

# PROGRESS REPORT

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## FOREWORD

The James R. Macdonald Laboratory (JRML) research program is dedicated to the study of atomic, molecular, and optical physics (AMOP). The focus of the laboratory has been to maintain a leadership role in experimental and theoretical AMOP collision physics with highly charged ions. During the current grant period, the program has been expanded to include the area of intense laser field-atom/molecule/surface interactions by hiring a new faculty member to establish an intense, ultra-short pulse laser facility and by drawing on the expertise of the ion-atom collision experiment and theory personnel of the JRML.

JRML is a DOE user facility located in the Physics Department of Kansas State University, KSU. The AMOP research program grew out of the early days of the JRML, formerly called the Nuclear Science Laboratory, accelerator program. The initial facility was constructed in 1969, with the installation of a 6 MV HVEC tandem Van de Graaff accelerator, and began operation in 1971. The original funding was from the AEC under the nuclear physics program. In 1975 the funding was transferred to the atomic physics program within Chemical Sciences with the agency name changing from AEC to ERDA and finally to DOE. The laboratory was renamed JRML in 1980. It was upgraded in 1985 with a new 120' X 50' experimental hall funded by KSU. The research facilities were enhanced with funding from DOE for the upgrade of the tandem from 6 MV to 7.5 MV, for the addition of a 9 MV superconducting LINAC booster accelerator, and for the addition of a new stand-alone ion source (CRYEBIS) for the production of low velocity highly charged ions.

The next major upgrade of the JRML AMOP program was in 2001 with the addition of a high power kHz Ti: Sapphire laser system, called the Kansas Light Source, which produces 4 mJ pulses with 25 fs duration at 1 kilohertz repetition rate. The facility was constructed with funds partly from a faculty start-up package from the university and partly from an NSF MRI grant. The laser laboratory was constructed in part of the "long room" which formerly housed beam lines for tandem-only experiments. The apparatus from these beam lines were moved to the new LINAC hall. The other part of the long room houses a new magneto optical trap (MOT) facility. The Kansas Light Source is operated under our DOE grant.

The next upgrade is in the process of being realized. The "square room," which is the other tandem-only beam vault, is being converted to a new laser lab for studies of supercontinuum radiation. This research program will be established by another new faculty member who will arrive in September 2003. The apparatus from this vault have been moved recently partly to the LINAC hall and partly to the CRYEBIS area.

*Pat Richard*  
*Principal Investigator and Director, JRML*  
*7/17/2003*

## TABLE OF CONTENTS

Foreword.....	i
Table of Contents .....	ii
I. Introduction.....	1
II. Progress Summaries.....	2
1. Molecular Dynamics with Ion and Laser Beams .....	2
1.1. Molecular Dissociation Imaging of Collision Induced Dissociation and Dissociative Capture in Slow $\text{H}_2^+ + \text{Ar}$ (He) Collisions, and a Few Other Simple Molecular Ions .....	2
1.2. High Intensity Laser Interactions .....	5
1.2.1. Evidence for Pondermotive-Gradient Field-Ionization in an Intense Focused Laser Beam.....	5
1.2.2. Photo Ionization and Photo Dissociation of $\text{H}_2^+$ by an Intense Short Pulse Laser .....	5
1.3. Ground State Dissociation of $\text{HD}^+$ .....	8
1.3.1. Charge Transfer and Elastic Scattering in Very Slow $\text{H}^+ + \text{D}(1s)$ “Half” Collisions.....	8
1.3.2. Separating the Momentum Transfer to a Hydrogen Molecule as a Whole from the Momentum Transfer to the Internal Motion of its Nuclei in the CM Frame .....	9
1.4. Isotopic Effects and Asymmetries in Bond-Rearrangement and Bond- Breaking Processes in Water Ionized by Fast Proton Impact .....	10
1.5. Formation and Decay Mechanisms of Doubly Charged Molecular Ions .....	11
2. Structure and Dynamics of Atoms, Ions, Molecules, and Surfaces: Atomic Physics Studies with a High Intensity Laser .....	13
2.1. High Harmonic Cutoff Extension Due to Ionization Suppression.....	13
2.2. The Effect of Orbital Symmetry on the Ellipticity Dependence of High Harmonic Generation.....	15
2.3. Extending High Harmonic Cutoff with an Optical Parametric Amplifier ...	18
2.4. A Sub-600 fs Streak Camera with <100fs Jitter .....	18
3. Structure and Dynamics of Atoms, Ions, Molecules, and Surfaces: Atomic Physics with Ion Beams and Synchrotron Radiation.....	23
3.1. COLTRIMS Measurements of Electron Spectra from Low Energy Ionization of Atomic H and He Targets .....	23
3.2. COLTRIMS Measurements of Electron Capture by Highly Charged Ions from Atomic Hydrogen.....	24
3.3. Ion-Ion Collisions Involving Molecular Systems .....	25
3.4. Identification of a Rescattering Mechanism in the Double Ionization of $\text{D}_2$ by Intense Laser Pulses.....	27
3.5. COLTRIMS Ionization Studies of Multielectron Systems Studied Through Synchrotron Radiation at the ALS .....	29
3.6. Photoelectron Diffraction from $\text{C}_2\text{H}_2$ , $\text{C}_2\text{H}_4$ and other Small Molecules ...	29
4. Studies of Charge Transfer Collisions and Photo-Ionization Processes using Innovative Methodologies.....	33

4.1.	Charge Transfer in Extremely Slow Collisions with Highly Charged Ions .....	33
4.2.	Magneto-Optical Trap Recoil Momentum Spectroscopy: MOTRIMS .....	34
4.2.1.	Excited State Fraction Measurements .....	35
4.2.2.	Differential Cross Section Measurements .....	36
4.3.	3-D Spatial Imaging Technique for the Study of Above-Threshold Ionization as a Function of Laser Intensity .....	38
4.4.	Stark-Induced X-Ray Emission from High Rydberg States of H-like and He-like Silicon Ions .....	38
5.	Time-Dependent Treatment of Continuum Phenomena .....	40
5.1.	Charge Exchange in $\text{H}^+ + \text{H}^-$ Collisions .....	40
5.2.	Intense Laser-Atom Interactions .....	43
5.2.1.	Scaling the Time-Dependent Schrödinger Equation .....	43
5.2.2.	Adiabatic Floquet Representation for Atoms .....	43
5.3.	Rearrangement Processes in Asymmetric Three-Body Systems .....	44
5.3.1.	Protonium Formation in $\text{H}^+ + \text{H}^-$ Collisions .....	44
5.3.2.	Diabatization Schemes .....	45
5.4.	Hyperspherical Approach to Four-Body Systems .....	45
5.4.1.	Low-Energy Ps+Ps Collisions .....	45
5.5.	Other Activities .....	46
6.	Theory of Ion and Laser Interaction with Atoms and Molecules .....	47
6.1.	Laser-Atom and Laser-Molecule Interactions .....	47
6.1.1.	Tunneling Ionization Theory for Molecules (MO-ADK) .....	47
6.1.2.	Alignment Dependent Tunneling Ionization Rates .....	48
6.1.3.	Rescattering Dynamics of $\text{H}_2$ and Molecular Clock at Sub-fs Resolution .....	48
6.2.	Hyperspherical Close-Coupling Method for Ion-Atom Collisions at Low Energies .....	50
6.3.	Triply Excited States of Three-Electron Atoms .....	52
6.4.	Ion-Atom Collisions at keV/amu Energies .....	54
6.5.	Other Activities .....	54
7.	Structure and Dynamics of Atoms, Molecules and Surfaces: Atomic Collisions with Highly Charged Ions .....	55
7.1.	Triply Excited States in Li-Like Ions .....	55
7.1.1.	Study of the Z-Dependent Autoionization Rates for the $2s2p^2\ ^2D^o$ Triply Excited States .....	55
7.1.2.	Formation of All Li-Like Triply Excited States by Triple Electron Capture .....	57
7.2.	Measurement of Triple Electron Capture in Fast Ion-Atom Collisions .....	58
7.3.	Production Mechanism and Fraction of Metastable $1s2s\ ^3S$ He-Like Ions Formed in Fast Cascading Ion-Atom Collisions .....	60
7.4.	Inelastic and Superelastic Electron Scattering Deduced from Ion-Atom Collisions .....	62
7.5.	Ionization of Atomic Hydrogen, Molecular Hydrogen, and Helium and Transfer Ionization with Highly Charged Ions at High Velocity; and Electron Capture with Highly Charged Ions at Low Velocity .....	64



8.	Interactions of Photons, Atoms, and Ions with Molecules, Clusters, and Surfaces .....	65
8.1.	Charge-Transfer Dynamics in Slow Atom-Surface Collisions: A New Close-Coupling Approach Including Continuum Discretization .....	65
8.2.	Interactions of Highly Charged Ions with Fullerenes and Surfaces.....	65
8.3.	Wave-Packet Propagation Methods Applied to the Neutralization of Negative Hydrogen Ions in Soft Collisions with Metal Surfaces .....	66
8.4.	Computation of Momentum Distributions Within Wave-Packet Propagation Calculations .....	68
8.5.	Fragmentation of $H_2^+$ in Strong Laser Pulses .....	68
8.6.	Mapping of Coherent and Decohering Nuclear Wave Packet Dynamics in $D_2^+$ with Ultrashort Laser Pulses .....	69
III.	Facilities Report.....	71
1.	Lab Operations Progress Report.....	71
1.1.	Tandem/LINAC, General Staff .....	71
1.2.	Low Energy Ion Collision Facility.....	72
1.2.1.	CRYEBIS .....	73
1.2.2.	ECRIS .....	74
1.3.	Data Acquisition System, LINAC Computer Control, and JRML Electronics Shop .....	75
1.3.1.	Data Acquisition .....	75
1.3.2.	LINAC Computer Control .....	76
1.3.3.	JRML Electronics Shop .....	76
2.	Laser Lab Operations Progress Report .....	77
2.1.	Development of the Kansas Light Source.....	77
2.2.	Applications .....	78
IV.	Financial Report.....	80
V.	JRML Personnel, Visitors/Users and Colloquia .....	81
VI.	Publications .....	91
VII.	Invited Talks by JRML Personnel .....	104

## I. INTRODUCTION

### P. Richard

This document summarizes the work carried out in the J. R. Macdonald Laboratory, JRML, over the past three years under the project entitled "Structure and Dynamics of Atoms, Ions, Molecules, and Surfaces" funded under DOE grant DE-FG02-86ER13491. The report presents a review of research performed by the personnel in the experimental and theoretical groups of the JRML in Section II entitled Progress Summaries, and of the technical assessments of the laboratory in Section III entitled Facilities Report. Section IV contains the financial report, Section V presents the list of JRML personnel, visitors/users and colloquia, Section VI contains the list of publications produced during the grant period, and Section VII contains the list of invited talks given by JRML personnel. The publication numbers appearing in the research summaries are taken directly from the list of publications given in Section VI. This report is prepared for the Atomic, Molecular, and Optical physics program of the Fundamental Interactions Branch of the Division of Chemical Sciences, Office of Science of the U. S. Department of Energy.

During the last three years, work from JRML research was published in 112 papers in refereed journals. This number is nearly identical to the 115 papers reported three years ago in our last three year Progress Report. There are at present 21 papers in various stages of the publication process. The faculty presented 54 invited lectures at professional meetings and universities.

The experimental program consists of 6 faculty, and 3 research faculty members. The experimental research program has been greatly enhanced during the last two years by the addition of the Kansas Light Source (see Section III), which was designed and installed by Zenghu Chang, who joined our faculty in August 2001. Two of the faculty members, Tom Gray and Siegbert Hagmann, retired as of July 2003. They have been replaced with new faculty members. Kristan Corwin will arrive in September 2003, and Igor Litvanyuk will arrive in January 2004. Igor has written a contribution to our renewal proposal and Kristan plans to submit an independent proposal after her arrival at KSU. Tom Gray was the Associate Director for Laboratory Operations until January 2003, after which time Kevin Carnes took over those responsibilities. We recently promoted Bing Shan from research associate to assistant research professor with the responsibility for the operation of the new Kansas Light Source facility.

The theoretical program consists of 3 faculty and 1 research faculty members. The theory group has long maintained a strong liaison with the experimental program as well as addressing other forefront issues in AMO physics. Xiao Ming Tong has been promoted to assistant research professor and brings a wealth of background in the theory of light scattering.

## II. PROGRESS SUMMARIES

### Itzik Ben-Itzhak

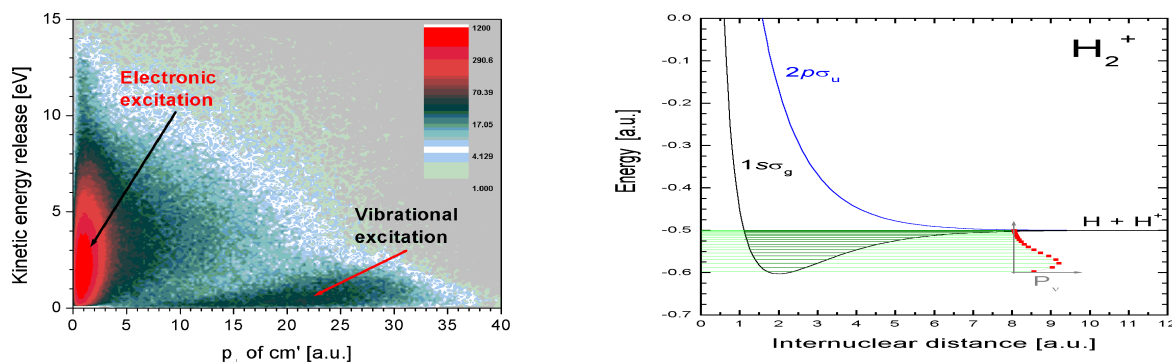
#### 1. Molecular Dynamics with Ion and Laser Beams – *Itzik Ben-Itzhak and Kevin D. Carnes*

*Our group effort in the last grant period focused on the study of mechanisms leading to molecular dissociation and charge exchange following fast collisions, slow collisions, or interactions with an intense short laser pulse as discussed below. The personnel in the group have changed during this time. My former graduate student Dr. Eric Wells graduated and took a Post Doc. position at the University of Virginia working with Professor Bob Jones. Dr. Dag Hathiramani worked as a Post Doc. in our group for one year, mainly on the collision induced dissociation project. Dr. Jiangfan Xia joined us recently as a Post Doc. and is learning our molecular dissociation imaging techniques for the intense laser experiment. A couple of new graduate students, Mark Smith and Max Sayler, joined our group last summer and are learning the basics of our experimental work. Note that Max did some experimental work with us as an undergraduate student. The same project is now being worked on by Matt Leonard, one of our freshman students. In addition, we had a few undergraduate students from other schools as part of our REU program. Some of our research was done in collaboration with other researchers from JRM or elsewhere as noted on each project.*

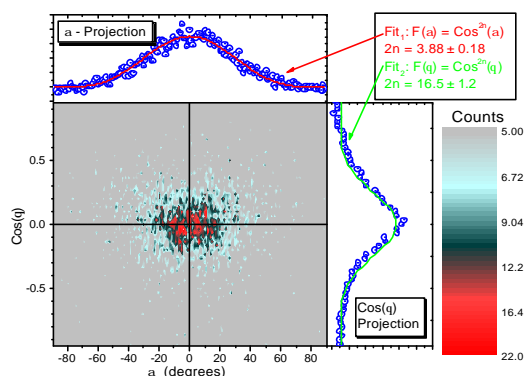
##### **1.1. Molecular Dissociation Imaging of Collision Induced Dissociation and Dissociative Capture in Slow $\text{H}_2^+ + \text{Ar}$ (He) Collisions, and a Few Other Simple Molecular Ions (A.3.5 in previous proposal) – *in collaboration with J.W. Maseberg (Fort Hays University)***

The dissociation of hydrogen molecular ions following a slow collision (keV) is studied by 3D momentum imaging of the fragments. The two main processes at this collision energy, collision-induced dissociation (CID, e.g.  $\text{H}_2^+ + \text{Ar} \rightarrow \text{H}^+ + \text{H} + \text{Ar}$ ) and dissociative capture (DC, e.g.  $\text{H}_2^+ + \text{Ar} \rightarrow \text{H} + \text{H} + \text{Ar}^+$ ), are experimentally separated in the method we recently developed (see schematic view of a similar apparatus in Fig. 1.2.2.1 of Section 1.2). Our experimental method is somewhat similar in its capabilities to the one used by Brenot *et al.* [1]. Using an electric field in the target region followed by a field free region, we managed to separate the CID from the DC in time. Thus, it is possible to evaluate the relative importance of these two processes, because both CID and DC are measured simultaneously. The same is true for the ratio of the two possible CID channels for heteronuclear molecules, i.e.  $\text{H}^+ + \text{D}$  or  $\text{H} + \text{D}^+$ . Moreover, this method allows one to distinguish experimentally between two different mechanisms of CID and thus study each one of them in detail. The two mechanisms differ in the momentum transfer to the projectile: (i) very small momentum transfer for CID caused by an electronic excitation to a repulsive state and large kinetic energy release (KER) upon dissociation; and (ii) very large momentum transfer for CID caused by a vibrational/rotational excitation associated with very small KER, as shown in Fig. 1.1.1. This distinguishes the present work from previous studies (see, for example, [2-4]), in which no such separation was possible. Results for CID of 3 keV  $\text{H}_2^+$  by an electronic excitation, shown in Fig. 1.1.2, indicate that the dissociating fragments align along the beam direction for “short” molecular ions and perpendicular to the beam for “long” ones, as predicted by Green and Peek. [5]. In contrast, the vibrational/rotational dissociation mechanism strongly favors molecular ions aligned perpendicular to the beam velocity (i.e.  $\theta=90^\circ$ ). Furthermore, the dissociation velocity is preferentially aligned along the momentum transfer for the latter mechanism, as shown by the strong peaking in Fig. 1.1.3. The probabilities for DC and CID are comparable for this collision

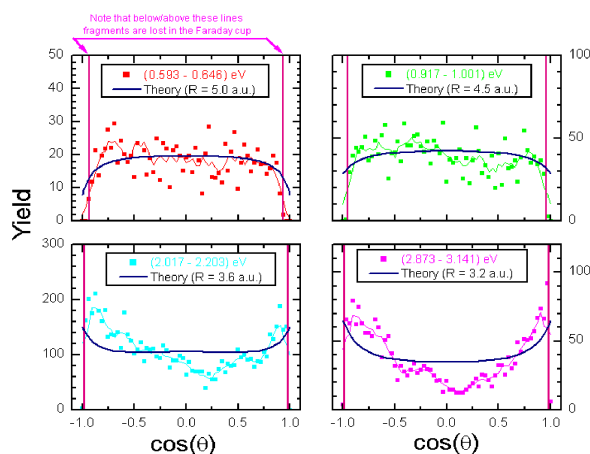
system; however, DC preferentially happens for molecular ions aligned parallel to their velocity. Further analysis of the DC and CID processes as well as model calculations of the vibrational CID mechanism are underway. These results were presented as invited talks in the CAARI 2002 and DAMOP 2003 meetings.



**Figure 1.1.1.** Left: a density plot of  $H^+ + H$  dissociation as a function of KER and transverse-momentum transfer; Right: A schematic energy diagram of an  $H_2^+$  molecule indicating the electronic and vibrational excitations.



**Figure 1.1.3.** A density plot of vibrational CID dependence on the molecular alignment,  $\theta$ , and the angle between the dissociation direction and the momentum transfer,  $\alpha$ .

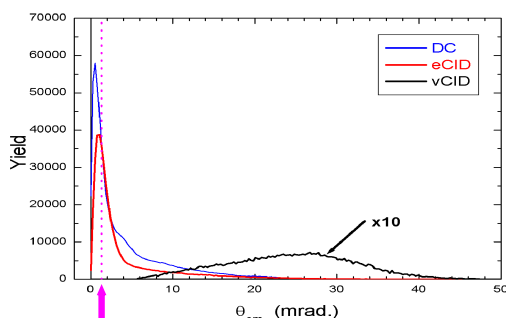


**Figure 1.1.2.** The angular dependence of the electronic CID for a few different “stretches” of the  $H_2^+$  molecular ion.

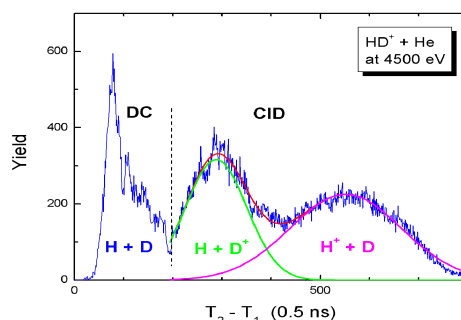
We also determine the scattering of the molecular ion as a whole, which is similar for electronic CID and DC; both are dominated by soft collisions. In contrast, vibrational CID occurs in close encounters, as shown in Fig. 1.1.4.

Recently we have conducted studies of CID of  $HD^+$  in similar collisions in search of the isotopic effects observed previously for this molecular ion (see, for example, [6-9]), namely, that the dissociation into  $H + D^+$  was favored over  $H^+ + D$ . The reported preference is very large for such isotopic effects, but the ratios differ significantly from about 2 [6-8] to almost 5 in the most recent report of Lehman *et al.* [9]. They also present a theoretical prediction based on the work of Rapp [10] in which the isotopic effect stems from the difference in vibrational excitation

energy transfer due to the different colliding masses in a head-on collision. The predicted branching ratio of 4 was found to be in reasonable agreement with the measured value. An additional interesting isotopic effect was reported by Đông and Durup [6], namely a forward-backward asymmetry in the collision induced dissociation of 4 keV  $\text{HD}^+$  on He. The deuteron fragment (D or  $\text{D}^+$ ) is preferentially emitted forward while the proton fragment (H or  $\text{H}^+$ ) is more likely to be emitted backward. In contrast, our preliminary results suggest that such isotopic preferences, if any, are very small, as can be seen from the raw time difference spectrum shown in Fig. 1.1.5.



**Figure 1.1.4.** The measured yield of dissociative capture as a function of the angle relative to the beam velocity for 3 keV  $\text{H}_2^+ + \text{Ar}$  collisions.



**Figure 1.1.5.** The time difference spectrum of  $\text{HD}^+$  dissociation following a collision with He at 1.5 keV/amu.

We also performed similar measurements for a few additional simple molecular ions, such as  $\text{HeH}^+$ ,  $\text{He}_2^+$  and  $\text{H}_3^+$  colliding with the same atomic targets. Further data analysis for all these collision systems is underway and is still needed before it can be compared to similar measurements (see, for example, [11-14]). Presently we are upgrading our experimental setup by adding a cold jet target, a new detector and improved electronics, as described in detail in our, recently approved, supplement proposal.

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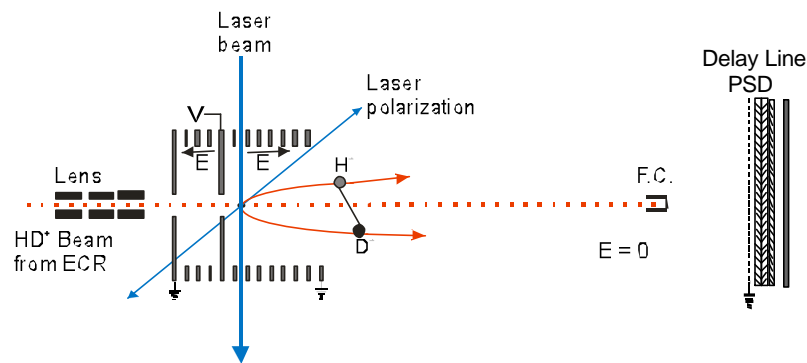
## 1.2. High Intensity Laser Interactions (A.6 in previous proposal)

### 1.2.1. Evidence for Pondermotive-Gradient Field-Ionization in an Intense Focused Laser Beam – in collaboration with E. Wells and R.R. Jones (University of Virginia).

We have measured the Rydberg-ion population produced during intense laser ionization in Xe, Kr, and Ar. The branching ratio for production of Rydberg ions,  $A^{(q-1)+*}$ , to ions  $A^{q+}$  has been measured as a function of laser intensity and polarization. Using 100 fs, 790 nm laser pulses, singly and double charged Rydberg ions are observed in Xe, but in Kr and Ar only singly charged Rydberg ions are seen. Model calculations of ionization by the gradient of the pondermotive potential ( $\nabla U_p$ ) of the focused laser beam suggest that the Rydberg population is inversely proportional to the ionization potential of the ion species. These calculations are in agreement with our data except for the  $\text{Xe}^{2+*}/\text{Xe}^{3+}$  ratio, which is anomalously large, approximately by a factor of two higher than the  $\text{Xe}^{+*}/\text{Xe}^{2+}$  ratio (see submitted 21a). Note that, this experience was very helpful as a first step toward my involvement in our new recent project involving the dissociation of molecular ions by intense short-pulse laser beams, and for that I am grateful. These results were presented as an invited hot-topics talk by E. Wells in the Multiphoton processes Gordon conference 2002.

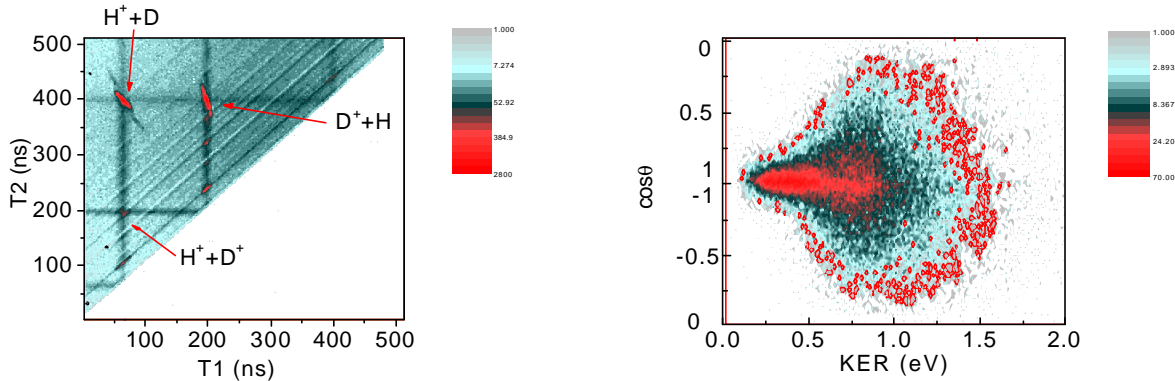
### 1.2.2. Photo Ionization and Photo Dissociation of $\text{H}_2^+$ by an Intense Short Pulse Laser – partly in collaboration with Z. Chang's group, C. Fehrenbach, and C.L. Cocke

We have recently begun measurements of ionization and dissociation of keV  $\text{H}_2^+$  beams crossed by an intense short-pulse laser beam using 3D molecular-dissociation imaging on a newly installed apparatus employing techniques similar to those described in Section 1.1. The experimental apparatus used for all our molecular dissociation imaging studies is shown schematically in Fig. 1.2.2.1. The triple coincidence (laser-pulse, ion, ion/atom) and the initial motion of the fragments separate them from ions produced by ionizing the much denser residual gas.



**Figure 1.2.2.1.** A conceptual figure of the apparatus for 3D molecular dissociation imaging of molecular ions exposed to intense laser fields. We also show, for example, the  $\text{HD}^+ + \text{He} \rightarrow \text{H}^+ + \text{D}^+$  reaction. Note that the extraction field modifies both trajectories.

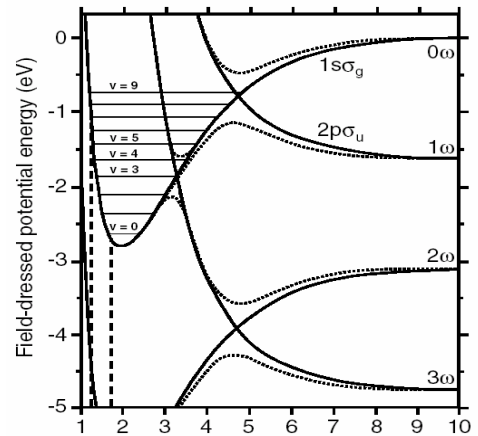
These measurements provide detail information about each reaction, like: (1) the kinetic energy release upon dissociation, from which we expect to learn about the vibrational states involved as well as the net number of photons absorbed; (2) the alignment and orientation ( $\theta, \phi$ ) of the molecular ion relative to the polarization vector; to this end we use linearly polarized light. In addition, note that the dissociation and ionization channels are separated by the longitudinal electric field, thus enabling their direct comparison. It can be seen from Fig. 1.2.2.2 (*Left*) that the ionization of  $\text{HD}^+$  is much smaller than its laser induced dissociation. Further data analysis is needed in order to compare quantitatively the measured ionization to dissociation ratio in order to compare it to previous measurements of Williams *et al.* [1] and to theoretical predictions of Kulander *et al.* [2], for example.



**Figure 1.2.2.2.** *Left:* Time correlation plot for  $\text{HD}^+$  exposed to a 45fs,  $3.9 \times 10^{14} \text{ W/cm}^2$  laser pulses. *Right:* A density plot of the angular dependence of  $\text{HD}^+$  dissociation for different KER values.

In Fig. 1.2.2.2 (*Right*) we show preliminary results for the angular distributions for different values of KER, i.e. different vibrational states. These results are in agreement with 2D-imaging measurements of Sändig *et al.* [3] who used longer pulses (of about 130-600 fs). It can be clearly seen that the lower vibrational states associated with lower KER values are aligned much more than the higher vibrational states, which exhibit approximately a  $\cos^2(\theta)$  distribution. We would expect the vibrational states (about  $v=9$ , see Fig. 1.2.2.3) that dissociate immediately when the energy gap between the dressed states opens to be less aligned, since they start dissociating way before the laser pulse reaches its peak intensity. In contrast the lower states are exposed to higher intensity before they dissociate and thus should be more aligned. Though the qualitative picture seems right, there is still much to do before we can predict quantitatively what would be the outcome of such measurements.

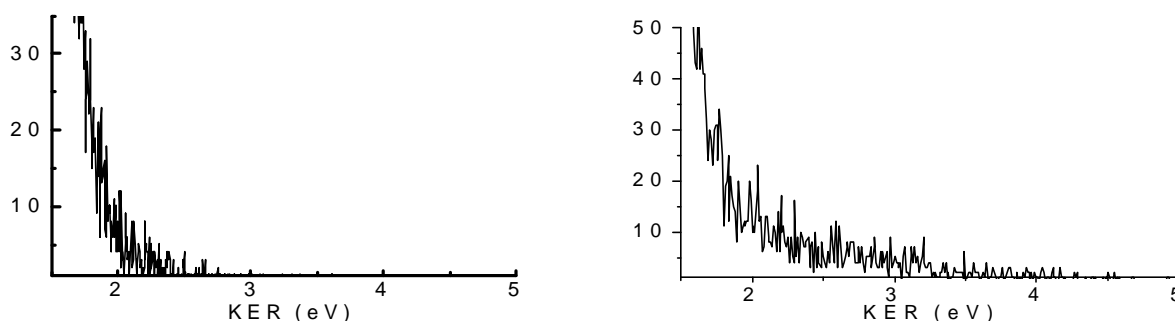
Our research on the interaction of intense short-pulse lasers with molecular ions is complementary to the research done in JRM with molecular targets (see Section 3.4 for studies



**Figure 1.2.2.3.** Typical dressed potential energy curves of  $\text{H}_2^+$ .

of molecules by *C.L. Cocks*). Interrogating molecules with such intense short-pulse lasers has resulted in a multitude of interesting new phenomena because the strength of the interactions of the electrons with the nuclei and the laser field are comparable. Among these phenomena are: tunneling ionization, above threshold dissociation (ATD), bond softening and bond hardening, charge resonance enhanced ionization (CREI), molecular alignment, and many more (see for example the review by Giusti-Suzor *et al.* [4]). The simplest molecular ion,  $\text{H}_2^+$ , is commonly studied by theorists [4-16], while experimentalists, for obvious reasons, prefer to study the naturally abundant  $\text{H}_2$  molecule [17-25]. In some of the experimental studies of  $\text{H}_2$  the experimental conditions have been tailored to enable the study of the behavior of the transient  $\text{H}_2^+$  formed early in the laser pulse (see, for example [24, 25]). However, some of the predictions about the  $\text{H}_2^+$  behavior are better tested using the molecular ion itself, and similar arguments hold for many-electron molecular ions. Only a handful of experimental studies of molecular ions have been conducted so far [2, 3, 26, and 27].

One of the interesting questions awaiting clear experimental evidence relates to the net number of photons absorbed in the process. In Fig. 1.2.2.4 we show experimental evidence for multi-photon absorption which is, as expected, more likely when we use a more intense laser pulse. Note that the KER distribution should terminate around 1.6 eV for 1-photon absorption, while 3-photon absorption is expected to start around 2 eV.



**Figure 1.2.2.4.** Dissociation of  $\text{H}_2^+$  by intense short-pulse laser *Left:* 135fs,  $1.3 \times 10^{14} \text{ W/cm}^2$ , *Right:* 45fs,  $3.9 \times 10^{14} \text{ W/cm}^2$ .

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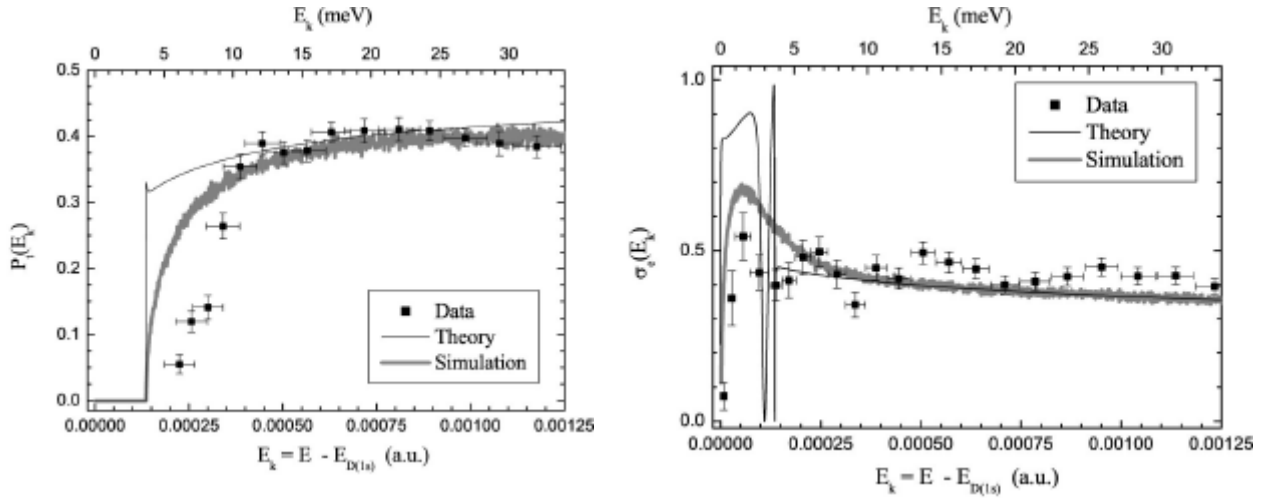
### 1.3. Ground State Dissociation of $\text{HD}^+$ (A.3.4 in previous proposal)

*The fast removal of one electron from a hydrogen molecule is followed by very slow dissociation if the vibrational continuum of the electronic ground state is populated in the vertical transition.* We name this process ground state dissociation (GSD). For the HD isotope of hydrogen the dissociation favors  $\text{H}^+ + \text{D}(1s)$  over  $\text{H}(1s) + \text{D}^+$  production due to the small, 3.7 meV, energy gap between these two dissociation limits (Pubs. #4 and 13). We have used this slow dissociation process of hydrogen to probe a couple of reaction mechanisms:

#### 1.3.1. Charge Transfer and Elastic Scattering in Very Slow $\text{H}^+ + \text{D}(1s)$ “Half” Collisions – in collaboration with B.D. Esry and H. Sadeghpour (ITAMP)

We have studied charge transfer and elastic scattering in the  $\text{H}^+ + \text{D}(1s)$  collision system. This system provides an interesting case study for theorists, since scattering calculations for this system depend in turn on  $\text{HD}^+$  structure calculations, which must correctly account for the difference in nuclear mass (see, for example, [1]). Our aim was to study the collision at energies from about 1 eV down to the charge transfer threshold at 3.7 meV, and below for the elastic channel. To accomplish this goal we used ground state dissociation (GSD) of  $\text{HD}^+$  to measure electron transfer from the  $1s\sigma$  to the  $2p\sigma$  state. Charge transfer occurs at an internuclear separation of about 12 a.u., around the avoided crossing, resulting in the  $\text{D}^+ + \text{H}(1s)$  final state (see Pubs. #12 and 50). In contrast,  $\text{H}^+ + \text{D}(1s)$  is the final state of elastic scattering. The energy of the resulting  $\text{H}^+$  or  $\text{D}^+$  fragment is typically less than 300 meV and is determined for each fragment by imaging its momentum vector using a COLTRIMS-style apparatus.

The measured relative yields of  $H^+$  and  $D^+$  fragments as a function of kinetic energy in the  $HD^+$  center of mass frame provide a direct measure of the electron transfer probability from the initial  $1s\sigma$  to the final  $2p\sigma$  state for very slow “half” collisions. Our experimental results, shown in Fig. 1.3.1.1, are in good agreement with our half collision calculations (Pub. #50) except near the charge transfer threshold where better resolution and subtraction of the  $H_2$  contamination are needed. Better subtraction of the  $H_2^+$  contamination so far has extended our agreement with theory down to about 12 meV (Pub. #97). Note that the full  $H^+ + D(1s)$  collision was measured only down to 120 meV by Newman *et al.* [2]. Further improvements of the experimental setup are needed in order to probe the threshold behavior of charge transfer and the resonances in the elastic channel. These results were presented as an invited talk by *E. Wells* in the CAARI 2000 meeting.



**Figure 1.3.1.1.** Absolute transition probability for: *Left* – charge transfer and *Right* – elastic scattering, as a function of the “collision” energy in very slow  $H^+ + D(1s)$  collisions. The simulation includes all relevant broadening effects.

### 1.3.2. Separating the Momentum Transfer to a Hydrogen Molecule as a Whole from the Momentum Transfer to the Internal Motion of its Nuclei in the CM Frame – in collaboration with C.L. Cocke, M.A. Abdallah, M. Stöckli and W. Wolff, H.E. Wolf (Universidade Federal do Rio de Janeiro)

In a collision, momentum can be transferred either to the CM motion of the molecule or to the internal motion of its nuclei in the CM frame. We have used the GSD process to probe and separate these two contributions from each other for slow  $He^+ + H_2$  (or  $D_2$ ) collisions ( $v \approx 0.25$  a.u.). The GSD fragments are very sensitive probes of small amounts of momentum transfer because of their small dissociation speed. It was found that for these collisions most of the momentum is transferred to the molecule as a whole for both electron capture and ionization processes. However, we observed some transverse momentum transfer to the motion of the nuclei in the CM system for the ionization process and none for electron capture. It is suggested that direct scattering off one nucleus is the cause of this momentum transfer (Pub. #82). We are planning to use the same technique in the future to probe angular alignment effects in other reactions such as single ionization and single capture.

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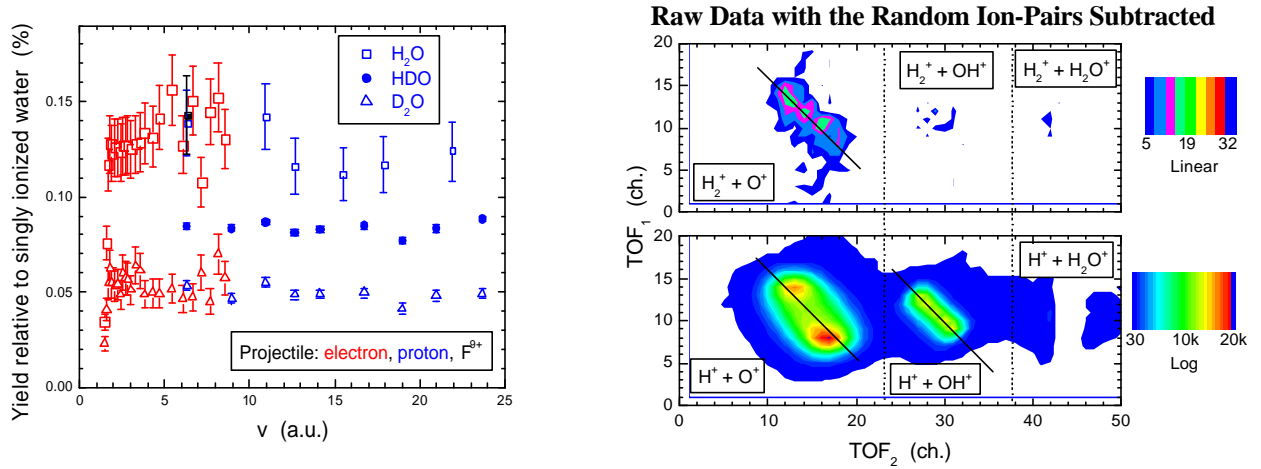
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### 1.4. Isotopic Effects and Asymmetries in Bond-Rearrangement and Bond-Breaking Processes in Water Ionized by Fast Proton Impact – in collaboration with J.W. Maseberg (Fort Hays University) and B.D. Esry

We continued some studies of interactions between fast ions and molecules, such as ionization of hydrogen molecules (Pub. #49) and fragmentation of water (Pub. #33 and 20a). We focus in this report on our studies of ionization and fragmentation of water molecules by fast protons and highly charged ions, because they have revealed an interesting isotopic preference for H-H bond rearrangement. Specifically, the dissociation of  $\text{H}_2\text{O}^+ \rightarrow \text{H}_2^+ + \text{O}$  is about twice as likely as  $\text{D}_2\text{O}^+ \rightarrow \text{D}_2^+ + \text{O}$ , with  $\text{HDO}^+ \rightarrow \text{HD}^+ + \text{O}$  in between, as shown on the left of Fig. 1.4.1. Our data is in agreement with equal velocity electron impact data [1-5] as one might expect, however, only Straub *et al.* [1] reported an isotopic difference in  $\text{H}_2^+$  production. Further investigations of this isotopic effect lead us to propose a similar isotopic effect following double ionization of water, namely we expect that the dissociation of  $\text{H}_2\text{O}^{2+} \rightarrow \text{H}_2^+ + \text{O}^+$  will be more likely than  $\text{D}_2\text{O}^{2+} \rightarrow \text{D}_2^+ + \text{O}^+$ . So far we have convincing evidence that this bond-rearrangement process does occur in double ionization, as shown on the right of Fig. 1.4.1. The observed  $\text{H}_2\text{O}^{2+} \rightarrow \text{H}_2^+ + \text{O}^+$  dissociation clearly exhibits the linear dependence expected from momentum conservation in a two-body breakup. The isotopic enhancement in the  $\text{H}_2\text{O}^{2+} \rightarrow \text{H}_2^+ + \text{O}^+$  dissociative double ionization channel requires further investigation to determine if it is similar in magnitude to that found in single ionization. In addition, we have observed large asymmetries in bond breaking in the HDO isotope. For example,  $\text{HDO}^+ \rightarrow \text{H}^+ + \text{OD}$  is more likely than  $\text{HDO}^+ \rightarrow \text{D}^+ + \text{OH}$  by about a factor of 1.5, suggesting that it is easier to break the O-H bond than the O-D bond. This preference is even larger in the dissociation of  $\text{HDO}^{2+}$ . Calculations are underway to determine the relative production rates for the different isotopes from the overlap of the initial and final vibrational wave functions and the time evolution of the final wave function. In addition, we determined the relative cross sections of all dissociation channels including  $\text{H}^+ + \text{H}^+ + \text{O}$  which typically are not measured by TOF techniques. These results were presented by Max Sayler as an invited undergraduate research talk in DAMOP 2002.

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**Figure 1.4.1.** *Left:* Ratio of H<sub>2</sub><sup>+</sup> (HD<sup>+</sup>, D<sub>2</sub><sup>+</sup>) to singly ionized water isotopes (electron data from [1]); *Right:* Time-correlation plots of a few dissociation channels of ionized water showing the H<sub>2</sub>O<sup>2+</sup> → H<sub>2</sub><sup>+</sup> + O<sup>+</sup> dissociation.

**1.5. Formation and Decay Mechanisms of Doubly Charged Molecular Ions (A.3.7 in previous proposal)** – in collaboration with: A. Bar-David, I. Gertner, B. Rosner (Technion) and partly with O. Heber and D. Zajfman (Weizmann Institute of Science)

*I continued my collaborative research of the formation and decay mechanisms of weakly bound molecular ions, specifically doubly charged ones. We used 3D molecular dissociation imaging to measure the mean lifetime and KER for a few molecular ions. For example, we measured a lifetime of 670±50 ns for the CO<sup>2+</sup> state with KER of 5.713 eV. Our results were consistent with a couple of other state specific measurements, though there is some ambiguity about the identification of this state due to some discrepancy with theoretical predictions (see details in Pub. #48). We also revisited our measurements of metastable N<sup>-</sup> and demonstrated that previous reports of its production in molecular dissociation were erroneous (submitted 19a).*

More interesting were the measurements of the decay rate of the doubly charged He dimer as they suggest that these molecular ions are spinning rapidly. The measured mean lifetime of <sup>3</sup>He<sup>4</sup>He<sup>2+</sup> molecular ions has been attributed to high angular momentum states. It has been suggested that the source of this angular momentum is the creation mechanism of the <sup>3</sup>He<sup>4</sup>He<sup>+</sup> parent molecular ions in the ion source. Using a 3D-imaging technique (Pub. #48) the mean lifetime and KER of long-lived <sup>3</sup>He<sup>4</sup>He<sup>2+</sup> molecular ions were determined to be τ=164±20 ns and 9.8±<sup>0.2</sup><sub>0.4</sub> eV, respectively, in nice agreement with the calculated values for a distribution of states around the v=1 and l=14,15 states. In order to determine if these high angular momentum states were measured just because they matched the range of high experimental sensitivity or because He<sub>2</sub><sup>+</sup> formation really peaks at high l values, we have recently conducted similar measurements of the homonuclear <sup>4</sup>He<sub>2</sub><sup>2+</sup> dimers. For this isotope low l-states as well as high l-states are within the high sensitivity range of our experimental setup. We have measured the decay rate and kinetic energy release upon dissociation of <sup>4</sup>He<sub>2</sub><sup>2+</sup> dimers formed in sub MeV He<sub>2</sub><sup>+</sup> + Ar charge stripping collisions. The measured mean lifetime indicates that He<sub>2</sub><sup>+</sup> molecular

ions are preferentially formed with high angular momentum, i.e. high  $l$  values, as suggested by our previous measurements of  ${}^3\text{He}{}^4\text{He}^{2+}$ .

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## **Other Contributions**

Finally, I have also been involved in projects reported by the project leader elsewhere in this document. I have added an impact parameter dependence to the Demkov model for charge transfer in slow collisions to help interpret the first charge transfer results from the MOT experiment by *B.D. DePaola* (see Section 4.2 and Pub. #69). I also participated in the studies of the ratio of transfer ionization (TI) to single electron capture (SC) by *P. Richard* (see Section 7.5 and Pub. #32). In addition, I presented 3 invited talks in 3 other Universities.

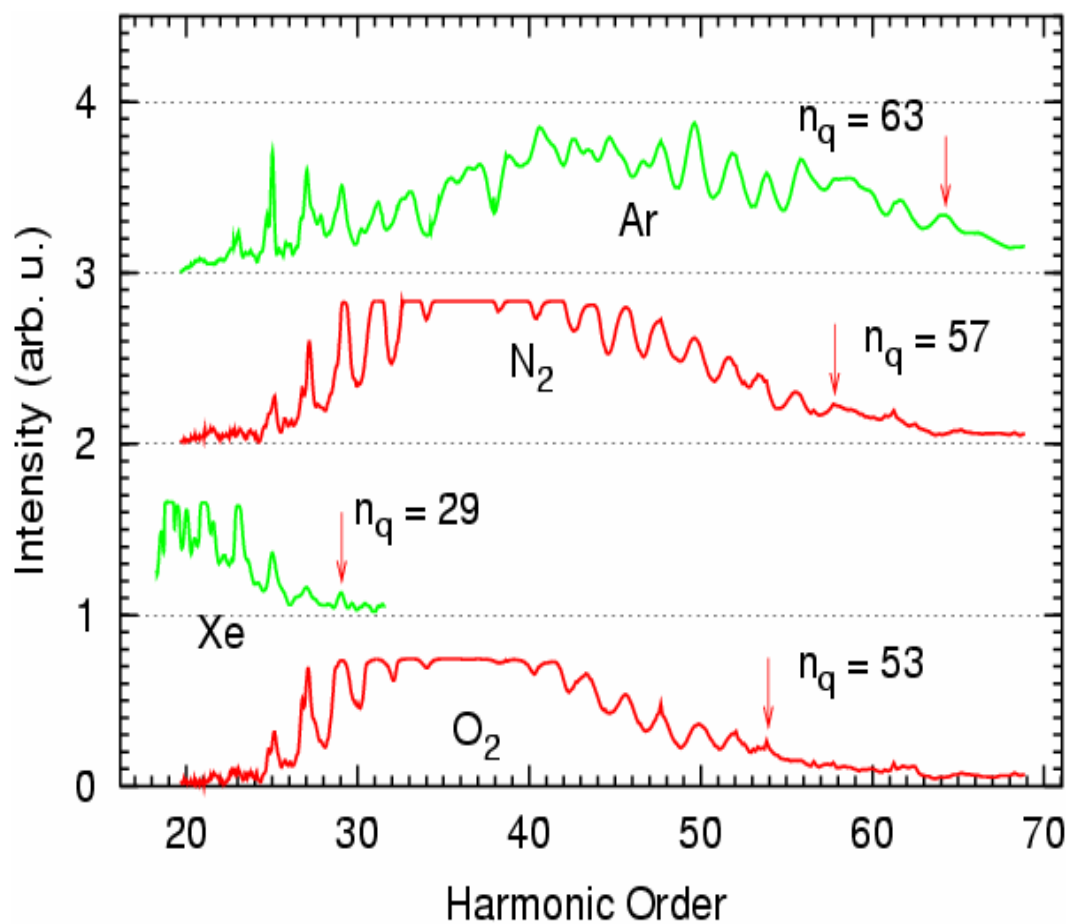
## 2. Structure and Dynamics of Atoms, Ions, Molecules, and Surfaces: Atomic Physics Studies with a High Intensity Laser

*The goals of this aspect of the JRML program were (1) to find out what determines the cutoff photon energy of the high order harmonic generation from molecules, (2) to explore the effect of orbital symmetry on the ellipticity dependence of high harmonic generation from molecules, (3) to determine the scaling of high harmonic cutoff as a function of laser wavelength, and (4) to develop a sub-picosecond x-ray streak camera operating in an accumulation mode.*

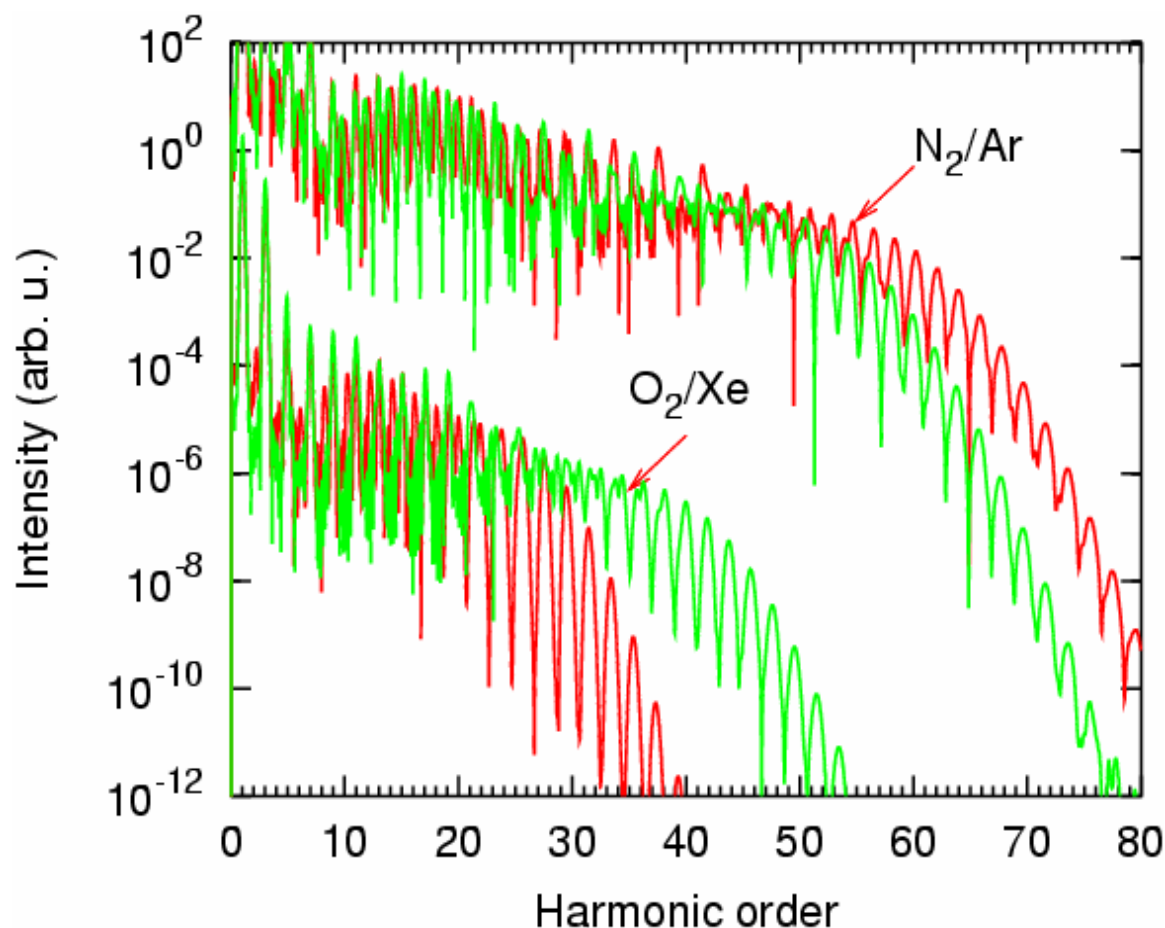
### 2.1. High Harmonic Cutoff Extension Due to Ionization Suppression -- Bing Shan, Xiao-Min Tong, Zengxiu Zhao, C.D. Lin and Zenghu Chang

Since the early discovery of high-order harmonic generation (HHG) at the end of the 1980s, most of the studies have been concentrated on rare gas atoms. There have been a number of experimental studies of HHG from molecules. In an earlier experiment, it was found that “the harmonic spectra from molecular gases are very similar to those obtained in atomic gases, with a plateau and a cutoff whose location is strongly correlated to the value of the ionization potential.” As an example, the HHG spectra of O<sub>2</sub> are close to that of Xe. Their ionization potentials are comparable (~12 eV). Compared to the preliminary study of HHG from molecules, the ionization of molecules has been studied more extensively. Recently, it was found that the ionization of O<sub>2</sub> is suppressed by about one order of magnitude when comparing with Xe. However, there is no ionization suppression for N<sub>2</sub> when comparing with Ar, which has nearly the same ionization potential as N<sub>2</sub>. As is known, the HHG is closely related to the ionization in the intense laser. The suppressed ionization of O<sub>2</sub> should lead to an increase of saturation ionization intensity, which should lead to a significant extension of harmonic spectra, which was not observed in the previous HHG measurements. Stimulated by such a controversy and the desire to further explore the relation between the HHG and ionization, we studied the HHG cutoff behavior for molecules and their companion atoms, for cases with a strong ionization suppression (O<sub>2</sub>, Xe), and for cases with no ionization suppression (N<sub>2</sub>, Ar).

The experiment was carried out with the newly established high intensity laser facility at the J. R. Macdonald Laboratory. We compared Ar and N<sub>2</sub>, which have nearly the same ionization potentials, at 15.76 eV and 15.58 eV, respectively, and we found they have nearly the identical harmonic cutoff (The cutoff positions for Ar and N<sub>2</sub> are  $q_c = 63$  and  $q_c = 57$ , respectively.). On the other hand, while Xe and O<sub>2</sub> have nearly the same ionization potentials, at 12.13 eV and 12.06 eV, respectively, the harmonic cutoff for O<sub>2</sub> ( $q_c=53$ ) is much higher than for Xe ( $q_c=29$ ). The spectra are shown in Fig. 2.1.1. We attributed this to the O<sub>2</sub> molecule being much harder to ionize than the Xe although they have the same ionization potential. Therefore, the harmonic cutoff extension and the ionization suppression are strongly correlated. The experiments were simulated using the Lewenstein model where the depletion of the ground state of the molecules is calculated using the ionization rate from the molecular ADK theory. The simulation results shown in Fig. 2.1.2 qualitatively agree with measured cutoff orders for both O<sub>2</sub> and N<sub>2</sub>. The cutoff extension caused by the ionization suppression provides another avenue for obtaining higher energy x-ray photons. This work is published in Phys. Rev. A Rapid communication [1 and Pub. #85].



**Figure 2.1.1.** The comparison of harmonic cutoff between atoms and their companion molecules. The cutoff photon energy of O<sub>2</sub> is two times higher than that of Xe though their ionization potentials are almost identical.



**Figure 2.1.2.** Numerical simulation of harmonic generation from molecules. The depletions of the ground states are calculated using the ionization rate of the molecular ADK rate.

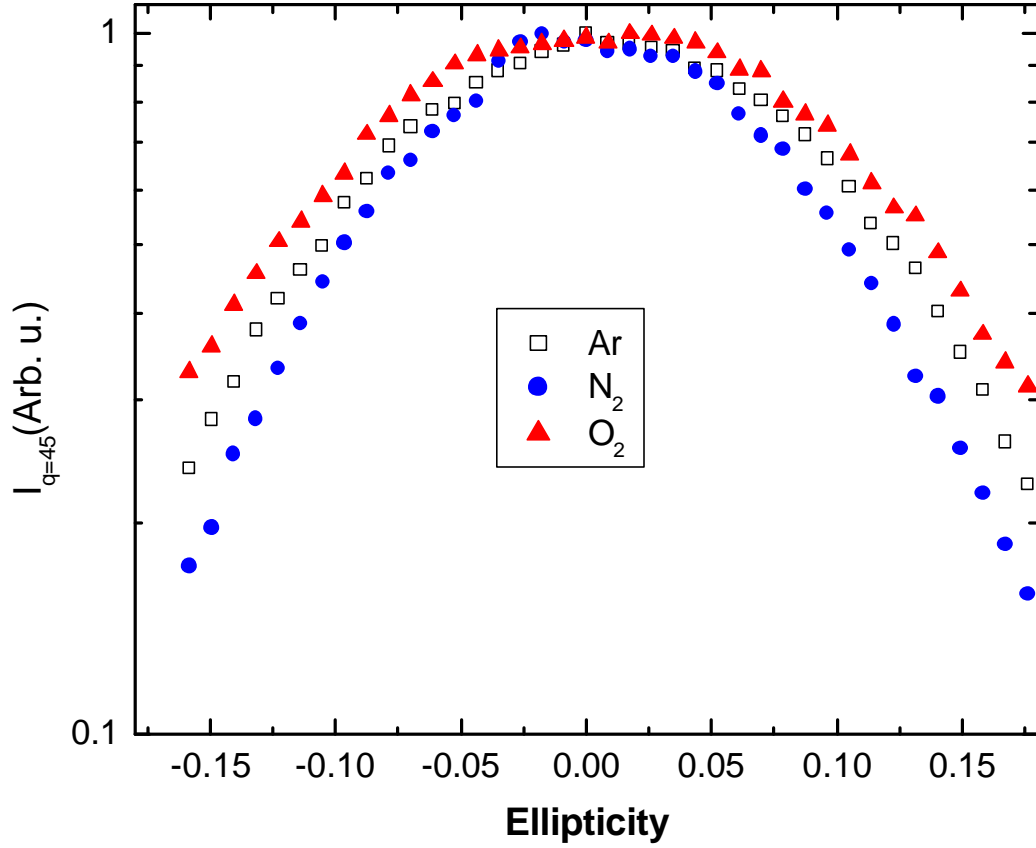
## 2.2. The Effect of Orbital Symmetry on the Ellipticity Dependence of High Harmonic Generation -- Bing Shan, Ghimire Shambhu, Chun Wang, and Zenghu Chang

The dependence of high order harmonic generation yield on the ellipticity of the driving laser field for  $O_2$  and  $N_2$  were compared experimentally for the first time. The results were also compared with that of Ar. It was found that the 45<sup>th</sup> order harmonic signal decreases slower for  $O_2$  than that for  $N_2$  with laser ellipticity, while that of Ar is in between. We believe that this is caused by the difference in the orbital symmetry between the two molecules.

The ellipticity dependence was measured using the *Kansas Light Source*. Figure 2.2.1 shows the results for the 45<sup>th</sup> order harmonics. We chose this order as close to the cutoff as possible but with a reasonably good signal-to-noise ratio. The results clearly show the difference of ellipticity dependence for the two molecules.

To understand what caused the difference, we applied the Lewenstein model to simulate high harmonic generation from *molecules*. The Lewenstein model can be considered as the quantum treatment of the three-step semiclassical model, i.e. electron first tunnels out the field-suppressed barrier of the atom, then the freed electron is accelerated in the laser field, and finally it recombines with the parent ion and emits a photon.





**Figure 2.2.1.** Measured ellipticity dependence for the 45<sup>th</sup> order harmonic from N<sub>2</sub> molecules, O<sub>2</sub> molecules and Ar atoms, respectively.

In the Lewenstein model, the harmonic spectrum is calculated by the Fourier transform of the dipole moment of an atom in the time domain:

$$\vec{r}(t) = i \int_0^\infty dt \left( \frac{\vec{p}}{\epsilon + it/2} \right)^{3/2} \vec{d}^*[\vec{p}_s(t) - \vec{A}(t)] e^{-iS(\vec{p}_s, t, t)} \vec{E}(t-t) \vec{d}[\vec{p}_s(t-t) - \vec{A}(t-t)] + c.c. \quad (1)$$

where  $\vec{d}[\vec{p} - \vec{A}(t)]$  is the field free dipole transition matrix element between the ground state and the continuum state.  $\vec{p} = \vec{v} + \vec{A}(t)$  is the canonical momentum and  $\vec{v}$  is the velocity of the electron in the continuum.  $\vec{A}(t)$  and  $\vec{E}(t)$  are the vector potential and the electric field of the laser field, i.e.,  $\vec{E} = -\frac{1}{c} \frac{\partial \vec{A}(t)}{\partial t}$ . Finally  $S(\vec{p}, t, t')$  is the quasiclassical action of the electron

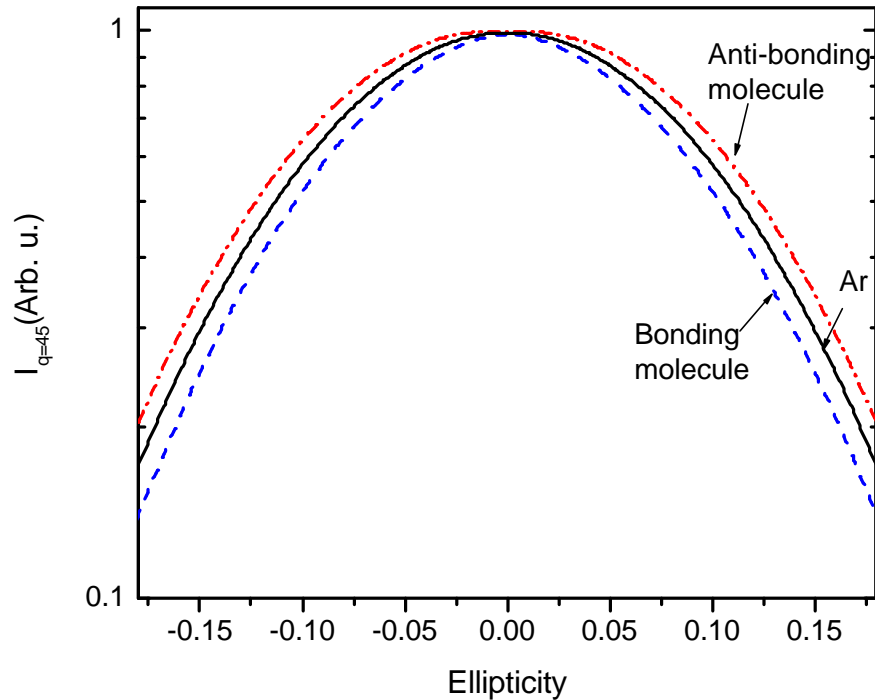
moving in the laser field,  $S(\vec{p}, t, t') = \int_{t'}^t dt'' \left( \frac{[\vec{p} - \vec{A}(t'')]^2}{2} + I_p \right)$ .  $\vec{p}_s = \vec{p}_s(t, t) = \int_{t-t}^t dt'' \vec{A}(t'')/t$  corresponds to the stationary phase,  $\epsilon$  is a small number.

Figure 2.2.2 shows the simulation that sums up the contribution from molecules with random orientation angles. It is clear that the ellipticity dependence difference between bonding and anti-bonding molecules exists for arbitrarily aligned molecules. This is consistent with our experimentally measured results. The above simulation results suggest that an ideal experiment to see the difference is to use molecules with perfect alignment. It has been shown that molecules can be partially aligned by a weaker laser pulse; such partial alignment should enhance the ellipticity dependence difference.

For the  $\Theta = 90$  degree molecule, the simulation results can be explained with a semi-classic theory. For an anti-bonding molecule, the electron tunnels out with a certain initial transverse velocity. For a linearly polarized laser pulse, the electron will draft away transversely from the parent ions, which results in a very small recombination probability in the recollision process. With an appropriate amount of ellipticity, the vertical component of the electric field can compensate for the effect of the transverse initial velocity and drive the drifting electron back to the parent ion, thus enhancing the recombination probability.

For a bonding molecule with the axis oriented perpendicular to the electric field of a linear light, the field does not change the *symmetry* of the system. This indicates that the probability of electron tunneling out with initial velocity along the electric field is larger than the other direction. In this case, when the electric field drives the electron back to the parent ion, the recombination probability is high for a linearly polarized light pulse.

A manuscript on this work was submitted to PRL.

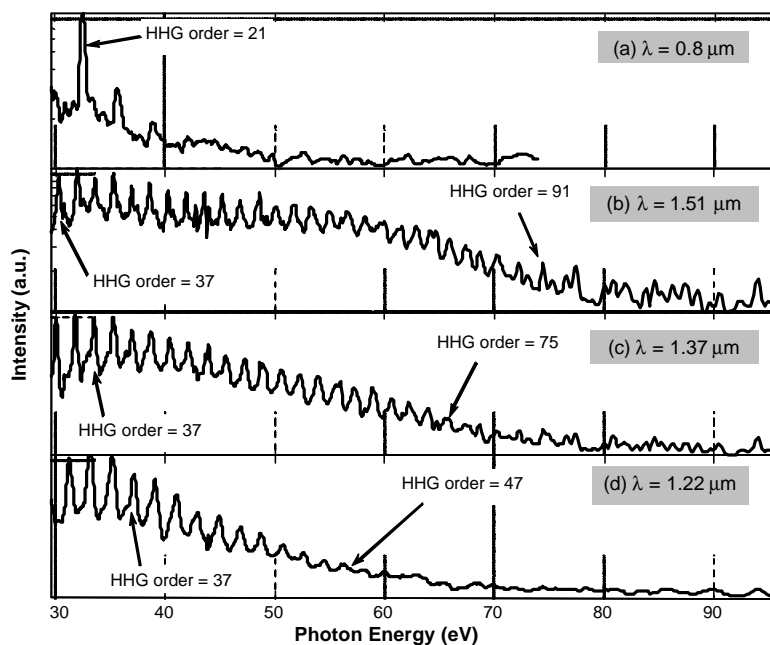


**Figure 2.2.2.** Calculated ellipticity dependence for the 45<sup>th</sup> order harmonic from bonding molecules, anti-bonding molecules and atoms, respectively.

### 2.3. Extending High Harmonic Cutoff with an Optical Parametric Amplifier -- Bing Shan, A. Cavalieri (University of Michigan), and Zenghu Chang

We demonstrated that by using a long wavelength ( $\sim 1.5 \mu\text{m}$ ) infrared pump pulse with  $10^{14} \text{ W/cm}^2$  from an optical parametric amplifier, the cut-off photon energies of Ar and Xe atoms were increased by a factor of two or more compared to that by a conventional 800nm pump laser. For Xe gas, the cutoff is  $\sim 40 \text{ eV}$  with 800nm pump and is  $\sim 80 \text{ eV}$  with a  $1.5 \mu\text{m}$  pump (Fig. 2.3.1). It also shows that a harmonic wavelength can be easily tuned to cover any wavelength from the 5<sup>th</sup> order to the cutoff by changing the OPA wavelength.

This work was published in Applied Physics B [2 and Pub. #94].



**Figure 2.3.1.** Harmonic spectrum using different pump wavelengths, constant pulse energy (50  $\mu\text{J}$ ) and focal point size.

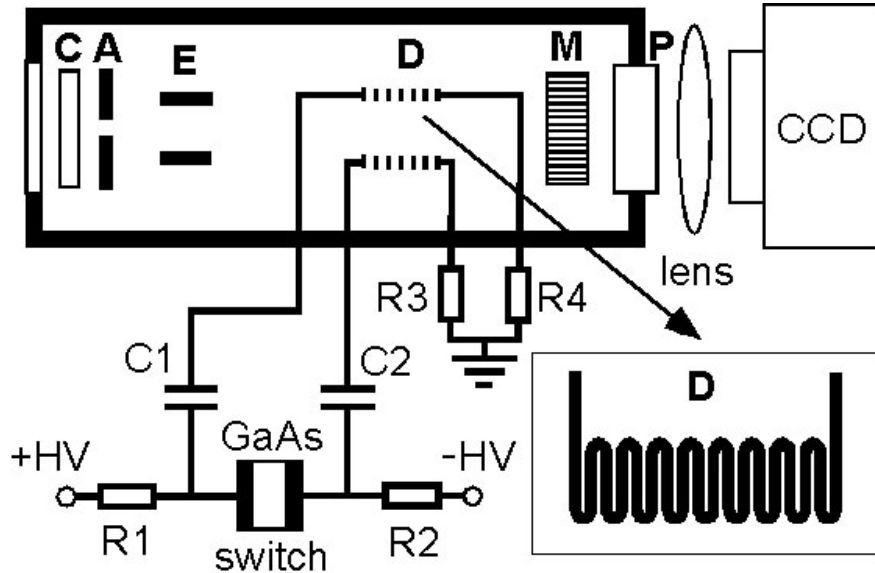
### 2.4. A Sub-600 fs Streak Camera with <100fs Jitter -- Jinyuan Liu (Argonne National Lab), Bing Shan, Mahendra Shakya, Jin Wang (Argonne National Lab) and Zenghu Chang

Ultrafast time resolved x-ray scattering and spectroscopy measurements have been proven powerful to study structural and electronic dynamics during laser-matter interactions on picosecond and sub-picosecond time scales. Although the development of ultrafast lasers advanced rapidly, the paucity of ultrafast x-ray detectors in the same temporal range has seriously limited the application of the x-ray measurements as a structure probe to elucidate those highly transient phenomena. Due to the relatively low instantaneous x-ray intensity and the low dynamic range of the streak camera accumulation over thousands of x-ray (and laser) shots is of absolute necessity. In the accumulation mode, temporal resolution of a streak camera is normally limited by the timing jitter caused by the shot-to-shot pulse energy fluctuation of the lasers which is 1-2% rms (root-mean-squared) for a typical kHz laser.

Currently, there are two methods to improve the time-resolution by means of reducing the synchronization jitter in the accumulating data collection mode. First, by improving the laser intensity stability to less than 0.5%, Naylor, et al., showed that the timing-jitter can be significantly reduced [3]. However, this approach seriously limited the portability of the x-ray streak camera for the synchrotron applications. Second, in a separate work, by employing multiple photoconductive switches to compensate for the laser fluctuations, an 0.8 ps time resolution can be achieved [4]. With many advantages, the more complicated photo-electronic circuitry and the requirement of more laser power to trigger the switches may limit its applications.

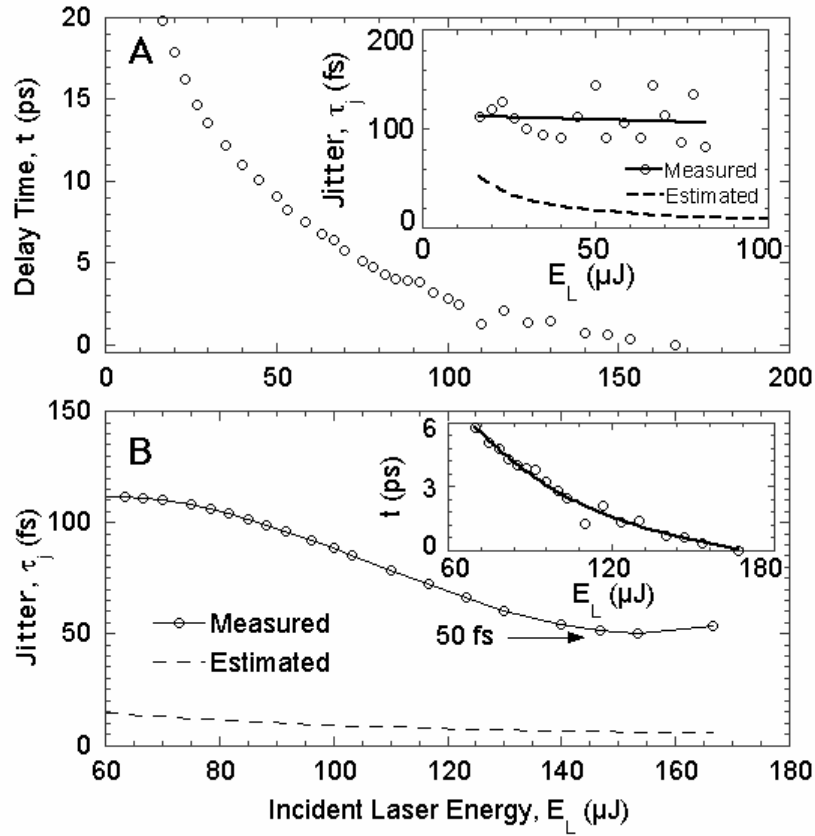
We demonstrated that the timing jitter of a classic streak camera can be reduced to 50 fs, even triggered by a laser with a 1.2% rms fluctuation, while retaining the simple structure of the camera with a single fast switch. In such a system, the timing jitter becomes irrelevant to the temporal resolution of the x-ray streak camera operated in the accumulation mode. Therefore, the time resolution of the accumulation streak camera is determined only by the intrinsic or the so-called single-shot resolution that has a theoretical limit of 200 to 300 fs in the hard x-ray regime.

The new x-ray streak camera, schematically shown in Fig. 2.4.1, was based on a classical camera with significant modifications and improvements on every component, given that the original device had a time-resolution of about 2 ps [5,6], primarily limited by the timing jitter. In the streak tube, the photoelectrons produced by the x-ray sensitive photocathode are accelerated by the high field (15 kV/mm) between the photocathode and the anode. The photo-electrons are focused by a set of quadrupole electrostatic lenses placed immediately before they enter the field between a pair of meander-type of deflection plates. The plates are driven by high ramping voltages generated in a single photoconductive switch circuit. Finally, the electrons are imaged on the microchannel plate/phosphor screen and the streak images are accumulated in a CCD chip coupled to the phosphor screen with a photographic lens.



**Figure 2.4.1.** Schematic of the x-ray streak camera. C: photocathode; A: anode, E: electrostatic lens; D: meander-type deflection plate; M: microchannel plate; P: phosphor screen;  $C_1$ ,  $C_2$ : DC blocks;  $R_1$ ,  $R_2$ : 1 M $\Omega$  resistors;  $R_1$ ,  $R_2$ : 50  $\Omega$  matching resistors;  $\pm$ HV: high voltage bias.

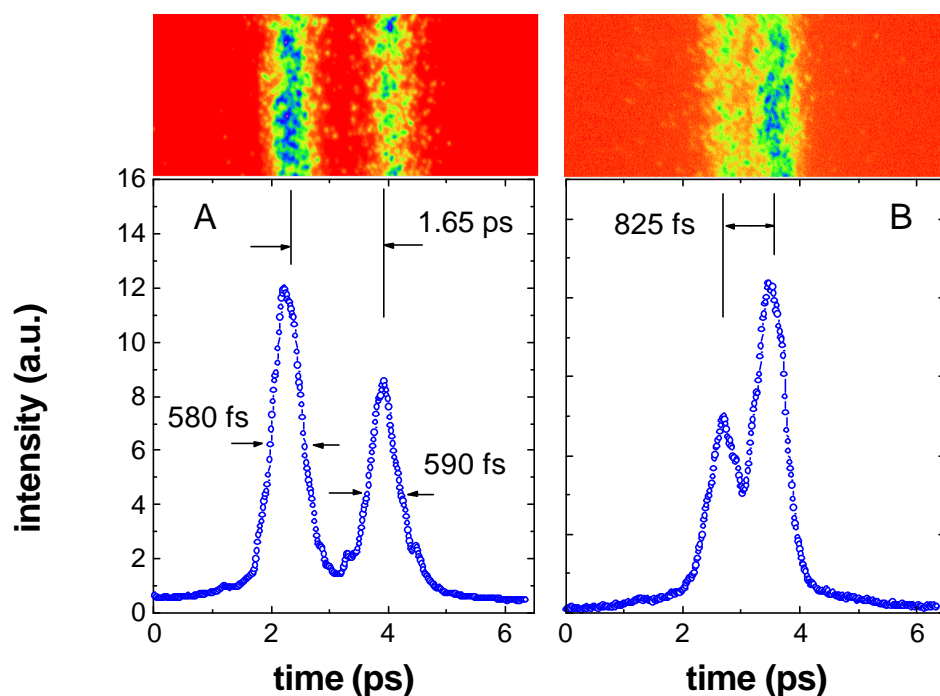
The jitter measurement was performed using the newly established high-intensity laser facility, *Kansas Light Source*, where the shot-to-shot laser pulse energy variation is measured to be 1.2% rms. This fluctuation value is typical to all current fs-laser systems. Figure 2.4.2A shows the measurement results of delay time vs. laser energy. In a lower laser energy region ( $E_L < 70 \mu\text{J}$ ) the jitter can be evaluated from the direct derivative of the measured curve. The jitter is determined to be varying around 110 fs ( $\pm 28$  fs) as shown in the inset to Fig. 2.4.2A. The jitter decreases from 110 fs (inset to Fig. 2.4.2A) to about 50 fs as the laser energy increases to 150  $\mu\text{J}$ . At this energy we did not observe any damage to the photoconductive switch. To the best of our knowledge, this is the lowest jitter ever demonstrated experimentally. Such a small jitter was the result of the extremely fast response time from the combination of the improved switch/deflection plates. Compared to the streak camera using multiple switches [4], the present single switch design requires much less laser energy to trigger. We also would like to emphasize here that the sub-100 fs jitter is achieved with a laser that has a similar fluctuation (1.2% rms) to most of the commercial lasers, therefore, it is easier to implement than to improve the laser stability.



**Figure 2.4.2.** Measured trigger delay and jitter of the photoconductive switch as a function of incident laser energy: A) trigger delay, and B) jitter at high incident laser energies and theoretical estimate of jitter in this energy range. The inset to (A) depicts the measured jitter at lower incident laser energies (open circle) with a linear fit (line) and theoretical estimate of the jitter (dashed). The inset to (B) illustrates a 3<sup>rd</sup> order polynomial (line) fit to the delay data taken at higher incident laser energies (open circle).

It was found that sweeping aberrations of the deflection plates limit the time resolution of our camera. We observed that the effect of the aberrations is significant for photoelectrons with large photoelectron beam divergence, which can be significantly reduced by collimating the electron bunches with a pair of slits. To conserve the photoelectron signal intensity, electrostatic lenses also were effective to collimate the photoelectrons. All these measures resulted in a much improved time resolution shown clearly in the lineout of the streak image accumulated with the 6000 UV shots (Fig. 2.4.3). After proper calibration, 30-fs UV pulses were recorded by the streak camera as 590 fs wide (full-width-at-half-maximum) streak strips. This shows that the x-ray streak camera has a better than 600 fs time resolution operating in the accumulation mode.

Since the streak camera can be operated reliably in sub-ps regime, it will not only make a significant impact on ultrafast science using the 3<sup>rd</sup> generation synchrotron x-ray sources but also will play an important role in timing diagnosis for experiments to be carried out at the 4<sup>th</sup> generation x-ray sources required by the unique timing structure of the x-ray pulses available at these sources. We have continued the collaboration with outside users to conduct research at the synchrotron facility using our streak camera [7]. This work is published in Applied Physics Letters and in a SPIE proceeding [8, 9].



**Figure 2.4.3.** Averaged lineout of the streak images with corresponding actual images (top) of two 30 fs UV pulses separated by 1650 fs (A) and 825 fs (B).

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C.L. Cocke

### **3. Structure and Dynamics of Atoms, Ions, Molecules, and Surfaces: Atomic Physics with Ion Beams and Synchrotron Radiation**

*The goals of this aspect of the JRML program were (1) to explore the dynamics of photoelectron emission from and the structure of small molecules, (2) to identify and explain basic mechanisms whereby electrons are removed from simple systems in capture and ionization processes involving charged particle beams and intense laser pulses.*

#### **Progress Over the Past Three Years on Individual Projects**

##### **3.1. COLTRIMS Measurements of Electron Spectra from Low Energy Ionization of Atomic H and He Targets -- E. Edgu-Fry and C. L. Cocke**

The goal of this project was to identify and characterize the process whereby a slow charged projectile promotes into the continuum an electron from a neutral target. The projectile velocity is sufficiently low that direct kinematic ionization is forbidden, and saddle-point electron promotion, in some form, is expected to be the major process. Theoretical attempts to deal with this process have led to several new approaches and formalisms, including hidden crossing theory (T and S processes) [1-4] and direct solutions of the time-dependent Schrodinger equation in both momentum-space [5,6] and configuration space [7] treatments, and have generated considerable discussion of the role of the Coulomb saddle formed by the two departing charged ions. Over the past six years we have applied COLTRIMS (Cold Target Recoil Ion Momentum Spectroscopy) techniques to the measurement of the momentum distribution of electrons produced in such collisions [8-11]. Our observations allowed new insights into this subject in the following respects: (1) They allowed us to measure the soft electron momentum spectra, down to electron energies well below one eV, which is the energy range which one must study to obtain the correct picture of the process. (2) They allowed us to experimentally fix the collision plane and impact parameter for each collision event. (3) They produced comprehensive maps of the momentum space distributions, in the form of images, which allow the recognition of the overall character of the continuum distribution for each case.

The main results of these measurements suggested that the continuum momentum distributions reflect directly the character of specific molecular orbitals which initiate the promotion process whereby the electrons finally reach the continuum. Experimental evidence for both  $\sigma$  and  $\pi$  orbital promotion has been seen, as well as evidence for interference from amplitudes of different symmetry [8-12]. An alternative theoretical interpretation of the data [5,6], however, suggested that some of the structure seen was to be associated directly with outgoing waves originating from the two final centers. No definite connection between these two approaches had yet been established.

At the beginning of this grant period (2000), all previous COLTRIMS work on this issue had been carried out with multielectron targets including He, Ne and H<sub>2</sub>. The experimental technique requires that the target be cold in order to obtain sufficiently high momentum resolution on the recoil ion. These targets are easy to prepare cold in a supersonic gas jet. Unfortunately, the theoretical problem of making definite predictions concerning the momentum distribution of the continuum electrons is difficult enough for a true one electron system, and



beyond the grasp of present theory for real two (or multi) electron systems. Thus the comparison between experiment and theory had thus far been largely qualitative, limited to comparing the general characteristics of the distributions found experimentally with the theoretical ones. Our proposal for the present 3 year period was to remove this uncertainty by carrying out the COLTRIMS ionization experiment using a *true one-electron hydrogen atom target* and bare projectiles, including p,  $\text{He}^{++}$  and eventually more highly charged species available from our CRYEBIS source. This work was the Ph.D. thesis work of Erge Edgu-Fry.

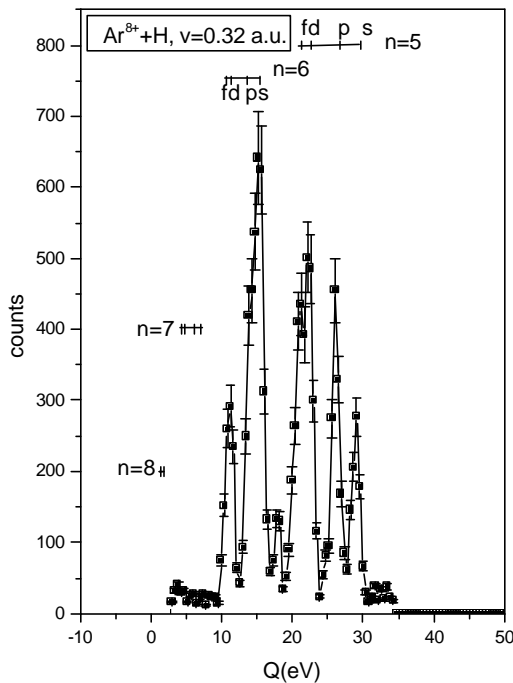
The experiment has finally been to a large extent successful, but with considerable struggles along the way. In preparation for the H-atom experiment, the previous He target work of Abdallah [10,11] was first extended to higher energies. At lower collision velocities (below .5 a.u.) the electron momenta had previously shown a  $\pi$  structure in the transverse momentum distribution [8-12] which oscillated as a function of  $v$  with respect to the nodal line in the structure. This behavior had been attributed to an interference between  $\pi$  and  $\sigma$  amplitudes [4] and had been predicted not to undergo further oscillations above  $v=1$  a.u. Our results for He confirmed this prediction, and showed a smooth evolution of the momentum distributions toward the target-centered one expected and previously measured at much higher ( $v>3$  a.u.) velocities. This work was published as Pub. #77.

The development of the H target was quite problematic. After more than a year of work it was finally decided to abandon the originally planned Slevin source in favor of a microwave discharge source. A further six months of development was required to make this source work adequately. Finally the source worked, providing a dissociation fraction in the quasi-cold jet of about 50%. The momentum resolution across the jet was excellent, below 0.1 a.u., while along the jet the source remained warm, 1.8 a.u. The ionization experiment was carried out for p on atomic hydrogen at  $v=0.77, 1.0$  and  $1.4$  a.u. Unfortunately, because of the low momentum resolution along the jet, it was not possible to obtain full impact-parameter information, and this limits the detail of the momentum-space images. In particular, only a washed-out  $\pi$  structure was observed, since it was not possible to clearly distinguish transverse direction of the recoil ion. This problem would have been much reduced had we been able to go to smaller  $v$ , but the rapid dying of the cross section as  $v$  is lowered and the thinness of the target made this impossible. Thus the comparison between experiment and theory will remain somewhat compromised, although for a different reason than had previously been the case. Dr. Edgu-Fry has written this up as part of her Ph.D. thesis, a paper is in preparation, and additional experimental work is continuing.

### **3.2. COLTRIMS Measurements of Electron Capture by Highly Charged Ions from Atomic Hydrogen -- E. Edgu-Fry and C. L. Cocke**

The presence on the EBIS of a working COLTRIMS atomic hydrogen target led us to carry out measurements of electron capture on this target. Previous studies of this process have been carried out by us and others [12; also see Pub. #36 and references cited therein] over the years, but never with a true one-electron target. Theoretical treatments of this process have become quite mature, but, as in the case of ionization discussed above, the comparison between theory and experiment was regularly compromised by the need to model a multielectron target with a core-plus-one-electron model. We therefore took advantage of our atomic H target to measure Q value distributions for  $\text{Ar}^{8+}$  on atomic hydrogen, similar to the work of Abdallah *et al.*, [12] but with a true one-electron target. The limitation in momentum resolution along the

jet was no obstacle in this case because only the momentum of the recoil along the beam is measured. The choice of  $\text{Ar}^{8+}$  was made because it is a closed-shell projectile which, at the large impact parameters for which capture occurs, appears nearly point-like to the target, yet it has sufficiently large quantum defects for the penetrating orbits for  $n=5$  and 6 (where the capture occurs) to allow us to resolve the  $\ell$  values for capture. Cross sections were measured for  $v=0.3, 0.5$  and  $0.7$  a.u. A sample spectrum is shown in Fig. 3.2.1. As predicted by an atomic-orbital-expansion calculation carried out by Lee and Lin [14], the major effect of increasing the velocity is to populate more and more the higher  $\ell$  states. However, the observed population of  $n=6$  was found to be substantially higher than the calculations predicted. This is a real surprise, since it was expected that this calculational approach to this kind of problem was essentially exact and that the agreement would be perfect. No such comparison has been made previously for a true one-electron target, however. The agreement is not perfect. These data are described in the Ph.D. thesis of Erge Edgu-Fry, are being prepared for publication, and further experimental work for bare oxygen on atomic hydrogen is presently being carried out by two undergraduates in the laboratory using the apparatus built by Dr. Edgu-Fry.



**Figure 3.2.1.** Q value spectra for electron capture from atomic hydrogen by  $v=0.32$  a.u.  $\text{Ar}^{8+}$  projectiles.

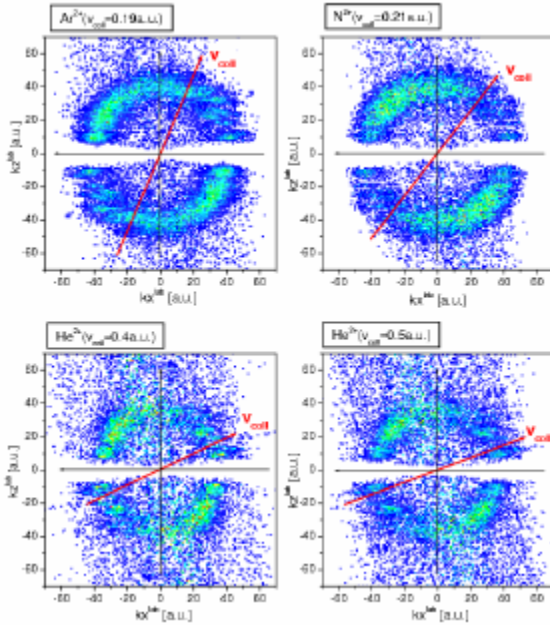
### 3.3. Ion-Ion Collisions Involving Molecular Systems -- *I. Reiser, C.L.Cocke, and H.Bräuning (Univ. Giessen)*

Another approach to studying a true one-electron-transition in atomic collisions is to use an ionic target: the  $\text{D}_2^+$  ion. [Note: deuterium is preferred to hydrogen for technical reasons and because its vibrational wave function is tighter]. As the Ph.D. thesis project of Ingrid Reiser, we had been attempting to measure the molecular-alignment-dependence of electron capture from this target by doubly charged He, N and Ar ions for several years. Such collision systems are of interest because they allow us to study capture from the simplest known molecule in a true one-electron process. The molecular target also offers the possibility to study the dependence of the

capture probability on the angle between the internuclear separation vector and the beam. On simple arguments, one would expect interference effects between amplitudes for capture from the two “atomic” centers intrinsic in the electronic wave function of the target [15-18], and these effects should reveal themselves in this angular alignment dependence. Total cross section measurements were first carried out at the Univ. of Giessen, in a collaboration between KSU and Giessen [Pub. #38], and found to be consistent with the predictions of such an interference model [19].

The doubly charged ions were produced in a 5 GHz ECR ion source and the  $D_2^+$  ions were produced in an Oscillating Electron Ion Source. Both ion beams were charge state analyzed by magnets before they entered the collision region where the two beams intersected each other at an angle of  $90^\circ$ . The reaction products were then separated from the parent ion beams by analyzing magnets and energy analyzed in an electric field before they were detected with 2D-position sensitive MCP detectors, one of which we equipped with a delay-line anode in order to observe both molecular fragments. Typical particle densities in the ion beams were of the order  $10^4 \text{ cm}^{-3}$ . Through improved differential pumping, we reduced the rest gas pressure by a factor of five down to  $2 \times 10^{-10}$  Torr, or a background particle density of  $7 \times 10^6 \text{ cm}^{-3}$ . Following capture from  $D_2^+$  by the doubly charged projectile, the molecule exploded into two protons. By detecting the impact times and positions on the molecule MCP detector, the angle of the molecule at the time of capture was deduced. Extensive analysis of the optics of the beam line was necessary to interpret these data.

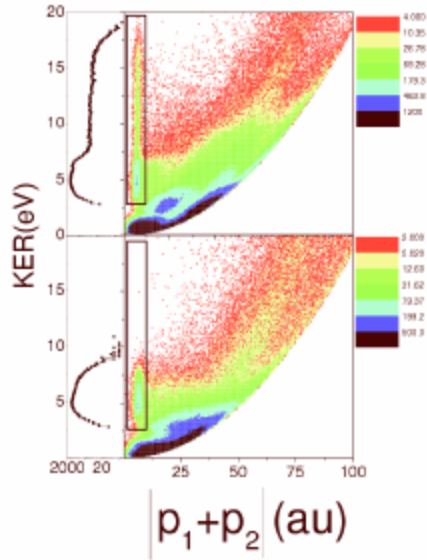
After considerable struggles (and in spite of the pronouncement by a recognized expert in the field that this experiment was impossible), the experiment worked. Figure 3.3.1 shows a momentum spectrum of the  $d^+$  ions from the exploding molecule, viewed in the plane defined by the direction of propagation of the initial  $D_2^+$  molecule and the relative collision velocity vector. This direction of this latter vector is also shown in the figure. The capture shows a propensity for enhanced capture when the molecule is perpendicular to the collision velocity direction. This result would be expected on the basis of the interference effect mentioned above: when the molecule is perpendicular to the beam, the longitudinal momentum transfer which accompanies capture causes no difference in phase between the amplitudes from the two centers, and constructive interference of the amplitudes occurs. For any other angle, some destructive interference occurs, reducing the capture probability. A detailed model based on this idea was developed and compared with the data, and found to be in qualitative, but not quantitative, agreement. This work is described in the Ph.D. thesis of Ingrid Reiser and two articles based on it have been published [Pubs. #6a and #112].



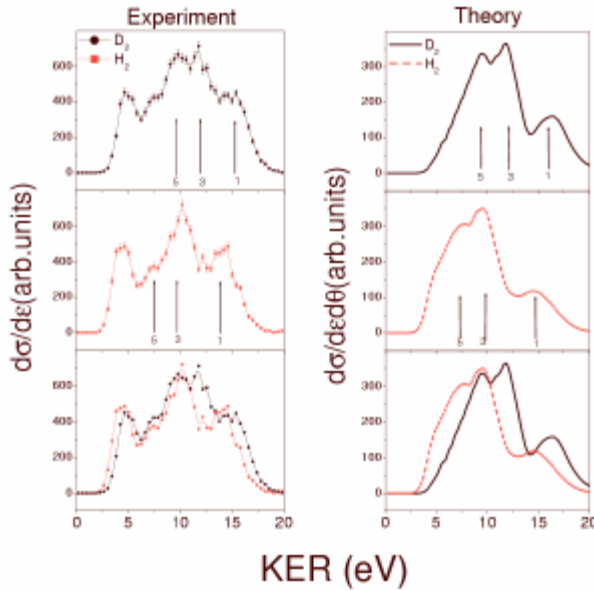
**Figure 3.3.1.** Momentum-slices in the plane determined by the collision velocity and the laboratory beam velocity for the capture from  $D_2^+$  molecules by different doubly charged projectiles. A propensity for capture from molecules aligned perpendicular to the beam is seen.

### 3.4. Identification of a Rescattering Mechanism in the Double Ionization of $D_2$ by Intense Laser Pulses – A. Alnaser, T. Osipov, E.P. Benis, A. Wech, C. Wyant, B. Shan, Z. Chang and C.L. Cocke

It is now well established that so-called “non-sequential” ionization of neutral atoms by femtosecond laser pulses with intensities in the range  $10^{13}$  -  $10^{15}$  watts/cm<sup>2</sup> can occur through a rescattering mechanism whereby the electron liberated in the single ionization process returns to the ion with sufficient energy to further ionize the singly charged ion through an (e,2e) process[20-29]. The equivalent process in the ionization of the  $D_2$  ( $H_2$ ) molecules has not been seen until very recently [30-32], partially due to the fact that charge-resonance-enhanced ionization [33-37] is usually the dominant process for multiple ionization. Using the newly installed fs light source in the JRM laboratory and COLTRIMS techniques, we have established, using linearly and circularly polarized light, that the high energy group reported by Staudte et al., [Pub. #68] is caused by a rescattering process. In Fig. 3.4.1 we show the kinetic energy release (KER) of  $d^+$  ion pairs for linearly and circularly polarized light on  $D_2$ , plotted versus the sum momentum of the two ions generated in the double ionization of deuterium by 35 fs light pulses at 800 nm with a peak intensity near  $2.5 \times 10^{14}$  W/cm<sup>2</sup>. Events lying near a sum momentum of zero are real coincidences, and those with KER between about 8 and 20 eV are due to rescattering. This process is turned off with circular polarization, for which the electron does not return to the molecule. The energy distribution of the resulting deuterons is consistent with the picture that the vibrational wave packet created in the single ionization of the  $D_2$  molecule, trapped in the gerade potential well of the  $D_2^+$  ion, is further ionized by the returning electron. This second step must itself proceed through excited states of the  $D_2^+$  ion, however, since the returning electron lacks sufficient energy to ionize the molecular ion in a single step. The observed deuteron energy distribution extends between limits that are consistent with the reflected energies from the double ionization potential evaluated at the turning points of the vibrational wave packet in the  $D_2^+$  gerade potential well.



**Figure 3.4.1.** The sum of the energies of two coincident  $d^+$  ions produced by double ionization of deuterium gas by a 35 fs laser pulse, plotted versus the magnitude of the vector sum of the momenta of the two fragments. The upper curve is for linear polarization and the lower one, circular polarization. The peak intensity in the stripe along the vertical axis corresponds to true coincidences, and the band of sum energies from 8 to 16 eV results from the rescattering process discussed in the text. This process disappears when circular polarization is used.



**Figure 3.4.2.** The spectrum of kinetic energy releases from the rescattering process. The structure is due to ionization of the  $1s\sigma$  wave packet at the first, third, fifth and so forth returns of the electron to the molecular ion. Left hand column: experiment; right hand column: model of Tong and Lin.

Figure 3.4.2 shows the KER for the rescattering process for deuterium and hydrogen targets. The structure is interpreted as due to the excitation on the first, third, fifth (etc.) return times of the electron. It is different for  $D_2$  and  $H_2$  because the evolution of the nuclear wave packet in the  $1s\sigma$  potential curve is different for the two cases, being slower for  $D_2$ . The rescattering process is believed to be a rescattering excitation of the  $1s\sigma$  electronic state of  $D_2^+$  to either the  $2p\sigma$  or  $2p\pi$  state, followed by ionization to the continuum by the laser field. A theoretical model based on this interpretation has been developed by Tong and Lin and the results of this model are also shown in the figure. This work has been submitted to Phys. Rev. Lett. [Pub. #4a].

**3.5. COLTRIMS Ionization Studies of Multielectron Systems Studied Through Synchrotron Radiation at the ALS** -- *R. Dörner, \* H. Bräuning, \* V. Mergel, \* O. Jagutzki, \* L. Spielberger, \* H. Khemliche, \*\* M. H. Prior, \*\* A. Staudte, \*\* J. Ullrich, \* C. L. Cocke, H. Schmidt-Böcking, \* A. Bräuning-Demian, \* K. Carnes, P. Richard, S. Dreuil, \* M. Achler, \* J. M. Feagin, T. Osipov, A. Cassimi, \*\*\*\* A. Landers, \*\*\* T. Weber, \* A. Czasch\**

This work is carried out in a collaborative project involving the University of Frankfurt\*, Lawrence Berkeley Laboratory\*\*, Kansas State University, Western Michigan University\*\*\*, and CIRIL\*\*\*\*. For two-electron systems He and D<sub>2</sub> the emphasis has been to use COLTRIMS techniques to investigate, in kinematically complete experiments, the photo-double ionization of He and D<sub>2</sub> by single photons. For more complex molecules, N<sub>2</sub>, CO, C<sub>2</sub>H<sub>2</sub> and C<sub>2</sub>H<sub>4</sub> the goal is to determine how the process depends on the alignment of the internuclear axis. Both linear and circular polarization have been used in many of these projects. The experiments are performed on “fixed-in-space” molecules, using *a posteriori* alignment. Control over this alignment has not been possible traditionally, with the first such experiments appearing only a few years ago. The experimental results show that the molecular alignment has a very large effect on the electron momenta. Partially not to overburden the reader, and also to clarify the KSU contribution to this collaboration, we describe below only the work on the molecular hydrocarbon molecules. This work has been analyzed and written up specifically by KSU personnel (Osipov and Cocke) and will form the Ph.D. thesis of Timur Osipov. In addition, KSU personnel (Osipov, Alnaser, Benis, Cocke) continue to participate regularly in ALS runs even when the specific project at hand will not be analyzed at KSU. In addition to the publications described in detail below, other publications from the collaboration include Pubs. #40, 58, 78, 83, 90 and 5a.

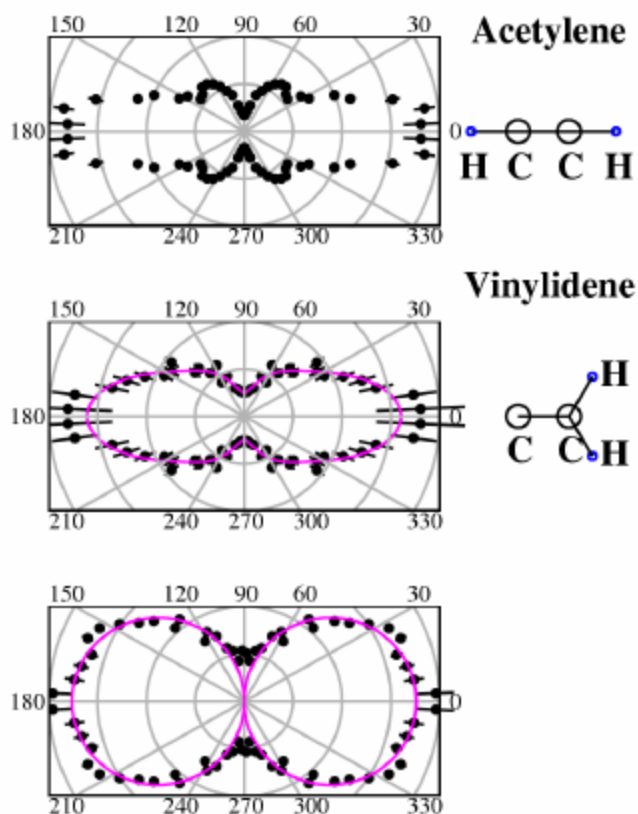
**3.6. Photoelectron Diffraction from C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub> and other Small Molecules** -- *T. Osipov, C. L. Cocke (KSU), A. Landers (Western Mich. Univ.), R. Doerner, Th. Weber, L. Schmidt, A. Staudte, H. Schmidt-Boecking (U. Frankfurt), M. H. Prior (LBL)*

Using beamlines 4.0 and 9.3.2 at the Advanced Light Source, we have measured the correlated momentum-space distributions of photoelectrons and charged photofragments ejected when the K-shells of C in acetylene and ethylene are photoionized. During the past year our work has centered on the analysis of diffraction patterns from C<sub>2</sub>H<sub>2</sub> and C<sub>2</sub>H<sub>4</sub>. Our attempt to identify in acetylene an f-wave shape resonance, well known in N<sub>2</sub> and CO [see Pub. #58 for example] but controversial for C<sub>2</sub>H<sub>n</sub> [39-41], was initially frustrated by the interesting observation that the dication of this molecule often undergoes isomerization to the vinylidene configuration before it dissociates. This isomerization had been observed previously [42] following ionization by soft x rays and considerable theoretical analysis of the reaction pathway and structure preceded this work [43; see also Pub. #3a and Refs. cited therein]. The separation of decays from the acetylene and vinylidene channels proved challenging, but has finally been accomplished. It turns out that, because of the very peaked photoelectron angular distributions associated largely with the strong f-wave character near the “resonance” region, the photoelectron distribution could be used as a clock to measure the time the isomerization process takes.

The major findings of the work are:

(1) Using only molecules decaying approximately along the polarization vector, the acetylene channel shows the expected f-wave structure near the predicted “resonant” energy (2)

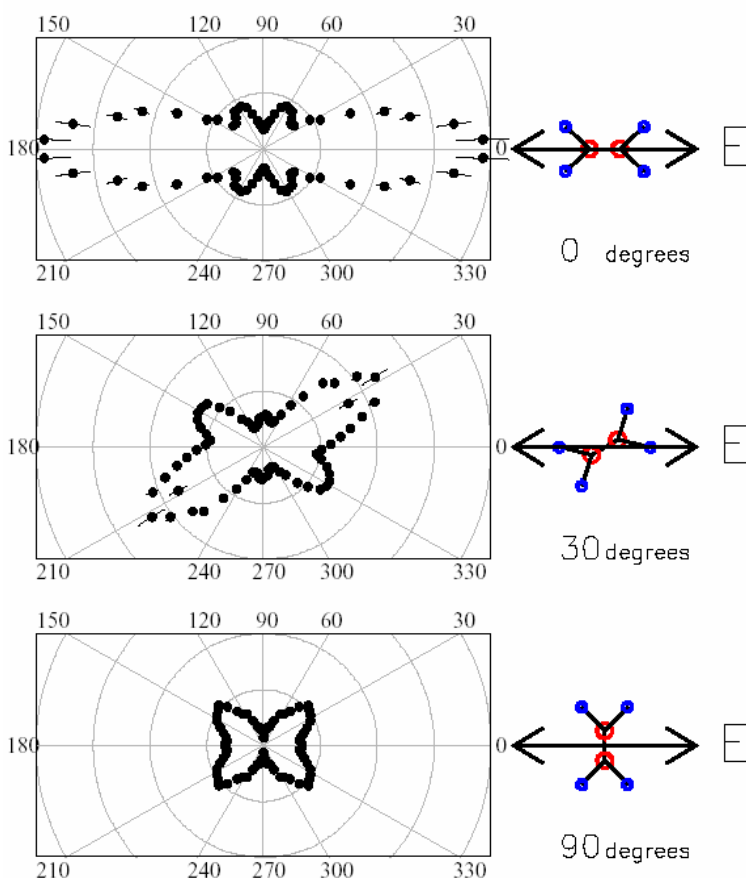
The vinylidene channel shows that this structure is considerably washed out (see Fig. 3.6.1). This occurs because the molecule rotates the bond angle after the photoelectron departs (a fast process) but before the dissociation is complete. This rotation angle, as seen through the extent to which the photoelectron distribution is washed out, provides information on the isomerization time: if the proton re-alignment occurs slowly, the correlation between axial dissociation and photoelectron emission will be entirely lost. Analysis of the data reveals that the rotation of the bond angle is very close to the minimum value consistent with the mass redistribution if the proton travels peripherally around the molecule to its new home. We deduce that the time scale for isomerization is no longer than approximately 60 fs. A Phys. Rev. Lett. on this work has been accepted for publication [Pub. #3a].



**Figure 3.6.1.** Angular distributions of photoelectrons from 310 eV photons on acetylene, measured in the body-fixed frame for the acetylene and vinylidene breakup channels. The latter distribution is washed out by rotation of the molecule between photoelectron emission and dissociation. An upper limit on the isomerization time of 60 fs can be placed from this data.

For the case of  $\text{C}_2\text{H}_4$ , no such complication occurs, and full photoelectron angular distributions for fixed-in-space molecules have been taken as a function of photoelectron energy spanning the range of the expected shape resonance. The data are extremely high quality and comprehensive. A small sample is given in Fig. 3.6.2. The angular distributions show definite enhancement of the f-wave partial wave in the “resonance” region for the sigma alignment, but strong enhancement in the p-wave channel as well. In spite of the high quality of the data, no unique extraction of the dipole matrix elements and phases from the data is possible, due to the

symmetric nature of the collision system. Nevertheless, by making reasonable assumptions about the smoothness of the contributing amplitudes, probable “best fit” amplitudes and phases have been extracted. A better way to make full use of such data is to take a definite theoretical calculation, deduce the appropriate dipole transition elements and from that calculate angular distributions to be compared with the data. Contact with two theoretical groups has been initiated to this end, and we expect to have complete comparisons available soon. This work is being written up in the Ph.D. thesis of Timur Osipov and a Physical Review article is in preparation.



**Figure 3.6.2.** Experimental angular distribution of photoelectrons from 302 eV photons on ethylene for three different alignments of the molecule with respect to the horizontal polarization vector. The statistical error bars are either visible or are smaller than the symbols.

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**Brett DePaola**

#### **4. Studies of Charge Transfer Collisions and Photo-Ionization Processes using Innovative Methodologies**

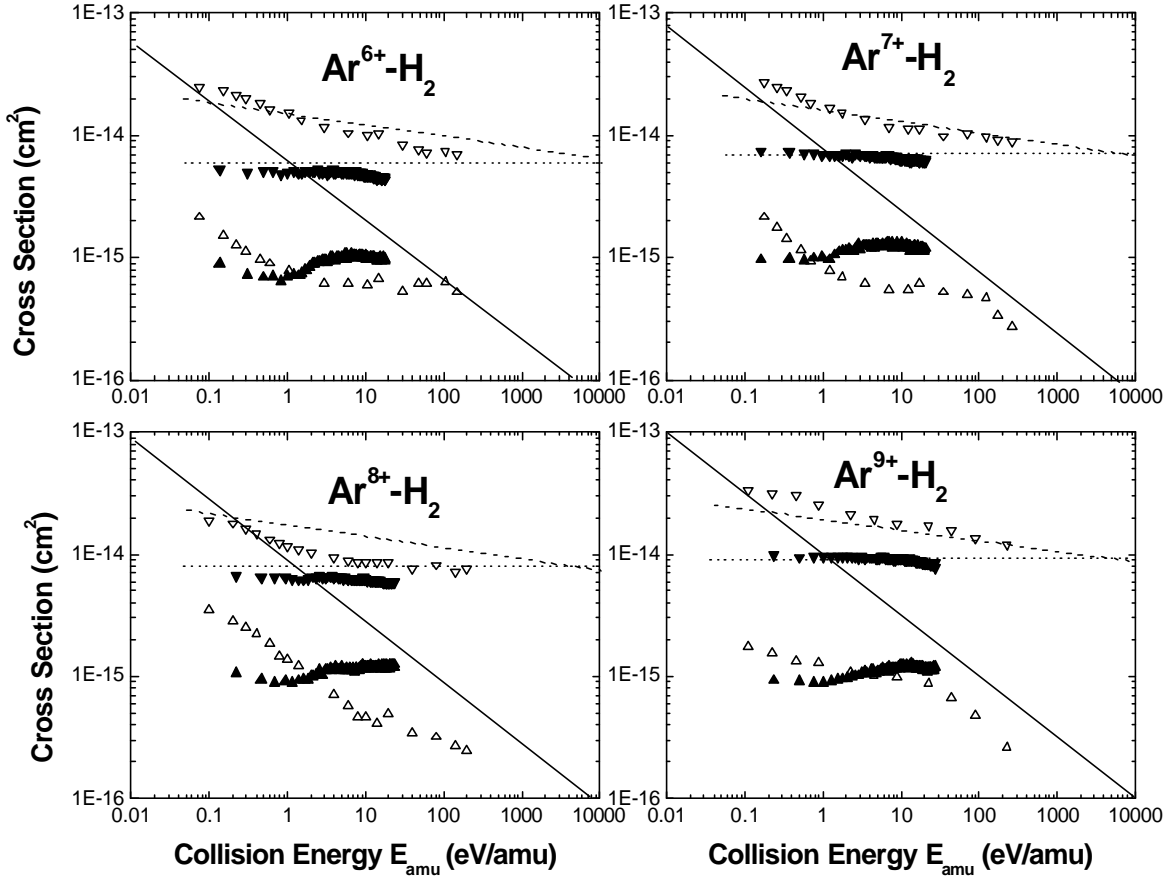
##### **4.1. Charge Transfer in Extremely Slow Collisions with Highly Charged Ions -- C. Verzani, K. Okuno, C. W. Fehrenbach, C. L. Cocke, and B. D. DePaola**

*We have measured total charge transfer cross sections in extremely slow (down to a hundred meV/u) collisions of multiply charged ions ( $q=2-26$ ) with ground-state He and H<sub>2</sub> targets.*

Measurements of charge transfer for very low energy, highly charged ions-atom/molecule collisions form an important topic of study since these collisions are important in astrophysical and fusion plasmas and upper atmospheric chemistry. Unfortunately, at energies in the few eV/u to few hundred eV/u range, these measurements are very difficult, and consequently few experimental data are available. Theoretical treatments are difficult as well, and there is a great need for experimental results against which to test calculations. At KSU we have developed, in collaboration with K. Okuno of Tokyo Metropolitan University, an octapole ion guide (OPIG) which is used to decelerate beams of highly charged ions, while keeping them radially confined. A target gas cell, located inside the OPIG allows the measurement of charge transfer cross sections in collisions between the highly charged ions and a neutral ground-state atomic or molecule target. We have chosen to concentrate our studies on single and double charge transfer from He and H<sub>2</sub> targets. (Net) single and double capture fractions are measured by directing the ion beams (primary, and once- and twice-less charged ions) exiting the OPIG onto a 2-D position-sensitive detector. Knowing the target thickness and detector efficiency allowed us to determine the absolute (net) single and double capture cross sections

In Fig. 4.1.1 we show some of the results our measurements. The hollow triangles represent our data (inverted is single capture; upright is double capture) and the solid triangles represent data from Okuno *et al.* in earlier measurements in which an OPIG is used, but a position-sensitive detection scheme is not used. The various lines represent different simple theoretical models. In general, the present KSU results are seen to be in very good agreement with the scaling law of Müller and Salzborn.

We have concluded cross section measurements for the following systems: Ar<sup>(5-11)+</sup> + He, H<sub>2</sub>, N<sup>(3-7)+</sup> + H<sub>2</sub>, O<sup>2+</sup> + He, H<sub>2</sub>, Ne, Ar, and Xe<sup>26+</sup> + H<sub>2</sub>. The experiment has served as the basis of a Ph.D. and the results will be submitted for publication.



**Figure 4.1.1.** Total single and double electron capture cross sections versus the collision energy in the laboratory frame for  $\text{Ar}^{(6-9)+}$  on  $\text{H}_2$ , and three simple theoretical models (single capture only).  $\nabla$  and  $\triangle$ , single and double capture from present results;  $\blacktriangledown$  and  $\blacktriangle$ , single and double capture data of Okuno; —, Langevin model; ----, Absorbing sphere model; ...., scaling law of Müller and Salzborn.

#### 4.2. Magneto-Optical Trap Recoil Momentum Spectroscopy: MOTRIMS -- H. Nguyen, H. Camp, X. Flechard, R. Bredy, S. R. Lundeen, and B. D. DePaola

*Using the MOTRIMS methodology, we have measured charge transfer cross sections, differential in initial and final state and in scattering angle, for singly charged alkali projectiles on ground-state and laser-excited Rb.*

In the past decade many beautiful experiments have been done using the technique of Target Recoil Momentum Spectroscopy (TRIMS). In these studies the momentum vector of the recoiling ions was directly measured using position-sensitive imaging and time-of-flight methods. The component of the recoil momentum perpendicular to the projectile axis ( $p_{\perp}$ ) is directly related to the collision scattering angle, while the component lying along the projectile axis ( $p_{\parallel}$ ) gives the collision Q-value, or energy defect (the initial minus final electron potential energy). For meaningful measurements to be made, the initial momentum spread of the target must be small compared to the momentum “kick” received by the recoil in the collision process.

To insure this, the target is often pre-cooled and made to undergo supersonic expansion prior to its collision with the projectile ion. The drawback of this powerful technique is that the study of collisions with laser-excited targets is difficult since systems with optically active electrons tend to condense or form clusters upon cooling. The solution implemented here is the use of a magneto-optical trap (MOT) to cool and hold alkali atom targets, in particular, Rb. Some fraction of the target is in an excited state as a natural consequence of the cooling and trapping process. Thus, in principle, one can simultaneously obtain relative state-to-state cross sections (total and differential in scattering angle) for ground-state and excited targets. In addition, because atoms in a MOT are more than 3 orders of magnitude colder than those in a pre-cooled supersonic expansion, the MOTRIMS methodology is not limited in resolution by target temperature.

The MOTRIMS studies carried out in the JRML during the past 3 years fall into two categories: **a)** determination of excited-state fraction, and **b)** differential cross section measurements. We present progress in these two categories in turn.

#### 4.2.1. Excited State Fraction Measurements

In a collision, the charge transfer rate out of some initial channel is proportional to the number of atoms in that channel times the cross section for charge transfer from that channel. An example of a Q-value spectrum is shown in Fig. 4.2.1.1. Here relative transfer rates are plotted versus Q-value for the 7 keV  $\text{Na}^+ + \text{Rb}$  collision system. The Rb has been partially excited to the Rb(4d) level, via the Rb(5p) level using two cw lasers. Each peak corresponds to a different state-to-state capture channel; the label on each peak indicates the final state in Na to which the electron is captured. A “\*” or “\*\*” in the label designates capture from Rb(5p) or Rb(5d), respectively. Each peak, then, is a relative measure of the product of cross section and initial state population. The problem is how to determine the separate constituents of this product.

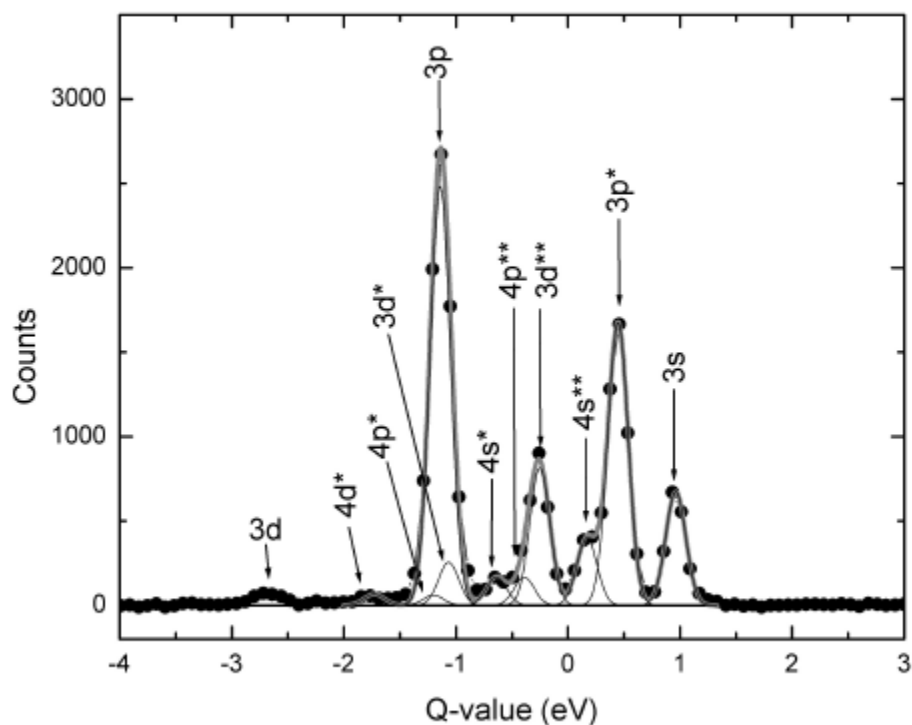
In a MOT, the cooled and trapped atoms move such a short distance in their decay lifetime that by chopping the lasers fast enough we can directly determine both the relative populations and the relative cross sections in the same measurement, since the projectile beam “sees” the same atoms with lasers on or off. Thus, changes in capture from Rb(5s) as the trapping laser is chopped on and off directly give us the excited-state fraction. For example, in a system containing only Rb(5s) and Rb(5p) targets,

$$f_s = \frac{A_s^{\text{off}}}{A_s^{\text{on}}}, \quad f_p = 1 - f_s = 1 - \frac{A_s^{\text{off}}}{A_s^{\text{on}}},$$

and

$$\frac{S_p}{S_s} = \frac{A_p^{\text{on}}}{A_s^{\text{on}}} \frac{f_s}{f_p},$$

where  $f_{s,p}$  is the fraction of atoms in the s (or p) state, and  $A_{s,p}^{\text{on,off}}$  is the measured area under a peak in a Q-value spectrum, corresponding to charge transfer from an s (or p) state, and with the exciting laser turned on (or off). This analysis can be trivially extended to N-levels, and we have already used it to measure incoherent, 2-photon, 2-color excitation efficiency of Rb to the 5d state (i.e., 5s-5p-4d).



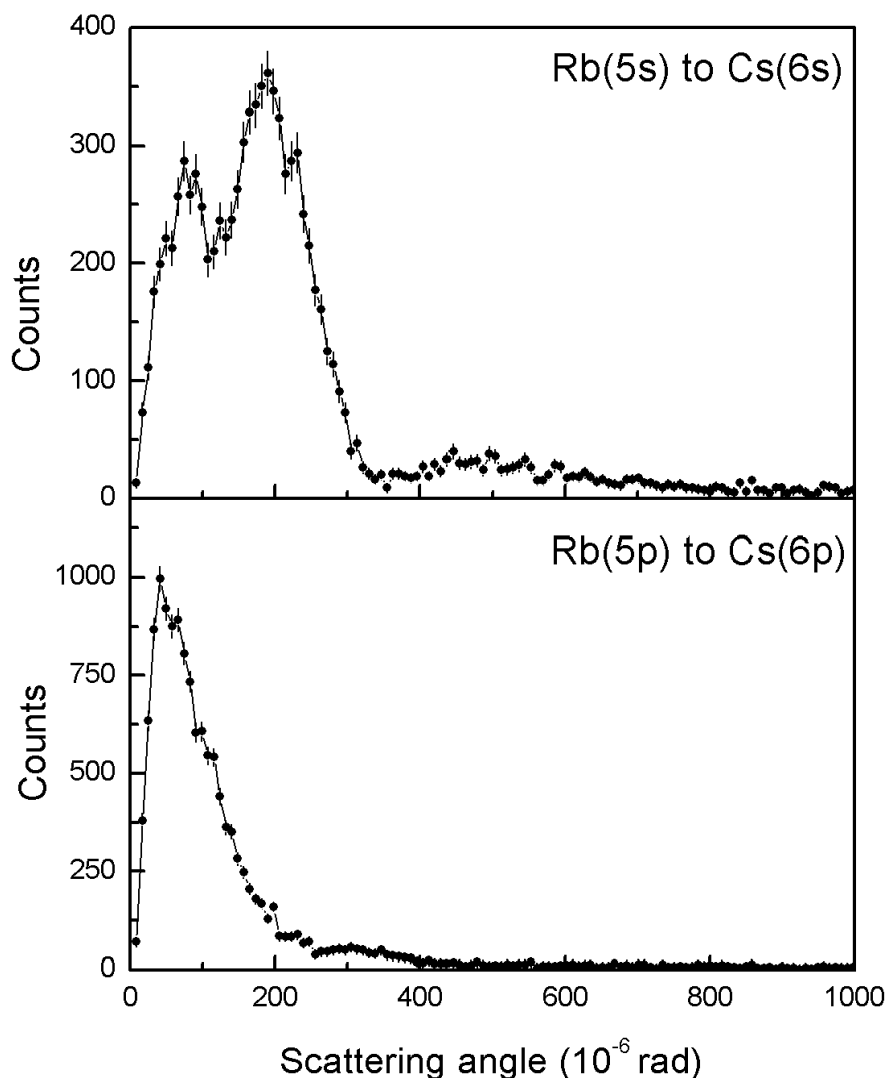
**Figure 4.2.1.1.** Typical MOTRIMS Q-value spectrum for the collision system of 7 keV  $\text{Na}^+ + \text{Rb}$ . The Rb has been laser excited, thus the spectrum shows capture from the ground state, Rb(5s), the first excited state, Rb(5p) (labeled with a single star, \*) and the next higher excited state, Rb(4d) (labeled with a double star, \*\*).

As the above discussion illustrates, knowledge of excited-state fractions is critical to the measurement of relative cross sections – and uncertainty in excited-state fraction translates directly into uncertainty in cross section. However, this methodology also represents a new tool for studying population dynamics in a cold sample of atoms. In the near future, we plan to exploit this methodology to study *coherent* excitation processes in 3- and 4-level systems. To this end, we have re-built the optical system, allowing us to introduce controlled, short pulse ( $\sim 30$  ns) temporally coherent pulses of narrow bandwidth ( $< 1$  MHz) laser light, having sufficiently high intensity both to efficiently trap and cool Rb atoms, and to apply and measure the results of a “stimulated Raman adiabatic passage” (STIRAP) process. This re-tooling resulted in negligible down-time for the cross section measurements described next.

#### 4.2.2. Differential Cross Section Measurements

Armed with this new tool for measuring the relative populations in the initial state of the target, we have completed a systematic study of charge transfer cross sections, channel by channel and differential in scattering angle, for singly charged alkali ions incident on Rb in the 5s and 5p states. The projectiles include  $\text{Li}^+$ ,  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Rb}^+$ , and  $\text{Cs}^+$ , over a range of collision energies from 2-7 keV. In Fig. 4.2.2.1, we show some results for a typical system, 6 keV  $\text{Cs}^+ +$

Rb. Here we plot relative capture cross section, differential in scattering angle for the two dominant charge transfer channels. The resolution in scattering angle is approximately 25 microns. These measurements will serve as the basis of a Ph.D. thesis for H. Nguyen, who is expected to graduate late in 2003. Some of these measurements played a significant role in the Ph.D. theory thesis of T. G. Lee, a student of C. D. Lin. Lee used a series of our measurements done on the  $\text{Na}^+ + \text{Rb}$  system to compare with his calculations.



**Figure 4.2.2.1.** Relative charge transfer cross sections, differential in scattering angle for the two dominant channels in the 6 keV  $\text{Cs}^+ + \text{Rb}(5s)$  and  $\text{Rb}(5p)$  collision systems. The indicated error bars are statistical, and the instrumental resolution in angle is about 25 microradians.

### 4.3. 3-D Spatial Imaging Technique for the Study of Above-Threshold Ionization as a Function of Laser Intensity -- R. Bredy, H. Nguyen, H. Camp, Z. Chang, and B. D. DePaola

*We have developed an efficient methodology for measuring above-threshold ionization rates as a function of peak laser intensity.*

In virtually all measurements of above-threshold ionization rate versus laser intensity, the ionizing laser beam has been focused down to some waist size in the interaction region. Thus, the target atoms or molecules are actually interacting with a range of laser intensities. The problem is that the ionization rate is known to be a non-linear function of laser intensity. We address this problem by using ion optics and time-of-flight techniques to obtain a 3-dimensional *spatial* image of the ionization region. (Recall that in a “momentum spectrometer”, such as used in the above experiments, one obtains a 3-D image in *momentum* space.) When compared with measured laser intensity profiles (also 3-D, using a translating CCD camera) one should obtain, in a single “snapshot”, a multiply redundant range of laser intensities along with the corresponding ionization rates.

In our implementation of this experiment we used the MOTRIMS “momentum spectrometer” from the above section. Potentials on the lens elements were adjusted such that instead of operation in “momentum imaging, position focusing” mode, as appropriate for TRIMS, we are in “spatial imaging, momentum focusing” mode, for the transverse directions ( $x$  &  $y$ ) as well as in time (which gives  $z$ ). The geometry of our apparatus is such that the ionizing laser beam, delivered to our experiment room from the Kansas Light Source femtosecond laser facility, enters our chamber in a vertical plane and at an angle of  $55^\circ$  from the horizontal. Through various manipulations of the beam position, we have calibrated the magnification of our lens system. In addition, this geometry has allowed us to directly measure the  $t \rightarrow z$  conversion required for true 3-D imaging. The status of this experiment is as follows: We have analyzed the laser beam and obtained 3-D characterization of its intensity profile. (It is a slightly astigmatic, 2-D Gaussian beam.) We have calibrated our 3-D spatial imaging system, and we have obtained 3-D images of the ionization region. We have experimentally verified that for our proof-of-principle system the spatial resolution in the  $x$ - $y$  plane (the detector plane) is just the spatial resolution of the detector (150 microns) divided by the ion lens magnification ( $\sim 6$ ) or  $\Delta x, y \approx 25 \mu m$ . Thus, should we choose to, an ion lens system with far greater magnification could be designed and constructed, and would result in a far greater spatial resolution. In the  $z$  (time) direction, the resolution is better, but more difficult to estimate. We find it to be  $\leq 1 \mu m$ . These measured resolutions are consistent with our estimates based on Simion calculations. In the near future, we plan to wrap up this series of measurements, and possibly to extend them to the study of photo-ionization of laser-excited Rb(5p), and then, possibly, spin-aligned Rb(5p).

### 4.4. Stark-Induced X-Ray Emission from High Rydberg States of H-like and He-like Silicon Ions -- S. R. Lundeen, C. W. Fehrenbach, M. A. Gearba, C. Verzani, R. Komara, B. D. DePaola

*We have measured the effects that small electric fields have on the products formed in charge transfer collisions between highly charged ions and laser-excited Rydberg target atoms.*

Electron capture by highly charged ions forms highly excited ions which may radiate substantial energy in the form of x-rays and become an important energy-loss (or energy transfer) mechanism in hot plasmas. The cross section for charge transfer scales like the fourth

power of the target principal quantum number, but previous studies here have shown that the capture is to relatively high- $L$  states. Thus, one might expect that the subsequent decay rate is low. On the other hand, the very high- $n$  ionic Rydberg states formed in these collisions are extremely susceptible to Stark-mixing which introduces “p-character” into the high- $L$  states, causing a more rapid decay. As part of a continuing collaboration with S. R. Lundeen and co-workers from Colorado State University, we have extended our studies of charge transfer between slow, highly charged ions and laser-excited Rydberg targets in order to study this very effect. Specifically, beams of H-like and He-like ions from the KSU CRYEBIS were made incident on Rb(10F) targets, and the x-ray emission was measured as a function of an externally applied electric field. As a result of these experiments, we have shown that the products of charge transfer by highly charged ions on Rydberg atoms are, in fact, very sensitive to small applied electric fields. Even with a nuclear charge of 14, the Rydberg H-like ions formed in these slow collisions show a marked change in the rate of x-ray emission in an applied field of only about 20 V/cm. The observed changes agree well with simple models. Based on these measurements, we have also published the first direct experimental evidence that charge transfer by highly charged ions on Rydberg atoms strongly favors states of low  $m$ , with respect to the ion beam direction. We are now in the process of modifying the basic apparatus to allow us to sweep the direction of the applied electric field. The goal of the new set of experiments is to directly measure the  $m$ -distribution in the Rydberg ion formed in charge capture from a randomly oriented atomic Rydberg target.



**B.D. Esry**

## **5. Time-Dependent Treatment of Continuum Phenomena**

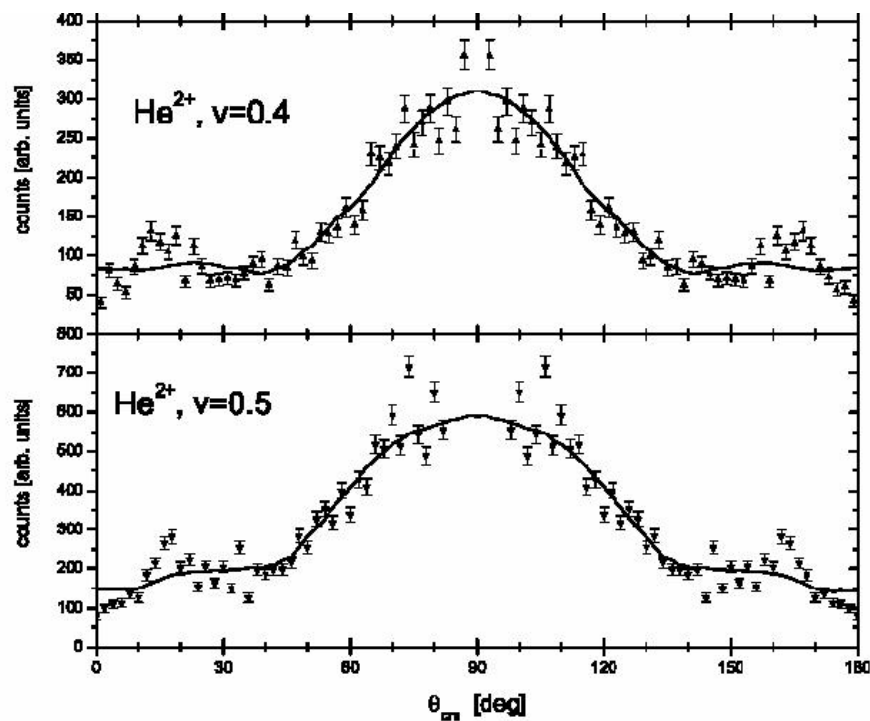
### **5.1. Charge Exchange in $\alpha + \text{H}_2^+$ Collisions**

*This work was motivated by experiments carried out by C.L. Cocke's group in our lab. The key feature in this system is its simplicity: it is a one electron problem. We have solved this problem using time-dependent propagation on a grid and have found that capture from molecules aligned with the projectile direction is favored--just the opposite of experiment! This work forms, in part, the Ph.D. work of Shu-chun (Amy) Cheng.*

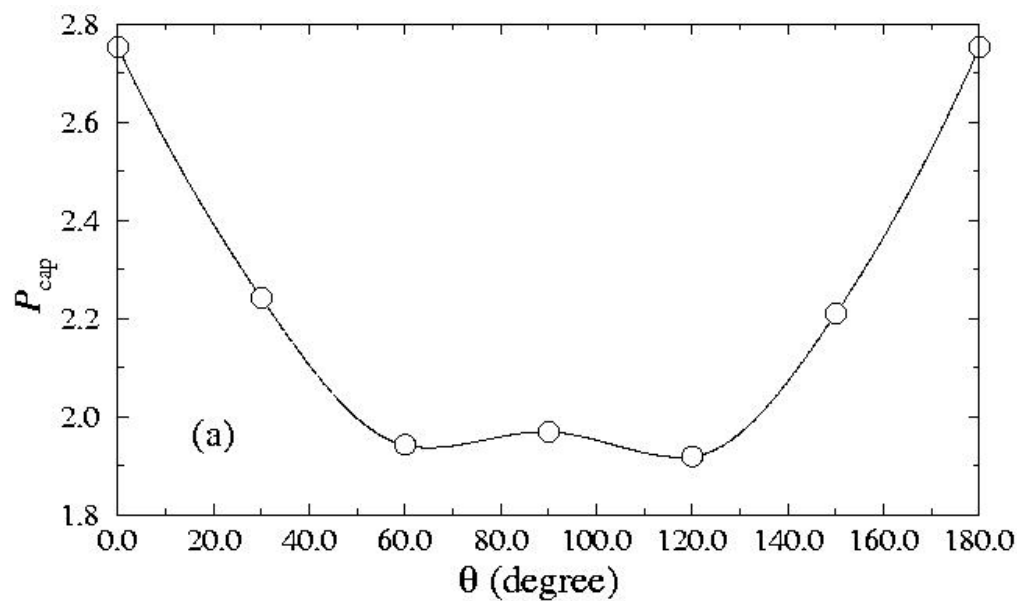
We have solved the three-dimensional time-dependent Schrödinger equation on a grid for the electronic motion in  $\alpha + \text{H}_2^+$  collisions. Our goal is to obtain the charge exchange probability as a function of the orientation of the  $\text{H}_2^+$  so that we may compare with the experimental results. Since the system has only a single electron, the signature of charge exchange is clear: the molecule dissociates.

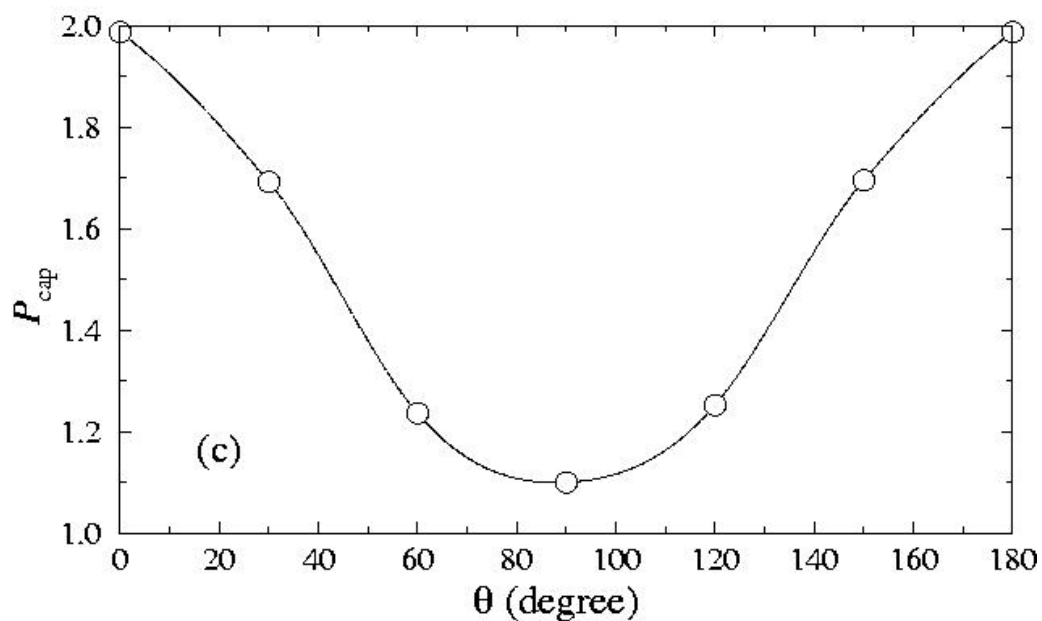
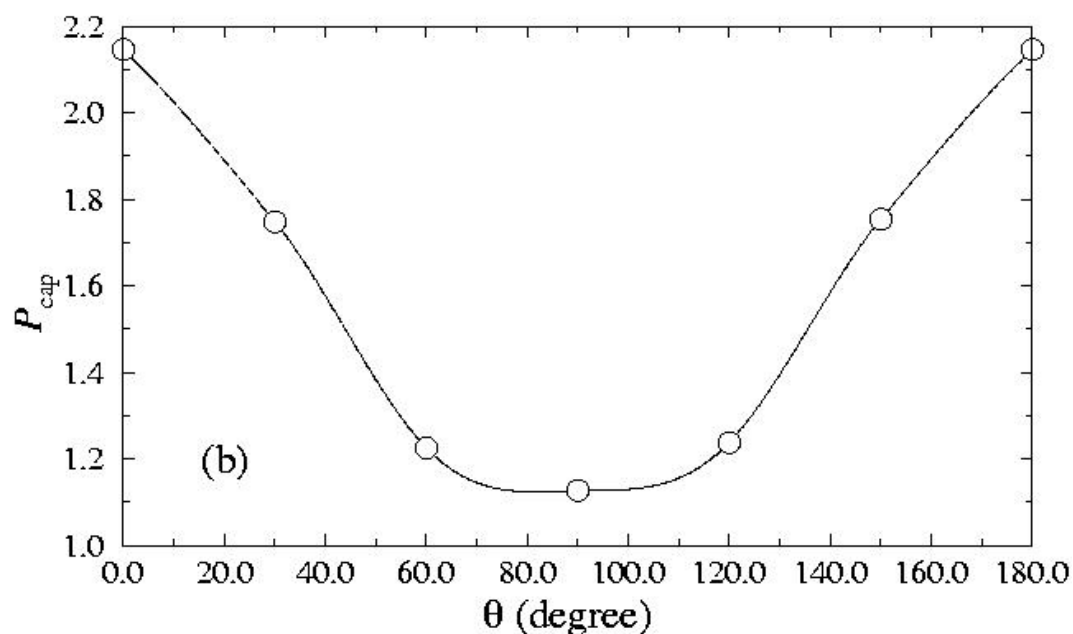
At the collision energies considered, the  $\alpha$  can accurately be assumed to travel along a straight line and the nuclei in  $\text{H}_2^+$  can be assumed fixed in space. The problem is thus a three-center problem, but this fact is of little import for the grid method employed. There are, however, five parameters upon which the capture probability depends. They are the three  $\text{H}_2^+$  nuclear coordinates, the impact parameter, and the impact velocity. Given that the calculation for a single set of parameters takes on the order of 10 hours, filling out this parameter space is a computationally expensive proposition.

Nevertheless, we have carried out a series of calculations for an impact velocity of 0.41 a.u. Figure 5.1.1 shows the experimental data from I. Reiser's thesis (carried out under C.L. Cocke's supervision). The main qualitative feature is that capture is largest when the molecule is aligned perpendicular to the projectile direction. In Fig. 5.1.2, we show our calculated results at two different values of the internuclear distance (the impact parameter and azimuthal angle of the molecule have been integrated over). The figures show a clear difference when compared to experiment--capture is smallest when the molecule is perpendicular.



**Figure 5.1.1.** The experimentally measured capture probability as a function of the molecular orientation angle  $\theta$  (relative to the projectile direction). The impact velocities are 0.4 a.u. and 0.5 a.u.





**Figure 5.1.2.** Our calculated capture probabilities as a function of the molecular orientation angle  $\theta$  (relative to the projectile direction). The circles indicate the calculated points; and the solid line, a spline fit to them. The impact velocity in each is 0.41 a.u. and the internuclear distance is fixed at (a) 2.2 a.u., (b) 1.8 a.u., and (c) 1.4 a.u.

The only other calculations carried out for this system are based on an old model from C.D. Lin's group that coherently superposes ion-atom scattering amplitudes. In principle, our calculation should include fewer approximations than this interference model, but implementing it on a grid introduces other approximations that perturb the spectrum of the constituent particles on the order of a few percent. Interestingly, the interference model predictions agree with the experiment for this system, but agree qualitatively with ours for other projectiles. This raises the question of whether a resonance effect is responsible for our disagreement with experiment. Since the grid perturbs the spectra of the  $\text{He}^+$  and  $\text{H}_2^+$  by a few percent, this could be enough to shift them out of any near resonance. We are in the process of evaluating this speculation as well as other sources of the discrepancy.

As long as only one electron is active, there is, in principle, no difficulty to extend the method to a polyatomic target, or even a molecular projectile. These cases would, of course, require careful modeling to reduce them to one active electron, but they could be quite interesting to study.

Publications from this work: in preparation.

## 5.2. Intense Laser-Atom Interactions

*Given the recent emphasis on intense laser physics in the lab, I have spent some effort on developing methods for treating these problems. My efforts have been two-fold: improving the direct solution of the time-dependent Schrödinger equation and developing the adiabatic Floquet representation for atoms in intense fields.*

### 5.2.1. Scaling the Time-Dependent Schrödinger Equation

I have developed a representation for the time-dependent Schrödinger equation that simplifies the problem considerably (see Pub. #14). The new representation, a combination of a coordinate and a wave function transformation, removes nearly all of the effects of kinetic energy from the wave function. This “scaling” representation frees us from the necessity of absorbing boundaries, allowing essentially boundary-free propagation of the wave function. It is then only necessary to propagate the relatively smooth envelope of the continuum wavepacket. We have applied the scaling method to the model problem of an intense laser interacting with a one-dimensional atom (Pub. #80). It was found there that the scaling does indeed reduce the computational burden by roughly an order of magnitude on average. To simplify the wave function even further, the wave function was transformed to the acceleration gauge to account for the effects of the oscillating laser field. We were thus able to propagate the wave function to very large times, allowing us to see directly in the wave function, localized continuum wavepackets corresponding to different numbers of photons absorbed, i.e., above threshold ionization.

Invited talks from this work: (see 3 talks in List of Invited Talks). Publications from this work: Pubs. #14 and 80.

### 5.2.2. Adiabatic Floquet Representation for Atoms

*This work was primarily carried out by an undergraduate student, Jesús Hernández. He will be attending graduate school in atomic physics at Auburn University beginning Fall 2003.*

The adiabatic Floquet representation has been used quite fruitfully to understand the dynamics of diatomic molecules in intense laser fields. The idea is to produce a set of Born-Oppenheimer potential curves that include the effects of the laser field. The result is a fairly intuitive picture in terms of the potential curves that permit identification of physical mechanisms in the ionization and dissociation of  $H_2^+$ , for instance. The presence of field-induced avoided crossings has led to the ideas of bond-softening and bond-hardening, among others.

We have begun developing the adiabatic Floquet representation for atoms in intense fields with the hope that the resulting potentials will provide similar insights as for molecules. The system that we have considered to date is the simplest: hydrogen in a CW laser. It turns out that the choice of gauge for the electromagnetic interaction is critical in producing simple potential curves. For  $H_2^+$ , on the other hand, the choice is not so critical, and the length or velocity gauges are typically used. Unfortunately,  $H_2^+$ —being a homonuclear molecule—is a special case that affords some simplifications.

For the atomic case, we have had to experiment with the gauge choice, settling finally on the acceleration gauge. The long range potential is then simple, but the short range part is still relatively complicated. The ideal choice would seem to be a mixture of gauges, changing from length gauge at short distance to acceleration gauge at large distance. We are currently working on implementing this approach.

Invited talks from this work: Jesús Hernández at DAMOP 2003 Undergraduate Session.

### 5.3. Rearrangement Processes in Asymmetric Three-Body Systems

#### 5.3.1. Protonium Formation in $\bar{p}+H(1s)$ Collisions

*Antiproton physics has recently gotten considerable attention with the production of cold antihydrogen at CERN. This project dealt with another aspect of antiproton physics, namely the production of protonium ( $p\bar{p}$ ). Protonium is one of the simplest forms of neutral hadronic matter and so could be of considerable interest for tests of fundamental theories.*

The low-energy, less than roughly 10eV, collision of  $\bar{p}$  with hydrogen is one of the most asymmetric systems one can consider. The difficulty lies in the fact that  $\bar{p}$  and  $p$  can form bound states with a ground state energy of approximately -459 a.u. By comparison, the energy in the incident channel is -0.5 a.u. The formation of protonium,  $Pn$  or  $\bar{p}p$ , occurs when the proton is captured by the antiproton, ionizing the electron in the process. Based on simple energy arguments, the most likely  $Pn$  states produced are in the  $n=30$  manifold. The extreme change in length and energy scales—going from truly quantum mechanical in the initial state to nearly classical in the final state—makes the problem extremely difficult to treat theoretically. Not surprisingly, the experiment is also difficult to do. Nevertheless, the ASACUSA collaboration at CERN predicts that they will make preliminary measurements of  $Pn$  formation in the near future. Unfortunately for us, the target will likely be hydrogen molecules rather than atoms since the  $Pn$  formation cross section is predicted to be larger from classical calculations.

It is tempting to apply the Born-Oppenheimer approximation to this problem, and many people have. The Born-Oppenheimer curves, however, do not allow for the formation of  $Pn$ ; the

united atom limit is a free electron. In collaboration with Hossein Sadeghpour at ITAMP, I have instead used the adiabatic hyperspherical approach to generate potentials that do indeed correlate to the  $\bar{p} + H(1s)$  limit as well as all of the  $Pn(n\ell) + e^-$  channels. Unfortunately, about 450 potential curves are required to cover the energy range of interest. This multitude of channels and the strong coupling between them is at the heart of the problems with asymmetric systems. To gain some insight into the physics, we have artificially reduced the masses of  $p$  and  $\bar{p}$  and carried out the scattering calculations with these simpler systems. By examining several values of the mass, we could identify the important channels.

Invited talks from this work: (see three talks in List of Invited Talks). Publications from this work: Pub. #96.

### 5.3.2. Diabatization Schemes

*Avoided crossings are the plague of any dynamical solution based on an adiabatic representation. There are many ad hoc procedures to produce diabatic curves that cross instead. We are taking the approach, however, of trying to design a diabaticization scheme that is exact.*

The vast majority of problems of current interest in atomic physics are described by a Schrödinger equation that is not separable in any coordinate system. Adiabatic approximations, such as the Born-Oppenheimer approximation, are convenient and powerful tools for dealing with such equations. Unfortunately, at the very points where the physics gets interesting—near the avoided crossings—the numerical treatment gets difficult. Theoretically, then, a representation that does not have avoided crossings would be desirable. Such representations are generically called diabatic, but it is difficult in general to generate a diabatic representation that includes as much physics as compactly as the adiabatic representation.

We have recently finished developing one possible diabaticization scheme. Standard, strict diabatic transformations are well known and require the nonadiabatic derivative coupling. We have dubbed our new representation the “split diabatic representation” as it is based upon the same equation as the strict diabatic transformation but with only part of the nonadiabatic coupling included. No approximations are made, however, since the remaining coupling is retained in its adiabatic form. The new representation can thus be considered a mixed representation since it is neither purely diabatic nor purely adiabatic, but the avoided crossings are eliminated. The split diabatic representation also avoids one of the problems of the strict diabatic representation, namely the unphysical behavior of the diabatic potentials at large distances. It turns out that because of long range nonadiabatic coupling—present for both the Born-Oppenheimer and the adiabatic hyperspherical representations—the strict diabatic potential curves oscillate sinusoidally at large distances. The long range portion of the nonadiabatic coupling need not be included in the definition of the split diabatic representation, though, so the asymptotic potential curves coincide precisely with the physically appealing adiabatic potentials.

Publications from this work: Esry and Sadeghpour (Pub. #7a).

## 5.4. Hyperspherical Approach to Four-Body Systems

### 5.4.1. Low-Energy Ps+Ps Collisions

*The three-body problem has received considerable attention to date, but the general four-body problem has only begun to be studied quantum mechanically. The Ps+Ps problem is among the most difficult since there is no mass difference ( $H_2$ ) or center of force (Li atom) to take advantage of. This study is thus a first attempt at the challenging problem of four interacting bodies.*

Roman Krems, a very capable Postdoctoral Fellow at the Center for Ultracold Atoms at Harvard, spent two weeks at Kansas State to begin implementing my formulation of an adiabatic hyperspherical approach for the low-energy collision of two Ps ( $e^+e^-$ ) “atoms”. The only four-body adiabatic hyperspherical treatments that have been done to date are for three electron atoms (see C.D. Lin's report). With an infinitely heavy nucleus, this system has a natural center about which to define approximately good angular momentum quantum numbers. In fact, four electrons can be treated in the adiabatic hyperspherical approach for this same reason. The equal mass problem that we are considering, however, does not have such a natural center, making the necessary expansion over partial waves much more slowly converging.

Because the adiabatic equation for the four-body problem in the center-of-mass (CM) frame requires eight coordinates, we must expand the wave function using partial waves. There is one spherical harmonic associated with each of the three relative position vectors in the CM frame, accounting for six coordinates. The other two coordinates are our hyperangles. In principle, then, coupled two-dimensional partial differential equations must be solved. This route very quickly becomes too computationally demanding. Instead, we are diagonalizing the adiabatic equation for a fixed set of  $\{\ell_1, \ell_2, \ell_3\}$ , then coupling these together to obtain the final result. Even though the  $\{0,0,0\}$  curve by itself recovers more than 90% of the asymptotic Ps+Ps energy, we are finding that the last few percent requires many partial waves.

We anticipate that the partial wave issue will soon be dealt with, and we will be able to produce adiabatic hyperspherical potential curves for Ps+Ps. With these curves and the coupling between them, we will be able to calculate both the bound states of the system as well as the low-energy scattering cross sections (both elastic and inelastic).

## 5.5. Other Activities

During this grant period, I have also contributed to the research efforts of other groups in the lab. In particular, I have performed calculations of the structure as well as full and half scattering calculations for  $HD^+$  in support of I. Ben-Itzhak's experimental efforts [Pubs. 4, 12, 13, and 50]. I am also on Pubs. #43 and 110 with C.D. Lin's group.

C.D. Lin

## 6. Theory of Ion and Laser Interaction with Atoms and Molecules

### 6.1. Laser-Atom and Laser-Molecule Interactions

*This is a new initiative started during this grant period. Following the tradition of the JRM laboratory, one of the goals in our theoretical effort is to provide support for the experimental works within the JRM.* Past experience demonstrated that such dialogue is beneficial for the whole program. In the meanwhile, we also developed new theoretical tools and ideas that are essential for the study of atoms and molecules in an intense laser field.

With the addition of Dr. X. M. Tong in the group as a Research Associate, we made great progress in this new direction in a short period of time. Within the current grant period, we have made three significant contributions. A graduate student, Z. X. Zhao, has also been fully involved in this effort.

#### 6.1.1. Tunneling Ionization Theory for Molecules (MO-ADK)

The tunneling ionization theory for atoms has been around for more than thirty years, under the name of the ADK (Ammosov-Delone-Krainov) theory. This theory calculates laser field ionization rates in terms of cycle averaged static field ionization rates. The ADK theory gives the ionization rate of an atom in analytical form with only a few parameters depending on the structure of the atom. Such a simple analytical expression previously was not available for molecules. Our first major contribution was to derive such an expression for the ionization rate of a molecule in a laser field, which we called the molecular ADK (or MO-ADK) theory, [see Pub. #89].

The main idea behind the MO-ADK theory is the recognition that ADK ionization rates depend on the electronic wavefunction in the asymptotic region. To derive an equivalent ADK theory for molecules, the electronic wavefunction of a molecule has to be expanded in terms of single-center functions. The expansion coefficients reflect the structure of the valence electron in a molecule.

According to the ADK theory for atoms the ionization rates depend primarily on the ionization energy. Thus a molecule with ionization energy comparable to that of an atom is expected to have nearly the same ionization rate. This is the case for Ar and N<sub>2</sub> which have nearly identical ionization energies and indeed their ionization rates have been shown to be nearly identical experimentally. On the other hand, Xe and O<sub>2</sub> also have nearly identical ionization energies, but the ionization rate for O<sub>2</sub> is much less than that for Xe. This is called ionization suppression in the literature.

In the MO-ADK theory we emphasize the geometric property of a molecular orbital of the valence electron. For O<sub>2</sub>, its valence electron is in a *p* orbital which is perpendicular to the axis of the molecule. When the molecule is aligned along the laser polarization direction, the electron density in the field direction is small such that the ionization rate is small. For N<sub>2</sub> the valence electron is in a *s* orbital such that the electron density along the laser field direction is large, and the ionization rate is not suppressed. This qualitative interpretation is further supported and refined by the quantitative MO-ADK model.



We have used the MO-ADK model to obtain the ionization rates for a number of molecules studied in the experiment by Wells *et al.*, [Phys. Rev. A **66**, 033402 (2002)]. The theory has been shown to explain all the molecules except for  $F_2$ . The origin of the difference is still not clear. We also note that the molecular structure for  $F_2$  is not as accurately known in the literature.

The MO-ADK theory has also been used to interpret the cutoff in the high-order harmonic generation. A reduced ionization rate for  $O_2$  implies that the cutoff of the high-order harmonic in  $O_2$  should be higher than the cutoff in Xe. This is indeed the case as shown by Shan *et al.*, in their first experiment using the new Kansas Light Source. The joint experimental and theoretical paper appears in Pub. #86.

### 6.1.2. Alignment Dependent Tunneling Ionization Rates

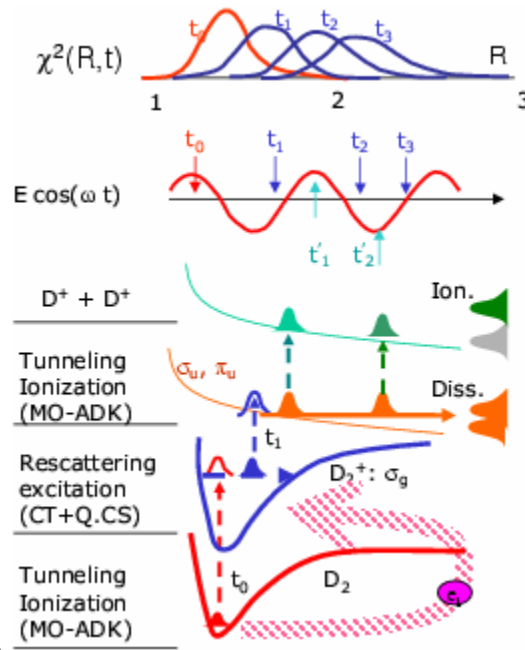
The ionization rate of a molecule in a laser field clearly will depend on the alignment or orientation of the molecule with respect to the direction of the laser polarization. Since in the experiment the molecules are randomly distributed initially, the measured ionization rate of molecules in a short laser pulse is obtained by averaging over the orientation of the molecules. The MO-ADK theory provides a prediction on the dependence of the ionization rate on the alignment of molecules. To test the theoretical prediction we proposed a pump-probe experiment where a short weak pulse is used to induce alignment of the molecules and another laser to ionize the molecules. Molecules can be periodically aligned at rotational revival times, during which time period the alignment changes rapidly. We proposed to ionize molecules during these time intervals. Our calculations show that the ionization rate will depend sensitively on the time delay between the two pulses, from which one can extract the dependence of ionization rates on the alignment of molecules. Although no such experiments have been carried out yet, an experiment with a similar idea has been performed by Corkum's group on  $N_2$  and their deduced alignment dependence is in agreement with the MO-ADK theory. Our paper reporting this work appears in Pub. #107.

### 6.1.3. Rescattering Dynamics of $H_2$ and Molecular Clock at Sub-fs Resolution

Following two recent Nature papers from Corkum's group [Niikura *et al.*, Nature **417**, 917 (2002); **421**, 826 (2003)] and the experimental work of Cocke's group, we had initiated a theoretical program for simulating the details of the ionization of  $H_2$  in an intense laser field. We focussed on processes which result in the emission of  $H^+$  with large kinetic energies (greater than 5 eV per ion). In particular, we concentrated on molecules which are aligned perpendicular to the direction of the linearly polarized laser field. This special geometry eliminates complications from the strong bond softening and enhanced ionization processes of  $H_2^+$  which would result in lower kinetic energies of the protons. The laser intensity was chosen at where the rescattering mechanism is important, i.e., in the nonsequential ionization regime.

The  $H_2$  molecule is ionized near the peak of the laser pulse. We then follow the physical processes that lead to the production of  $H^+$  ions. First the ionization rate of  $H_2$  is calculated using the MO-ADK theory. This initial ionization creates a correlated electron wave packet and a vibrational wave packet which propagates and broadens in the  $S_u$  potential curve of  $H_2^+$ . The electron, which is in the field of the molecular ion and the laser field, will return to collide with the  $H_2^+$  ion at about  $2/3$  cycle of the optical period later and every  $1/2$  period after that, to excite or

ionize the other electron. The excited electron of  $H_2^+$  will dissociate into  $H+H^+$  if it is not further ionized by the laser. If it is further ionized by the laser, then two  $H^+$  ions are formed. Since the rescattering and/or ionization occur at relatively well-defined times, the dissociation or ionization energy of each  $H^+$  ion has its own characteristic value. By measuring the kinetic energy of the  $H^+$  ion, the recollision time can be read if the physical processes leading to the dissociation and the ionization are properly understood. The whole reaction is illustrated in Fig. 6.3.1.1.



**Figure 6.1.3.1.** Schematic of the rescattering process in laser- $D_2$  interactions. The time dependence of the laser pulse is shown in the second row. The  $D_2$  is first ionized at  $t_0$ , creating an electron wave packet which propagates in the laser field and the residual field of the  $D_2^+$  ion and a nuclear wave packet shown on the top line. The electron returns to recollide with  $D_2^+$  ion at time  $t_1$  to excite  $D_2^+$  to the excited electronic states when the nuclear wave packet has already expanded to the positions shown at  $t_1$ . The excited  $D_2^+$  can be ionized by the laser at  $t'_1$  when the laser reaches the peak strength again. Recollision and Ionization can also occur at later returns. The event, when each occurs, is marked by the kinetic energy distribution of the  $D^+$  ions. In other words, the kinetic energy distributions can be used to clock the time when the rescattering occurs or at what internuclear distances.

To simulate the physical processes leading to the dissociation and ionization of  $H_2$ , we need to have: (1) Ionization rates of  $H_2$  and  $H_2^+$  by lasers at different internuclear separations. We need to derive the MO-ADK rates for  $H_2^+$  from the ground and the excited electronic states at different  $R$ 's; (2) The classical trajectory from the rescattering process where the electron is under the field of the laser and the Coulomb field of the ion; (3) The excitation and ionization cross sections of  $H_2^+$  from the ground state to the excited electronic states at different internuclear separations.

From our simulation we conclude that for  $H_2$  at peak field near  $2 \times 10^{14}$  w/cm<sup>2</sup>, a large fraction of  $H^+$  ions are produced by the ionization of excited  $H_2^+$ , in agreement with the recent experiment from Cocke's group at the JRM laboratory. This result is in contradiction with the assumptions made in the experiment of Niikura *et al.*, where the  $H^+$  ions were assumed to come from the dissociation of  $H_2^+$ . Thus they attributed the peaks in the  $D^+$  ion kinetic spectra (the experiment of Niikura *et al.*, used  $D_2$  target) to incorrect physical processes and hence the molecular clocks were not read correctly. We have used the rescattering model to simulate the kinetic energy spectra of the ions for different laser peak intensities, and have also shown that a shorter laser pulse would allow the clock to be read more accurately. Based on our analysis, we showed indeed that the molecular clock can be measured with attosecond accuracy. A report on this work has been submitted to Physical Review Letters.

During this grant period we have also tested different numerical methods for treating laser-atom collisions and investigated the pulse length dependence of laser ionization of alkali atoms for future experiments in DePaola's group. These papers appear in Pubs. #1,56,80,108.

## 6.2. Hyperspherical Close-Coupling Method for Ion-Atom Collisions at Low Energies

*Despite the lack of broad interest in ion-atom collisions at low energies in the AMO community in recent years, this field is of importance in many areas such as in astrophysics and in laboratory plasmas, as exemplified by a workshop at ITAMP this year (2003) under the title of "Topical Group on EUV and X-Ray Emission from Comets, Planets, and Heliospheric Gas."* The recent observations of X-rays from comets were postulated to come from charge transfer between solar wind ions with the gas in the comet followed by radiative deexcitation.

While the field is old, from the theoretical viewpoint, the fundamental theory of ion-atom collision has remained incomplete for more than half a century. For collisions at low energies, molecular orbitals are the natural representations for describing slow ion-atom collisions. The well-known perturbed stationary state (PSS) approximation, first introduced by Massey and Smith in 1947, is known to have many fundamental deficiencies, namely, the theory is not Galilean invariant. Since then, many remedies have been suggested, including the so-called switching functions or the reaction coordinates, which were introduced to remove the Galilean dependence, but these remedies are unsatisfactory since they are not based on first principles.

An elementary ion-atom collision system consisting of one electron and two heavy nuclei is a special class of the general Coulomb three-body systems. It has long been believed that the hyperspherical coordinate approach would avoid the difficulties encountered in the PSS approximation. The hyperspherical close coupling method (HSCC) has been used to calculate electron-atom, positron-atom and atom-diatom collisions in the past, but extending the standard HSCC to ion-atom collisions encounters a number of practical difficulties because of the large number of partial waves needed to achieve a converged cross section calculation.

In the last grant period, we have developed the HSCC method to study ion-atom collisions. The new computer codes are fully working and have been used to test a number of ion-atom collision systems. In the new HSCC package, we employed modern powerful computational techniques in the formulation. This includes using the B-spline basis functions to obtain adiabatic hyperspherical potential curves (from Brett Esry), and the R-matrix propagation method and the slow-variable discretization method (SVD) in the solution of hyperradial functions. We have also employed a rigid-rotor approximation which allows us to calculate partial wave cross sections without the need to solve the adiabatic channel functions for each

partial wave, and a two-dimensional interpolation procedure within the SVD method so calculations can be carried out at higher energies.

So far we have studied a few collision systems:  $\text{He}^{2+}+\text{H}$ ,  $\text{H}^++\text{D}$ ,  $\text{H}^++\text{Na}$ ,  $\text{Si}^{4+}+\text{H}$  and  $\text{Be}^{4+}+\text{H}$ , from a few meV/amu to about 1 keV/amu. These collision systems have been studied by other theorists using reaction coordinates or switching functions and these calculations are considered to be the more reliable ones available. In general, we did not find great discrepancies between the present HSCC calculations and results from using the reaction coordinates for the total cross sections or cross sections to the dominant channels. However, we did find discrepancies in the small channels and in the partial wave cross sections. Thus it appears that calculations based on the reaction coordinate method are capable of providing reliable cross sections for ion-atom collisions, despite that ad hoc switching functions have been used in the formulation of the theory. In the last year we have carried out studies for these systems:

(i) The detailed formulation of the HSCC theory and the results for  $\text{He}^{2+}+\text{H}$  are now published, see Pub. #110. We found that the earlier MO calculations using electron translational factors are not in good agreement with the present HSCC results, while our calculations at low energies do agree with distorted wave atomic orbital calculations. The latter method, however, is much more difficult to calculate and has not been widely adopted.

(ii) For  $\text{H}^++\text{Na}$  collisions, we found that the recent calculations by Dutta *et al.*, [Phys. Rev. A **63**, 022709, (2001)] were incorrect. Instead the earlier calculations by Croft and Dickinson [J. Phys. B **29**, 57 (1996)] agree with ours. However, we did find discrepancy with the latter at the very low energies near the threshold. This calculation also establishes that the existing experimental low-energy collision data are not correct.

(iii) For  $\text{Si}^{4+}+\text{H}$  and  $\text{Be}^{4+}+\text{H}$ , we performed the calculation because there are experimental data for  $\text{Si}^{4+}+\text{H}$  for collision energies down to about 0.01 eV/amu from ORNL. This allows us to investigate the isotope effect and to examine the Langevin model. We found good agreement with the experimental data of Pieksma *et al.*, [Phys. Rev. A **54**, R13 (1996)] and the theory result presented in that paper calculated using the reaction coordinate method. We did find that the partial electron capture cross sections to 4s and 3d did not agree with the measurement of Wu and Havener, J. Phys. B **30**, L213 (1997). For  $\text{Be}^{4+}+\text{H}$ , we did the calculation in order to check with the detailed calculations published by Errea *et al.*, J. Phys. B **31**, 3527 (1998) using the reaction coordinate method. It turns out that we agree well in the total electron capture cross sections from a few eV/amu up to few keV/amu, and the good agreement prevails even for the J-dependent cross sections. On the other hand, at low energies we did note differences in the J-dependent cross sections. Thus we tend to believe that the reaction coordinate method works well in general, except at low energies and for small cross sections.

(iv) Excitation and charge transfer cross sections to H(2p) in  $\text{H}^++\text{H}$  or  $\text{D}^++\text{H}$  collisions. For this elementary system, the resonant charge transfer cross sections have been well studied both experimentally and theoretically for collision energies down to about 1 keV. Below that, few such studies are available. For energies below 1 keV, the resonant charge transfer cross section depends weakly on the energy. The only other important transitions are excitation and charge transfer to H(2p) where the cross sections also change little as the collision energies drop below 1 keV. The question is at what energy will the H(2p) cross section begin to drop. We carried out the HSCC calculation and found that this occurs at about 200 eV, and below 100 eV, the cross sections drop exponentially with energies. Our calculations also indicate that existing experimental data for H(2p) capture or excitation cross sections are questionable; so are the

results from the triple-center atomic orbital calculations by McLaughlin *et al.*, J. Phys. B 30, 1043 (1997).

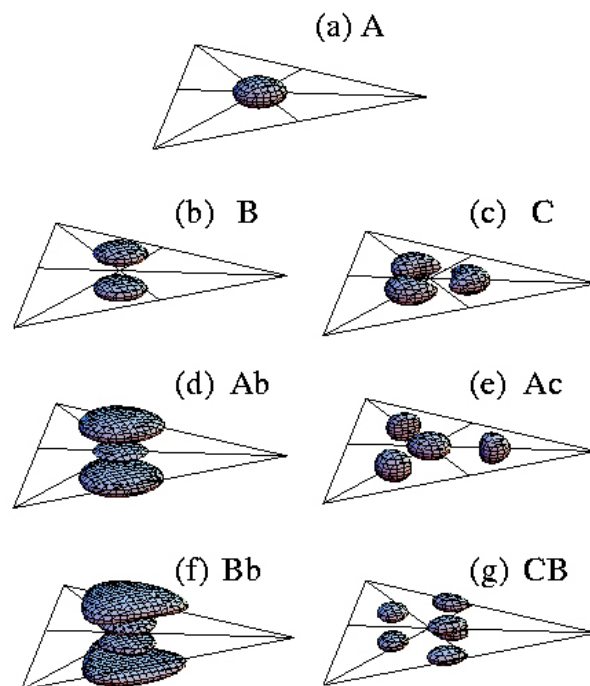
(v) Earlier two-channel calculations for muons colliding with H atom can be found in Pub. #11.

(vi) Using hyperspherical coordinates we also have searched for the possible existence of rotational excited states. The calculation concludes that there are no rotational excited states for helium trimers. This paper is in Pub. #43.

### 6.3. Triply Excited States of Three-Electron Atoms

*During this grant period we have completed the classification of intrashell and intershell triply excited states of atoms.* For intrashell states, we have classified the eight 222 (such as  $2s^22p$ ,  $2s2p^2$ ,  $2p^3$ ) states, that is, the states where the principal quantum number of each electron is in  $n=2$ , into three groups, called A, B and C, where each group is characterized by its bending and stretching modes of an  $XY_3$  molecule. For states in group A, the three electrons form an equilateral triangle with the nucleus at the center. For states in group B, the three electrons form an equilateral triangle, but the wavefunction vanishes when the plane of the electrons coincide with the nucleus. Thus they resemble the ammonia molecules. For states in group C, the electrons and the nucleus can be coplanar, but the electrons can form isosceles triangles only. When the three electrons are at the equilateral triangle configuration the wavefunction vanishes. Note that for states in group B and C, their wavefunctions have one nodal surface such that they have higher bending excitation energies. Within each group, states of different angular momentum form rotational multiplets similar to that of a symmetric top.

In the last grant period we managed to generalize the classification of the 222 triply excited states to the 333 triply excited states. There are 54 such intrashell states. We have been able to classify these 54 states. The details are published in Pub. #55. Basically we were able to identify the bending excitations for each group A, B and C and their combinations. With the properly chosen angular coordinates, the internal structure, or more precisely, the density distributions of the relative angles between the three electrons can be displayed. In Fig. 6.3.1 we show such examples. Besides A, B and C, we note Ab, Ac, Bb and CB groups. For states belonging to the same group, their energy levels exhibit rotational structure similar to approximately that of a symmetric top. With these new bending vibrational quantum numbers we were able to reclassify all the 54 intrashell 333 states. The classification has been confirmed by rearranging the calculated energy levels of  $N^{2+}$  and  $N^{4+}$  into the rotational manifolds. The details are described in Pub. #55.



**Figure 6.3.1.** Surface plots showing the different bending modes of triply excited states. For a detailed explanation, see Pub. #55.

In this grant period, we have also investigated the correlations of the electrons in intershell triply excited states. We have used the hyperspherical coordinates to calculate the wavefunctions and have analyzed the hyperspherical channel functions for the intershell states. Due to the large multiplicity of the number of states, we focused only on the 223 intershell states, i.e., two of the electrons in the  $n=2$  shell and the other in the  $n=3$  shell. Within this group, there are already 49 states. We have been able to show that in addition to A, B and C, which classify the bending motions of the three electrons, additional “+” and “-” quantum numbers are needed to describe the symmetric or antisymmetric stretches of the outer electron with respect to the two inner ones. The “+” and “-” are similar to those used earlier in the classification of doubly excited states. The full description of this classification can be found in Pub. #109.

From the works supported under this grant, we claim that the general classification for the low-lying triply excited states are now complete. For higher manifolds, similar methods can be used but the full analysis will be too complicated.

We have also used the hyperspherical close coupling method to calculate the excitation energies and widths of some intrashell triply excited states of  $F^{6+}$  ions that have been studied experimentally by Pat Richard's group at the JRM. The experimental and theoretical results are published together, see Pub. #111.

In the last grant period the papers published in this area are: Pubs. #47, 55, 57, and 109.

## 6.4. Ion-Atom Collisions at keV/amu Energies

We continued to study a few ion-atom collision systems during this grant period in view of some recent experiments in the JRM laboratory and elsewhere. This includes:

(i) Impact Ionization at low energies. A few papers were published at the early stage of this grant period that dealt with electron momentum distributions by ion impact at low energies using the direction solution of the time-dependent Schrödinger equation in momentum space. The ejected electron spectrum of He by proton impact has been calculated and compared to experiments carried out at the JRM. The electron spectra from  $\text{He}^{++}$  colliding with H also have been calculated to probe the role of saddle point electrons, which play a dominant role in ionization at low energies. The importance of electron capture to the continuum is also examined for this system.

(ii) In view of the experimental study of angle-differential cross sections in low-energy ion-atom collisions in a MOT performed by Brett DePaola's group, we have engaged a related theoretical study. We have found generally good agreement between theory and the experimental data. For low energy collisions between  $\text{Na}^+$  with Cs, from the ground state or from the excited states, charge transfer occurs at very small scattering angles. With the improved resolution from the laser-cooled target, the angular resolution remains not adequate enough to resolve all the oscillatory structures predicted from the theoretical calculations. When the theoretical angular distributions are convoluted with the experimental angular resolution, good agreement with experimental data was found.

(iii) A number of papers were published for the charge transfer processes for a variety of collision systems during this period, including alignment dependent cross sections in ion and  $\text{H}_2^+$  collisions, the alignment of the  $1snp$  states in proton impact excitation of He, and the inner-shell ionization cross sections by heavy ions. The calculations were carried out in response to the demand from the experimentalists. A few other calculations were performed because of existing discrepancies between experiments and some other calculations.

The list of publications in this area are in Pubs. #2, 7, 8 9, 10, 18, 37, 46, 54, 77, 79, 84, and 88.

## 6.5. Other Activities

In the last grant period we have also carried out several theoretical studies on subjects that do not fit into the above categories. These problems were addressed in response to new experiments. In Pub. #44 we studied the radiative decay of doubly excited states of He. Doubly excited states of helium decay primarily by electron emission but for some states they decay mostly by radiative transitions. In Pub. #44 we investigated the radiative transitions and compared that to experiments carried out recently. In Pub. #45 we calculated the alignment of the excited states of He after they have been collisionally excited by protons. In Pub. #87 we reexamined the shakeoff theory in order to explain the measurement of the ratio of transfer ionization cross section to single electron capture cross sections in high energy proton-helium collisions. In the period we also wrote a chapter titled "Fast and Slow collisions of Ions, Atoms and Molecules" for the *Encyclopedia of Scattering* published by Academic Press, see Pub. #81.

P. Richard

## 7. Structure and Dynamics of Atoms, Molecules and Surfaces: Atomic Collisions with Highly Charged Ions

### 7.1. Triply Excited States in Li-Like Ions

*This is a new initiative in which we have demonstrated that strongly-correlated, triply excited three-electron states can be studied effectively and clearly by triple electron capture in bare-ion atom collisions at high velocity by a proper choice of target projectile-ion pairs. The key to the method is that an ion velocity may be found where the relative momenta distributions of the target electrons overlap the momentum distribution of one of the excited shells of the projectile. Such a case is 16 MeV  $F^{9+} + Ar$  in which  $2l^3$  capture is prominent. These studies open the door for making detailed comparisons with new theories for strongly correlated three-electron systems. These studies include an extension of our previous studies of resonance electron scattering to triply-excited states by using two-electron metastable-ion beam collisions. This work forms part of the Ph. D. thesis of Mikhail Zamkov.*

The study of triply excited states of atoms and ions presents new opportunities to probe multi-particle excitations of a quantum system. For these states, interelectronic correlation plays a crucial role in determining their properties, thus the description of their atomic structure as well as excitation and decay dynamics, provides unique challenges to theory. The advances in synchrotron radiation technology in the last decade have stimulated considerable experimental and theoretical interest in the subject. In particular, the recent investigations using high-resolution photoelectron spectroscopy have provided some of the most detailed information on the partial photoionization cross sections for a number of triply excited states. Until now, however, studies of triply excited states have focused almost exclusively on neutral lithium, mostly due to the insufficient densities of ionic targets, which ruled out the possibility to investigate triply excited resonances in Li-like ions. Furthermore, the selective nature of the photoexcitation technique prohibited the population of quartet states, recently considered an ideal probe for photodetachment studies. The absence of available experimental data for three electron ions has prevented theorists from pursuing a global understanding of triply excited states, such as new classification schemes, approximate quantum numbers, and possible approximate selection rules for the formation and the decay of these states.

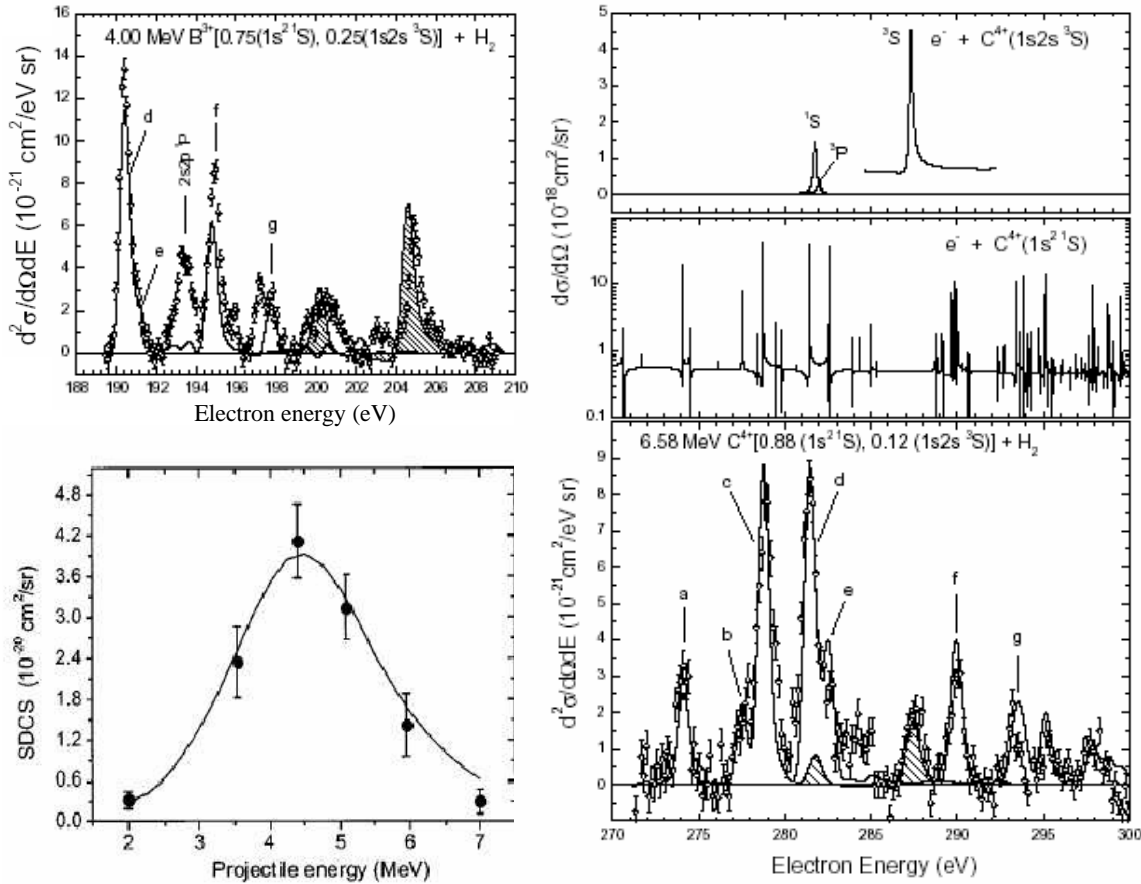
We have introduced two novel experimental techniques that provide efficient ways to populate triply excited states in Li-like ions as well as to study their decay dynamics. In the first approach, the  $2s2p^2\ ^2D^e$  state is selectively populated by  $180^\circ$  quasi-free resonant electron scattering (RES) from the  $1s2s\ ^3S$  metastable state of He-like ions. In the second approach, all  $2l2l'2l''$  intrashell states can be formed via triple electron capture to bare ions. This technique has been demonstrated by studying triply excited  $2s2p^2\ ^2S^e$ ,  $^2,4P^e$ ,  $^2D^e$ , and  $2p^3\ ^2P^o$ ,  $^2D^o$  states of fluorine.

#### 7.1.1. Study of the Z-Dependent Autoionization Rates for the $2s2p^2\ ^2D^o$ Triply Excited States -- E. P. Benis, M. Zamkov, T. J. M. Zouros, T. Gorczyca, K. R. Karim, and P. Richard

Initially, the formation of the  $2s2p^2\ ^2D^e$  state was experimentally observed in high resolution Auger spectra obtained in collisions of  $B^{3+}$  beams with  $H_2$  targets. The  $B^{3+}$  ions were



prepared in mixed ( $1s^2\ ^1S$ ,  $1s2s\ ^3S$ ) ground and metastable states, respectively. Previously, two techniques for determining and controlling the fraction of metastable  $1s2s\ ^3S$  ions in He-like beams were developed. The results of these studies were published [Pubs. #26, 51, 70, 71, see section 3]. The  $2s2p^2\ ^2D^e$  state is formed via resonant electron scattering (RES), where the loosely bound target electron interacts with the  $1s$  projectile electron resulting in the transfer of the target electron to an excited projectile state with the simultaneous excitation of the projectile's  $1s$  electron. Thus the ion is promoted to excited states with an empty K-shell, from which it relaxes primarily via Auger decay.



**Figure 7.1.1.1.** Formation of the  $2s2p^2\ ^2D^e$  resonance in Li-like Boron and Carbon beams. **Left Top:** Zero-degree electron spectra for 4.0 MeV  $B^{3+}$  ( $1s^2\ ^1S$ ;  $1s2s\ ^3S$ ) collisions with  $H_2$ . Theory: R-matrix calculations within the ESM and convoluted with electron spectrometer resolution. **Left Bottom:** Measurements of single differential cross sections for the  $1s2s\ ^3S$  to  $2s2p^2\ ^2D$  excitation followed by the Auger decay back to the  $1s2s\ ^3S$  state as a function of the ion-atom collision energy. The theoretical single differential cross section (solid line) was calculated using the available autoionization rates, and was multiplied by a factor of 0.61 to fit the experimental data. **Right Top:** R-matrix calculations for  $180^\circ$  RES from the  $C^{4+}(1s2s\ ^3S)$  metastable state leading to the formation of the triply excited  $C^{3+}(2s2p^2\ ^2D)$  state. Both elastic (decay back to the  $C^{4+}(1s2s\ ^3S)$  state) and inelastic (decay to the  $C^{4+}(1s2s\ ^1S, 1s2p\ ^3P)$  states) RES channels are shown. **Middle:** Same as top, but for elastic RES from the  $C^{4+}(1s^2\ ^1S)$  ground state leading to  $C^{3+}(1s2ln)$  resonant states lying on top of the non-resonant continuum. **Bottom:** Data (open circles): Zero-degree electron spectra for 6.58 MeV  $C^{4+}(1s^2\ ^1S; 1s2s\ ^3S)$  collisions with  $H_2$ . Theory: R-matrix calculations within the ESM and convoluted with electron spectrometer resolution.

Measurements of Auger electron emission in the direction of the ion beam were used to determine the absolute cross sections for the formation of the  $2s2p^2\ ^2D^e$  state and the branching ratios of the corresponding elastic ( $^2D^e$  to  $1s2s\ ^3S$ ) and the two inelastic ( $^2D^e$  to  $1s2s\ ^1S$ ,  $1s2p\ ^3P$ ) electron scattering channels. The results have been compared to the recent theoretical prediction of the  $1/Z$  expansion method.

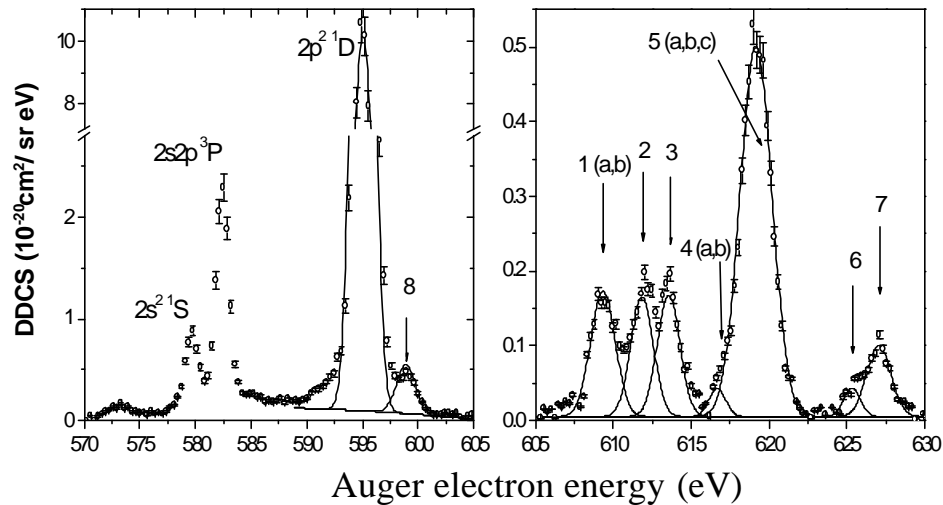
The success of the first study motivated us to proceed to the next step, i.e., to extend the investigation to ions with higher atomic numbers. The first measurement of the production and subsequent Auger decay of Li-like triply excited states as a function of an atomic number  $Z=5-9$  was performed. The R-matrix calculations were utilized within the electron scattering model (ESM) in which the quasi-free  $H_2$  electrons scatter from the ion as free particles with a momentum distribution given by their Compton profile. The comparison between the experiment and the calculations is shown in Fig. 7.1.1.1. Auger rates for the elastic decay scattering channel also were extracted from the experimental data and compared to a number of theoretical calculations.

An excellent overall agreement between the measurements and the R-matrix calculations has been observed. The complete isoelectronic study has been submitted for publication in Physical Review Letters [Pub. #15a].

### 7.1.2. Formation of All Li-Like Triply Excited States by Triple Electron Capture --

*M. Zamkov, E.P. Benis, C.D. Lin, T. Morishita, T.J.M. Zouros, T.G. Lee and P. Richard*

The second experimental technique relies on a strong projectile-Coulomb interaction to populate *all* triply excited states in Li-like ions. The states are produced by triple electron capture in energetic ion-atom collisions and observed by the subsequent Auger decay to the continuum states of He-like ions. The method has been demonstrated by studying triply excited  $2s2p^2\ ^2S^e$ ,  $^2,4P^e$ ,  $^2D^e$ , and  $2p^3\ ^2P^o$ ,  $^2D^o$  states of fluorine formed in fast collisions of bare  $F^{9+}$  ions with Ar atoms both experimentally, using zero-degree Auger projectile electron spectroscopy and theoretically, using the hyperspherical close coupling method (HSCC). (See Fig. 7.1.2.1.)



**Figure 7.1.2.1.** Present experimental measurements of Auger decay channels from the triply excited states of Li-like fluorine into the continua of  $F^{7+}$  ions. The solid line represents the Gaussian fit to the experimental data. A summary of present experimental results and theoretical calculations as well as figure peak notations is given in Table 7.1.2.1.

The Auger decay branching ratios have been extracted from the electron spectra and compared to the limited calculations available in the literature (see Table 7.1.2.1). Differential cross sections for triple electron capture are calculated in the independent electron approximation and are shown to be in good overall agreement with the experimental data. Finally, the energies for the observed triply excited states were calculated using the HSCC method and compared to both the present experimental data and other available calculations.

Present results demonstrate that triple electron capture can offer an efficient method for the study of triply excited states in different ions.

**Table 7.1.2.1.** Present experimental results and theoretical calculations for the observed triply excited states of  $F^{6+}$ . Single differential cross sections (SDCS) are given in units of  $10^{-21} \text{ cm}^2/\text{sr}$ . Auger energies are calculated relative to the ground state of Li-like fluorine ( $E = 2242.2 \text{ eV}$ ).

Peak	Auger electron energy (eV)			SDCS ( $\text{cm}^2/\text{sr}$ )		Branching ratios		
	Present measurement	Theory from Ref [1]	Theory from Ref [2]	Experiment	IPM calc.	Present measurement	Theory from Ref [1]	Theory from Ref [3]
1a	609.4 (0.5)	609.38	609.56	3.3 (0.6)	6.05	0.41	0.44	0.52
1b		609.77	609.77					
2	611.9 (0.6)	611.51	611.16	2.9 (0.7)	3.19	0.45	0.39	0.44
3	613.6 (0.6)	613.90	612.34	2.9 (0.8)	1.02	0.32	0.25	0.24
4a	616.7 (0.5)	616.97	616.89	0.5 (0.2)	0.99	0.50	0.50	0.52
4b		617.36	617.10					
5a		617.89	618.10			0.55	0.60	0.60
5b	619.1 (0.8)	618.42	618.62	12.7 (2.9)	15.19	0.59	0.56	0.48
5c		619.34	619.28			0.68	0.74	0.75
6	625.4 (0.5)	625.62	625.95	0.5 (0.2)	1.35	0.50	0.37	0.47
7	627.1 (0.5)	627.26	627.39	1.8 (0.4)	1.86		0.78	0.60
8	599.0 (0.7)	599.51	599.09	9.5 (1.9)	3.10	1.00	1.00	1.00
1	U.I. Safronova and R. Bruch, Physica Scripta <b>57</b> , 519 (1998)							
2	M.J. Conneely and L. Lipsky, Atomic Dat. And Nucl. Tables to be published (2002)							
3	K.T. Chung, Phys. Rev. A <b>59</b> , 2065 (1999)							

**Publications from this work: Pubs. #69, 111, 11a, 13a and 15a.**

## 7.2. Measurement of Triple Electron Capture in Fast Ion-Atom Collisions -- M. Zamkov, E.P. Benis, T.J.M. Zouros, T.K. Lee, and P. Richard

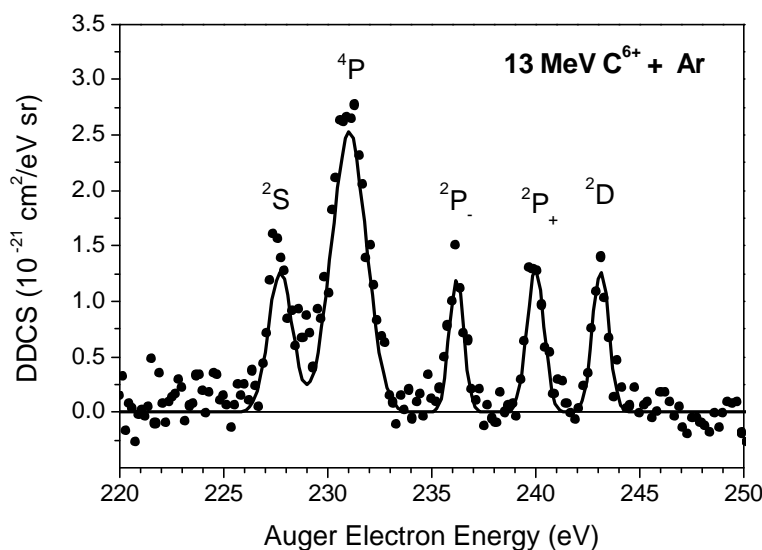
*The study of strongly-correlated, triply excited three electron states by triple electron capture was a direct follow up on an observation and proof that electron decay following triple electron capture was measurable. This section outlines that work.*

Multiple electron capture in collisions of highly charged ions with multielectron atoms or molecules has become a very active area of atomic physics research in the last decade. Transfer processes with more than two active electrons represent a fundamental problem of a many-body dynamic system, thus providing tests for most contemporary atomic models. The present understanding of multiple electron transfer has come from numerous experimental and theoretical studies primarily in terms of the classical quasimolecular description of the process.

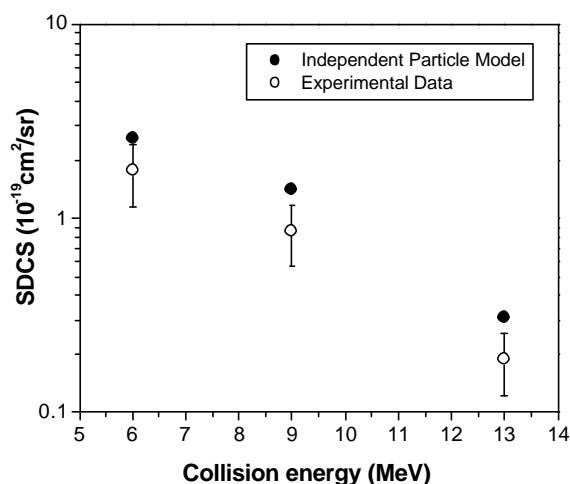
To date, however, a general approach, suitable for a wide range of impact velocities, has not yet been presented. In particular, the role of electron-electron correlation effects in multielectron capture still remains unclear, raising the demand for a more comprehensive model.

In the present work, high resolution zero-degree Auger electron projectile spectroscopy was used to study true triple electron capture to doubly excited KLL states of carbon. The states are produced in fast collisions ( $v = 4.5\text{-}6.6$  a.u.) of bare  $\text{C}^{6+}$  projectiles with Ar gas targets, see Fig. 7.2.1. High resolution measurements of differential cross sections for individual KLL states provided a unique tool for testing the predictions of the independent particle model for the triple electron capture. Single electron capture probabilities, employed by the model, were calculated using the two-center semiclassical close-coupling method, based on an atomic orbital expansion. In order to allow comparison of the measured zero-degree differential cross sections with calculated total cross sections, the Auger electron emission from the doubly excited KLL states was assumed isotropic.

In Fig. 7.2.2 single differential cross sections for triple electron capture calculated within the model are compared to the experimental measurements. The observed agreement is quite acceptable in view of the complexity of the process. This confirms that doubly excited states are formed mostly without relying on the electron-electron correlation. The observed agreement also signifies that the projectile's energy levels do not fully readjust in the course of the collision due to the insufficient interaction time, and the projectile charge remains only partly screened by captured electrons.



**Figure 7.2.1.** Absolute Auger electron DDCS spectra for the collision system of  $13 \text{ MeV } \text{C}^{6+} + \text{Ar}$ , recorded at zero-degree with respect to the beam direction. The formation of the  $\text{C}^{3+}(1s2l2l')$   $^2\text{S}$ ,  $^4\text{P}$ ,  $^2\text{P}_-$ ,  $^2\text{P}_+$  and  $^2\text{D}$  doubly excited states by triple electron capture, which Auger decay to the  $\text{C}^{4+}(1s^2)$  ground state, is prominent.



**Figure 7.2.2.** Absolute SDCS measurements of triple electron capture to the  $C^{3+}$  KLL states, populated in fast collisions of bare carbon ions with Ar targets (open circles). Independent particle model calculations (solid circles) are seen to be in fairly good agreement with the data.

**Publications from this work: Pubs. #91 and 10a.**

### 7.3. Production Mechanism and Fraction of Metastable $1s2s\ ^3S$ He-Like Ions Formed in Fast Cascading Ion-Atom Collisions -- M. Zamkov, E.P. Benis, H. Aliabadi, H. Tawara, T. Gray, T.J.M. Zouros, and P. Richard

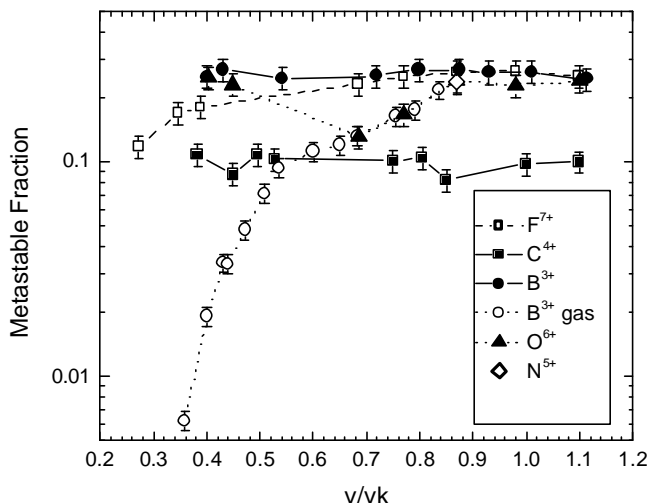
*The mechanism for the formation of  $1s2s\ ^3S$  metastable beams in high velocity beams is developed in this work.*

Experimental measurements of various collision cross sections for He-like beams require quantitative information on the non-negligible fraction of ions in a long-lived  $1s2s\ ^3S$  metastable state. The knowledge of the metastable  $1s2s\ ^3S$  fraction is crucial for the absolute cross section measurements of numerous processes in He-like ions including dielectronic recombination, impact excitation, transfer excitation, capture of the target electron, inelastic scattering or recently discovered superelastic scattering of target electrons from highly charged metastable ions.

A number of experimental techniques have been developed for the calculation of the metastable fractions over the years and several measurements of the metastable fraction have been reported in the literature for various He-like ions. Until now, however, the unified treatment, which accounts for a wide range of beam energies and target densities that dramatically affect the metastable population in two-electron ions, has not yet come forth. That creates a major problem in determining absolute cross sections for collisions with He-like ions, since theoretical calculations are very often unable to predict the correct fractions. Therefore, the goal of the present investigation was to measure the metastable fraction for the He-like isoelectronic sequence to establish a benchmark for various absolute measurements in metastable ion-atom collisions.

In this work, a universal technique for the determination of the metastable  $1s2s\ ^3S$  ion fraction, which is based on measurements of Auger electron emission from doubly excited states of Li-like ions formed in collisions of investigated beams with light targets, is outlined. The method was used to measure the fraction of metastable  $1s2s\ ^3S$  ions in fast He-like B, C, N, O, and F beams produced in collisions with thin carbon foils as a function of both the incident energy, in the range of 0.5 to 2 MeV/u, and the foil thickness, in the range of 1-5  $\mu\text{g}/\text{cm}^2$ . Some

differences were observed both in the energy dependence and the absolute value of metastable fractions for different ion beams. In particular, the metastable content in  $C^{4+}$  ions produced in carbon foils was found to be significantly lower than that of other investigated beams (see Fig. 7.3.1). The observed deviation has been explained as due to K-vacancy sharing, which is known to have the highest probability for symmetric collisions.

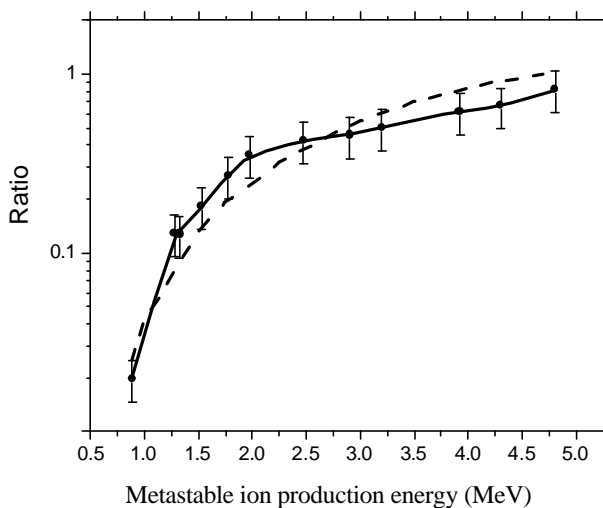


**Figure 7.3.1.** The fraction of metastable ions in He-like B, C, N, O, F beams versus the projectile velocity in units of K-shell electron velocity. The error bars correspond to the statistical uncertainty and are plotted at the 90% confidence level.

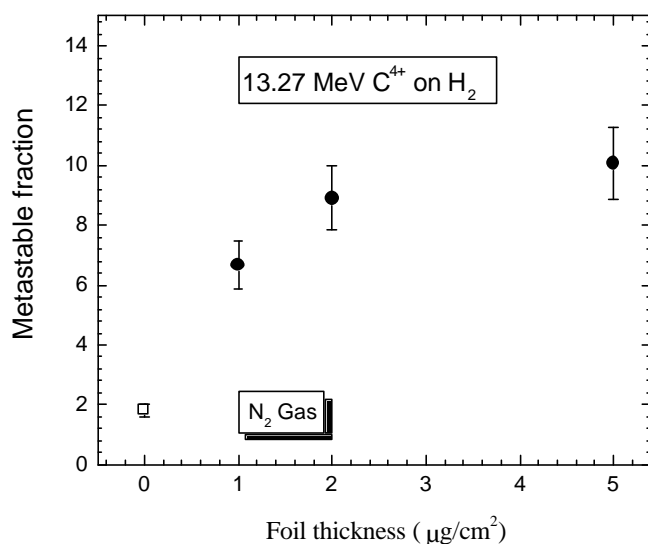
We have identified the dominant process contributing to the formation of metastable  $1s2s\ ^3S$  ions in collisions with atomic targets. It was demonstrated that the K-shell vacancy production in He-like beams, that leaves ions in the  $I^{(Z-1)+}$  charge state, followed by subsequent electron capture into the  $2s$  electron state is the only significant contribution to the formation of the metastable  $^3S$  ions in both solid and gas targets. In Fig. 7.3.2 the ratio predicted by this model is compared to present experimental data.

The first theoretical model for the predictions of metastable  $1s2s\ ^3S$  ion fractions has been developed and successfully applied for predictions of absolute values and energy dependence of the metastable fraction.

A different experimental technique also has been developed to allow for a more accurate determination of the metastable fraction. Similar to the first method it utilizes measurements of the Auger electron yield from the doubly excited states of Li-like ions,  $^4P$  and  $^2D$ . However, contrary to the first technique, where the fraction is determined in a single measurement, incorporating theoretical cross sections for the production of the doubly excited states, in the new approach, the metastable beam fraction is determined by relating the Auger yields obtained in two successive measurements taken at the same beam energy but with beams having different metastable fractions. The resulting value of the metastable fraction is therefore independent of the theoretical cross sections that largely affect the accuracy of the first technique. It has to be noted that although both techniques are applicable within the limits of the RTE energy region, the first technique can be applied in general with no experimental restrictions resulting in an upper limit for the absolute uncertainty of 45%. The second technique can be applied only in cases where the two metastable fractions, obtained for the same ion beam energy, are significantly different (>50%). Its accuracy increases with the increase in the difference of the metastable fractions.



**Figure 7.3.2.** The calculated ratio of the metastable  $1s2s\ ^3S$  ion fraction resulting from collisions with  $N_2$  gas to the metastable fraction produced in carbon foils, using the proposed model, is compared to experimental data.



**Figure 7.3.3.** The metastable fraction  $F$  in 13.3 MeV  $C^{4+}$  beams as a function of foil thickness. The error bars correspond to the statistical uncertainty and are plotted at the 90% confidence level.

**Publications from this work: Pubs. #26, 51, 70, 71 and 8a.**

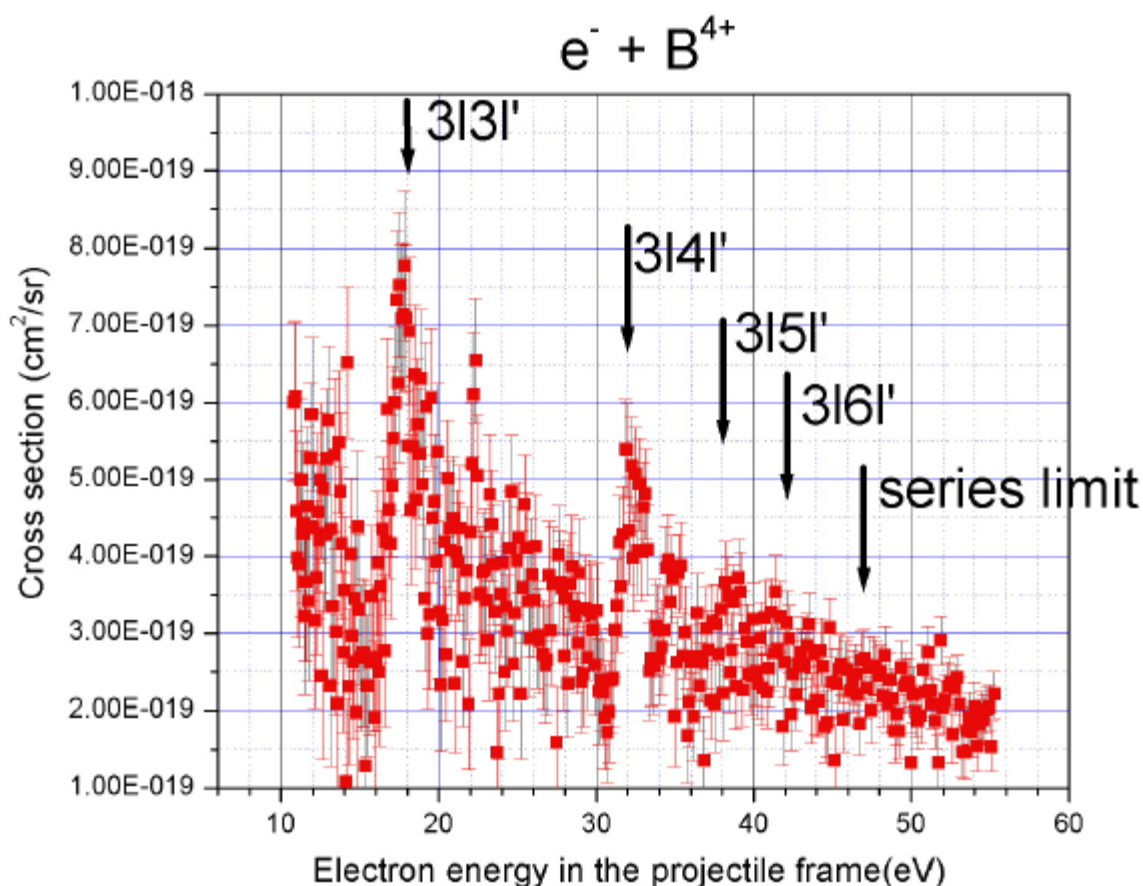
#### 7.4. Inelastic and Superelastic Electron Scattering Deduced from Ion-Atom Collisions

*We have measured the inelastic and superelastic scattering of electrons from highly charged ions by the RES method. Part of this work forms the Ph. D thesis of Habib Aliabadi.*

In previous grant periods, we have presented the results of the inelastic electron scattering from highly charged ions. Absolute double differential cross sections, DDCS, were measured for  $e^- + O^{7+}$  and  $e^- + F^{8+}$  collision systems. The  $3l3l'$  resonances were observed for  $0^\circ$  and  $180^\circ$  scattering in the c.m. frame. R-matrix calculations gave an overall good agreement with most of the observed resonances [Toth *et al.*, Phys. Rev. A 54, R4613, (1996), Grabbe *et al.*, Nucl. Instrum. and Methods in Phys. Res. B 124, 347 (1997) and Zavodszky *et al.*, J. Phys. B: At. Mol. Opt. Phys. 32, 4425 (1999)]. In our last renewal proposal, we proposed to study these resonances in  $e^- - Mg^{11+}$ ,  $-Al^{12+}$ , and  $-Si^{12+}$  collisions, which are of interest in fusion modeling,

with a newly constructed electron spectrometer capable of handling higher voltages required for the measurements. We were able to measure the electron elastic scattering DDCS, but had insufficient count rates from the LINAC beams to be able to successfully observe the electron inelastic scattering channels. As a recourse, we were able to measure the resonances in  $e^- - B^{4+}$  collisions. The energy resolution required to separate the resonances in this system is difficult to reach. Figure 7.4.1 shows the obtained spectra. To obtain higher resolution data, attempts were made to measure inelastic electron scattering spectra with the off-center hemispherical spectrometer, which has a zoom lens and position sensitive detector. These efforts failed due to the large background of electrons coming from cusp electrons hitting the plates of the analyzer and scattering onto the position sensitive detector.

We have also reported for the first time the measurement of electrons scattered superelastically from highly charged ions having an initial K-shell vacancy. In this process, the scattered electron gains  $\sim 725$  eV of energy from the deexcitation of an excited He-like  $F^{7+}(1s2s^3S)$  metastable ion to its ground state. A theoretical calculation based on an R-matrix approach agrees well in position, shape, and magnitude with the experimental results [Pub. #35].



**Figure 7.4.1.** The inelastic scattering DDCS for  $B^{4+} + H_2$  plotted vs. the inelastic electron energy in the projectile frame.

**Publications from this work: Pubs. #27, 30, 35, 9a and 12a.**



**7.5. Ionization of Atomic Hydrogen, Molecular Hydrogen, and Helium and Transfer Ionization with Highly Charged Ions at High Velocity; and Electron Capture with Highly Charged Ions at Low Velocity**

*These three projects are either completed or nearly completed. Due to lack of space, write-ups are not provided, but a list of the published results sorted by the projects is given.*

**Ionization of Atomic Hydrogen, Molecular Hydrogen and Helium with Highly Charged Ions at High Velocity** -- *L.C. Tribedi, L. Gulyas, M.E. Rudd, R. Moshhammer, and P. Richard*

**Publications from this work: Pubs. #24 and 25.**

**Transfer Ionization with Highly Charged Ions at High Velocity** -- *R. Unal, H. Aliabadi, H. Tawara, C.L. Cocke, I. Ben-Itzhak, M.J. Singh, A.T. Hasan, and P. Richard*

**Publication from this work: Pub. #32.**

**Electron Capture with Highly Charged Ions at Low Velocity** -- *H. Tawara, K. Okuno, C.W. Fehrenbach, C. Verzani, M.P. Stockli, B.D. DePaola, P.C. Stancil, U.I. Safronova, A.A. Vasilyev, S. Hansen, A.S. Shiyaptseva, and P. Richard*

**Publications from this work: Pubs. #23, 66, 74, 75 and 100.**

## 8. Interactions of Photons, Atoms, and Ions with Molecules, Clusters, and Surfaces

### 8.1. Charge-Transfer Dynamics in Slow Atom-Surface Collisions: A New Close-Coupling Approach Including Continuum Discretization

*We have developed a new two-center close-coupling approach in which the time-dependent Schrödinger equation is solved for an active electron interacting with a slow projectile and a metal surface.* The continuum of metal conduction band states is discretized by using Weyl wave packets. This wave packet description explicitly takes into account electronic couplings inside the metal (electron-hole pair excitation) and evaluates the population of both atomic and metal states. In numerical applications to H/Al collisions, we calculated the evolution of the atomic and metallic population amplitudes and discussed the main elementary hybridization, electron transfer, and excitation processes occurring during the collision [Pubs. #84, 101, 103].

### 8.2. Interactions of Highly Charged Ions with Fullerenes and Surfaces

*In collisions with complex targets, such as large atoms, clusters, and surfaces, slow highly charged ions may capture many electrons into highly excited states, thereby leading to the temporary formation of unstable, multiply excited projectiles, commonly referred to as “hollow ions”.* Recent recoil-coincidence collision experiments with fullerene targets have made it possible to distinguish between hard collisions, which strongly favor fragmentation of the fullerene, and soft collisions, which primarily (multiply) ionize the fullerene. We continued to investigate soft collisions of slow highly charged ions with gaseous C<sub>60</sub> targets. Our models for multiple electron transfer and emission yield fair agreement of our numerical applications with a variety of recent measurements of electron capture cross sections, charge-state distributions, projectile deflection angles, and projectile kinetic energy gains. This comparison makes static and dynamic properties of fullerenes, such as ionization potentials and polarizabilities, observable in scattering experiments with charge-state and energy-selected beams of highly charged ions [Pub. #102].

While for C<sub>60</sub> targets modern coincidence experiments allow for the selection of distant projectile trajectories that do not result in the destruction of the target's carbon cage, even in the most grazing collisions between highly charged ions and surfaces, close encounters cannot be avoided. This complicates the study of collisions with surfaces to the extent that the interaction mechanisms which dominate while the ion is close to (and possibly inside) a surface are not yet understood in full detail. For collisions of slow multiply-charged ions with solid surfaces, we therefore extended the well-know classical over-the-barrier model to take into account important interactions mechanisms that operate at small ion-surface distances, such as electron peel-off, side feeding, and continuum promotion. We calculated the population dynamics of the projectile by Monte-Carlo sampling along the entire ion trajectory over a large number of trajectories. For the classical motion of the projectile we included all relevant binary interaction potentials between the projectile and individual surface atoms. Our results are in reasonable agreement with various experimental observables for different combinations of projectiles, target types,

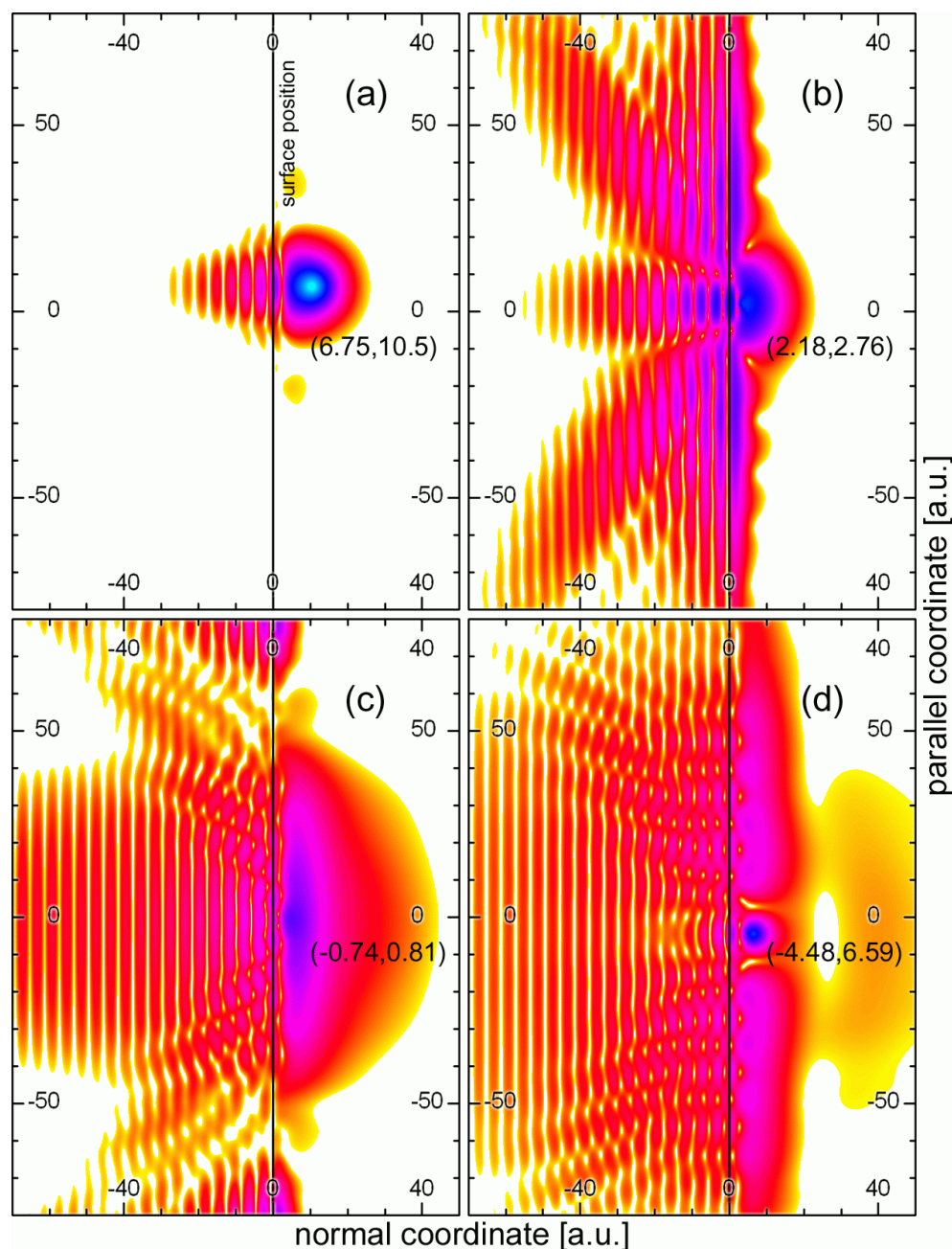
incident angles and beam energies. This has been achieved without adapting the free parameters involved in the simulation to a particular collision system [Pubs. #95 and 103].

### **8.3. Wave-Packet Propagation Methods Applied to the Neutralization of Negative Hydrogen Ions in Soft Collisions with Metal Surfaces**

*In this project we continued our investigation of the resonant transfer of a single electron, initially bound to the projectile, during the reflection of a slow incoming ion or atom on a metal surface.* Apart from contributing to the qualitative understanding of the interaction mechanisms through computer animations, this project has led to the quantitative assessment of charge transfer and wave function hybridization in terms of level shifts and decay widths.

Using a wave packet propagation approach, we find that the resonant charge transfer process of H near a Cu(111) surface is strongly influenced by transient hybrid states. These states originate from an ion-induced confinement parallel to the surface. The lowest members of this set of states have lifetimes of the order of the interaction times in typical particle-surface scattering experiments. The propagation of the electron probability density provides clear evidence for this effect in visualizing the evolution and the decay of these transient states (Fig. 8.3.1).

Interestingly, it appears that the existence of these laterally confined states is i) linked to the existence of a Cu(111) surface state within a band gap of bulk states and ii) leads to a strong increase of the negative survival probability in comparison with (under otherwise identical conditions) the neutralization of H at Cu(100), where the surface state is degenerate with the valence band. This leads to the simple interpretation that laterally confined states at the Cu(111) surface retain electronic probability density that eventually swaps back to the reflected projectile [Pub. #1a].



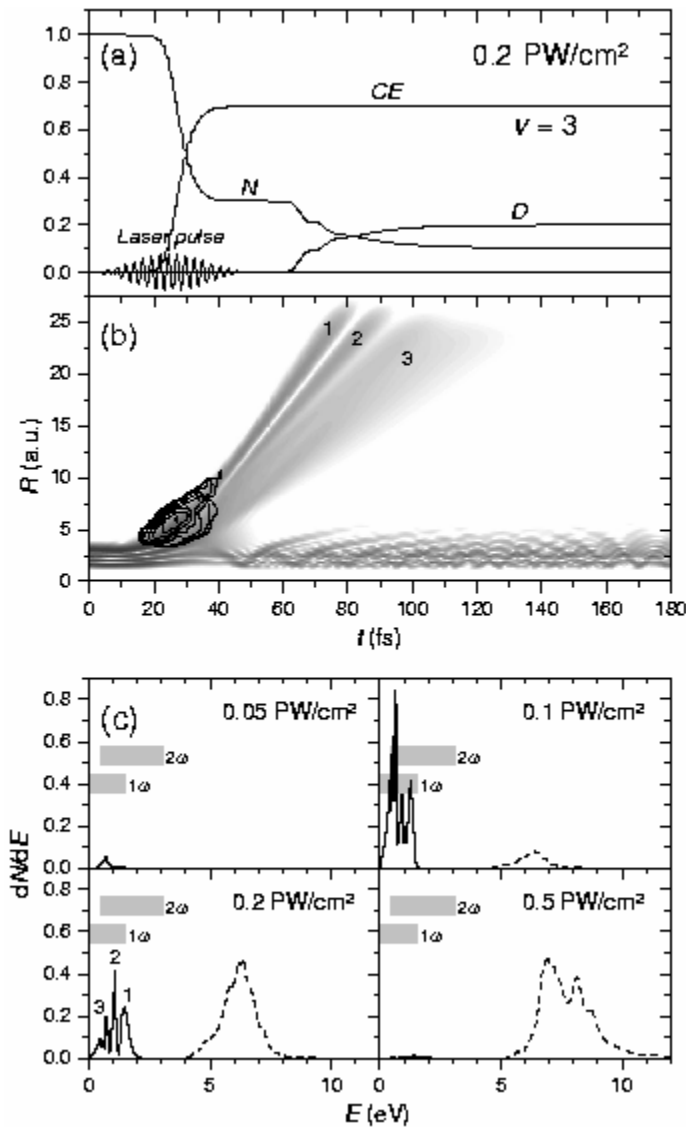
**Figure 8.3.1.** Probability densities (logarithmic scale) at times -320 a.u.(a), -110 a.u.(b), 20 a.u.(c), and 180 a.u.(d), relative to the time ( $t=0$ ) at which the point of closest approach is reached. The H<sup>+</sup> ion approaches the Cu(111) surface at an angle of  $60^\circ$  with respect to the surface plane and with an energy of 50 eV. Positions (X,D) in a.u. are given in parenthesis, with X being relative to the point of closest approach in the surface plane. D is the ion-surface distance.

#### 8.4. Computation of Momentum Distributions Within Wave-Packet Propagation Calculations

*We designed and programmed a new method to extract momentum distributions from time-dependent wave packet calculations.* In contrast to the established Fourier transformation of the spatial wave packet at a fixed time, this method examines the time dependence of the wave packet at a fixed position. Due to the analogy of this method to the experimental sorting (binning) of events into small momentum intervals, we refer to it as “virtual detector” method. In first applications to the ionization of model atoms and the dissociation of  $\text{H}_2^+$ , we found a significant reduction of computing time and derived fragment momentum distributions by using a comparatively small spatial numerical grid for the time-dependent wave function [Pub. #105].

#### 8.5. Fragmentation of $\text{H}_2^+$ in Strong Laser Pulses

*We investigated the fragmentation of the  $\text{H}_2^+$  molecular ion in 25 fs, 800 nm laser pulses in the intensity range 0.05 to 0.5 PW/cm<sup>2</sup> by means of wave packet propagation calculations.* We used a collinear reduced-dimensionality model that represents both the nuclear and electronic motion by one degree of freedom, including non-Born-Oppenheimer couplings. In order to reproduce accurately the properties of the “real” 3D molecule, we introduced a modified “soft-core” Coulomb potential with a softening function that depends on the internuclear distance. Using virtual detectors (see above) to derive and analyse the flux of outgoing nuclear and electronic probability density, we obtained fragmentation probabilities and kinetic energy spectra (Fig. 8.5.1). Our results show that the relative probabilities for dissociation and Coulomb explosion depend critically on the initial vibrational state of the molecular ion [Pub. #104].

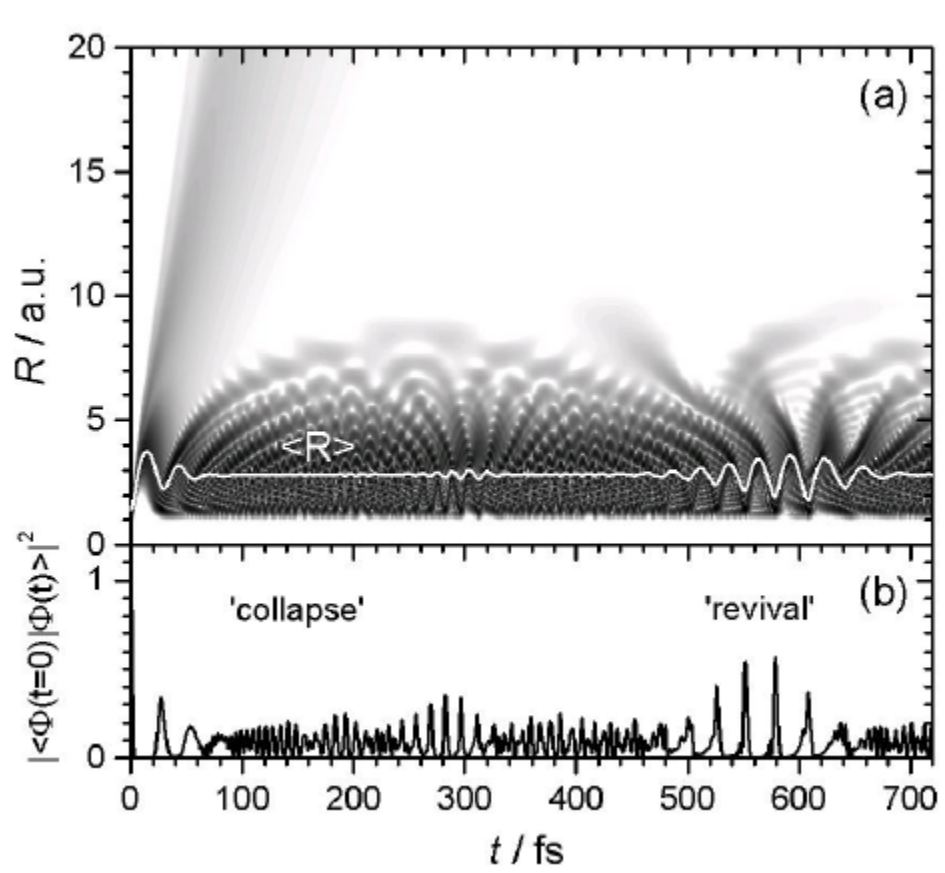


**Figure 8.5.1.** Fragmentation of  $\text{H}_2^+(v=3)$  in a 25 fs laser pulse. (a): Time-dependent norm (N) and probabilities for Coulomb explosion (CE) and dissociation (D) for a peak intensity of 0.2  $\text{PW}/\text{cm}^2$ . (b): Corresponding probability density  $P(R,t)$  (logarithmic gray scale) and ionization rates (contour lines). (c): Kinetic energy spectra for dissociation (solid lines) and CE (dashed lines) for intensities in the range from 0.05 to 0.5  $\text{PW}/\text{cm}^2$ .

## 8.6. Mapping of Coherent and Decohering Nuclear Wave Packet Dynamics in $\text{D}_2^+$ with Ultrashort Laser Pulses

*Fast ionization of  $\text{D}_2$  leads to the coherent population of many vibrational states of  $\text{D}_2^+$ .* Usually, only the squared absolute values of the vibrational state amplitudes, known as Franck-Condon factors, are observed since insufficient experimental time resolution averages out all coherence effects. We proposed a Coulomb explosion imaging method to visualize the coherent motion of bound nuclear wave packets using ultrashort (5 fs), intense pump-probe laser pulses.

With this type of experiment decoherence times in the fs to ps range may become directly observable and provide essential information for coherent control (Fig. 8.6.1) [Pub. #106].



**Figure 8.6.1.** Coherent motion of the  $\text{D}_2^+$  nuclear wave packet following ionization of  $\text{D}_2$  ( $v = 0$ ) in a 5 fs, 1  $\text{PW}/\text{cm}^2$  laser pulse. (a): Probability density  $|\Phi(R,t)|^2$  (logarithmic gray scale) and expectation value  $\langle R \rangle$ . (b): Autocorrelation function.

### III. FACILITIES REPORT

#### 1. Lab Operations Progress Report -- *Kevin Carnes, Associate Research Professor*

##### 1.1. Tandem/LINAC, General Staff -- *Kevin Carnes*

Tom Gray, who has been Associate Director for Laboratory Operations for the past thirteen years, retired as of June 2003. In February 2003, I took over his Associate Laboratory Director position so that we would have a few months to overlap. Tom has done an excellent job and leaves big shoes to fill. I find that I am taking over direction of operations at a time of tremendous change in the laboratory.

The usage of laboratory accelerators over the last contract period has been heavily influenced by the construction of the new Kansas Light Source, the high power femtosecond laser laboratory reported on separately by Zenghu Chang. All experimental groups in the laboratory have begun doing experiments with the laser beam. As a result, requests for tandem and LINAC beam times has waned, at least for the present. This is reflected in the operation hours for our High Voltage Engineering Corporation (HVEC) model EN tandem Van de Graaff accelerator.

For the 2001 contract year, the tandem operated for approximately 2500 hours. In 2002, that dropped to 1750, and so far this year (Feb.-Jun.), it has had 267 hours of operating time. This year's numbers have been affected by a shutdown over the last couple of months as we've tried to fix a problem with the tandem fast control system. The LINAC last ran beam in December of 2001. Due to lack of demand, we shut down the liquid helium refrigeration plant in April of 2002. The additional cost of buying liquid helium for the EBIS has been offset by reduced liquid nitrogen consumption and less demand on technical staff, freeing them to focus on implementing the numerous laboratory changes that have come about as a result of the new laser program. The tandem remains a vital part of the laboratory, and the LINAC could be restarted if beam time is desired, but the change of emphasis in the laboratory has meant a large change in responsibilities for the technical staff.

Two developments in particular have altered the way our staff interacts with the experimenters in the lab. In the past, experiments revolved around two large machines: the tandem/LINAC, and CRYEBIS. Staff spent most of their time maintaining the machines, and researchers largely worked on their own beamlines and experimental apparatus. Even before the addition of the laser lab, we had begun to develop more stand-alone experiments that had their own small ion sources and didn't rely on the accelerators. This has meant that staff has become more involved in building apparatus associated with individual experiments rather than with a general purpose accelerator. Their expertise has been invaluable in supplementing our limited pool of research associates and graduate students. With the addition of the laser lab, the amount of new construction, both for the laser lab itself and for associated experiments, has increased greatly. In addition, experimenters have wanted to have the laser beam delivered to experiments throughout the laboratory in much the same way as an ion beam is delivered. Staff has therefore spent time developing and constructing a laser beam transport system, learning about the necessary optics and mirror control assemblies along the way. As usual, our technical staff (Bob Krause, Al Rankin, and Mike Wells) has proven its flexibility and competency in accomplishing a great deal in a relatively short time.



The HVEC EN tandem is still being used regularly. Besides atomic collisions experiments, we have begun irradiating samples of silicon strip detectors for the KSU High Energy Physics group. The group is interested in the characteristics of these semiconductors after being irradiated with different fluences of 10 MeV protons. These beams simulate neutron radiation damage received by these strips after installation as part of the upgrade to D0 at Fermilab. The HEP group has been quite pleased with the performance of our laboratory. In the process of testing, they have confirmed an early observation of a discrepancy in a scaling factor used to convert intermediate energy proton fluence into equivalent neutron dose.

In the summer of 2002, we were able to install a new Danfysik magnet power supply for our 90 degree analyzing magnet. The old HVEC supply had failed some years before and we were working with an old Alpha supply purchased from another laboratory. We have retained the Alpha as a backup. As of this writing (June, 2003), we are awaiting delivery on a replacement for our inflection magnet power supply. This magnet is used to bend beams from either of our two ion sources into the tandem. This magnet, also, used an old HVEC supply that was no longer repairable. The replacement supply will be a new Alpha supply. This leaves only one old power supply in the laboratory, namely the HVEC switching magnet power supply. It has been running without problems and hopefully can continue in operation for the next three year grant period with parts from the old, identical analyzing magnet supply which is now available for troubleshooting/repair if necessary.

As mentioned earlier, we have spent the last two months troubleshooting a problem with the tandem's fast feedback slit control system. The problem results in terminal ripple of up to 6kV, whereas the usual ripple is approximately 800 V. So far, no clear cause has surfaced. We are in contact with accelerator engineers from around the world through the SNEAP network to solicit their help in diagnosing the problem. Since the electronics in the system are over 30 years old, repair may prove difficult even if we can find the cause. Fortunately, we have in house a replacement control system from High Voltage Engineering Europa that should work, although there may be some issues in adapting it to work with our new Pelletron chain charging system instead of a belt. If further attempts to repair the existing system fail, we will install the HVE Europa system.

When construction on the new femtosecond laser lab began in the summer of 2001, one of the tandem target rooms was cleared of beam lines to make way for the lab. That left only the "Square Room" with its three beam lines for tandem experiments that did not need to go through the LINAC. With our recent hiring of Kristan Corwin as a new faculty member, the Square Room is being cleared out as well to make room for her lab. Experiments that were set up in those two rooms have been moved to beam lines on the LINAC, where they can use beams from the tandem only or higher energy beams from the tandem LINAC system.

### **1.2. Low Energy Ion Collision Facility -- C.W. Fehrenbach**

The Low Energy Ion Collision Facility (LEICF) is comprised of two ion source/accelerator systems that are available for general user experiments. The Cryogenic Electron Beam Ion Source (CRYEBIS) has been in operation for over 10 years. It is designed to deliver highly charged ions to experiments at low to medium beam energies (1-160 keV/q). We also have a second ion source, an Electron Cyclotron Resonance Ion Source (ECRIS) which was installed in the lab for dedicated use in ion-ion collision studies. With those experiments being

completed, the ECRIS has been reconfigured as a general user facility for providing beams of low charge state ions ( $1 \leq q \leq 6$ ) at low energies (1-10 keV/q).

Both facilities are running stably as production sources with little down time being needed for development. Over the three year period of 2000-2002, the CRYEBIS was providing ion beams to users for a total of 547 days or about 50% of the time, on average. The ECRIS delivered beams to users during 305 days (or 28%) over that same time span. The amount of time that beam was delivered to users was set by user demand, not by facility capability. It is worth noting first, that with the conversion of the ECRIS system to a more general user facility, demand for beams from that source has been increasing recently. As well, on a run-time basis, the LEICF has become one of the major sources for ion beams for user experiments in the Macdonald Laboratory.

### 1.2.1. CRYEBIS

The CRYEBIS has been operating as a stable user facility. The source has been kept cold and functioning except for maintenance.

The electron beam system was upgraded to permit use at higher electron beam energies. A new electrical feedthrough system into the electron-gun vacuum chamber was installed which is rated to 15 kV. This system was designed by Dr. Martin Stockli who has moved to the Spallation Neutron Source at Oak Ridge. Since installation, the system has been tested to 5 kV, which is the maximum that our current power supplies can reach. Stable operation was achieved at this potential, and the electron beam was transported through the trap region without showing large beam power being lost to the cryogenics system.

In addition to upgrading the feedthroughs to the electron gun, higher test feedthroughs were installed on drift tubes in the trap region. This was necessitated by failure of the old insulators which resulted in break down at high voltage. A new feedthrough flange was obtained which fit the same form factor as the old system, and has insulators rated for continuous use at 5 kV, whereas the previously used insulators were rated for use at 3 kV.

With both new sets of electrical feedthroughs installed, we have been able to operate the CRYEBIS with an electron beam going through the trap at an energy of 9.5 keV. This allows us to extend the production of bare nuclei up to  $Z=25$ . Greater e-beam energy is needed, however, for efficient production of such ions. The existing power supplies can go to higher voltages; however, above 9.5 kV we start to see some beam transport problems, which show up as beam current lost to the trap electrodes and as increased liquid He consumption. These issues will have to be studied further before the source can be modified to operate at the higher energies.

In response to requests from users, we have been trying to make bare or hydrogen-like ions with  $Z$  greater than 18. This has required running the electron beam at the higher energies as well as experimenting with new seed gasses. Using a metal-chloride compound, we were able to make beams of H-like and bare vanadium. Thus far, these beams have not been suitable for the user's experiments because of problems with the seed-gas leak valve and because of overlaps in the charge-to-mass ratio between V and Cl ions. We are looking into improvements to the seed gas system to try to prevent the clogging of the leak valve from metal-halide vapors and to allow the use of F compounds instead of the Cl-containing substances.

One of the user experiments that has been running on the CRYEBIS has required high fluxes of proton beams for calibration purposes. As the CRYEBIS is not suitable for this, a small hot-filament source has been added to the HV platform on an auxiliary port on the

analyzing magnet. This source is configured for easy switch over between the EBIS and the hot-filament source.

Improvement has also been taking place in the control system for the CRYEBIS. A computerized system is being developed to replace some of the analog controls as they wear out. This system is being developed to address several problems. One is reliability. There are potentiometer controls (mostly on the analyzing magnet) that wear out frequently and must be replaced. The new system uses optical shaft encoders and DAC's to duplicate the functionality, but with better reliability. Another problem the computer helps with is fault detection. The computer monitors source operations continuously and will send warnings to the operators if something goes wrong, whereas in the past, we had to wait for the user or technical staff to notice that the source had shut down or was not operating in its normal mode. The last important feature of the computer control system is to facilitate efficient operation of the source with fewer staff people. In particular, the system makes use of wireless communication technology to inform technical staff remotely of source status and technical problems.

### 1.2.2. ECRIS

The ECR Ion Source facility has undergone a change from being a dedicated part of a single ion-ion collisions experiment to being a general facility. The number of independent beam lines which can be used on this facility is limited to three. We have used all three of these ports for user experiments in the past year. This reconfiguration to a multi-user system has prompted some refinements in the control system for the ion source. The problems reported previously with the independent supplies on the ECR axial field coils have been fixed and a control system was developed that lets the user adjust independently the central field and the front to back mirror ratio. The seed gas system was redesigned for easier change over of gas species (this system also had to be designed with special purge capabilities so that it could be used with silane gas, which ignites on contact with air.) The rf amplifier for the ECR was replaced along with its waveguide isolator in order to increase drive power to the source. In addition the waveguide system was modified to incorporate a dual directional coupler on the source side of the isolator so that the rf power actually being absorbed in the source can be monitored.

Two other things are worth noting in regard to the operation of the ECRIS system. One is that while the facility is configured to support only two complete user beam lines, the lab staff was able to rig a third beam line off of a zero degree port on one of the inflection magnets. This permitted a visiting researcher from an outside institution to do a proof-of-principle experiment on the ECRIS looking into X-ray yields from ions interacting with solids. This experiment is attempting to provide data relevant to astronomical observations. The experiment was set up with relatively little overhead either to the lab or the user. The other significant point is that one of the ECRIS experiments is using the femtosecond laser to look at photo dissociation of molecular ions. This exploits one of the unique features of the J. R. Macdonald Laboratory, the ability to combine state of the art pulsed lasers with dense ion beams.

### 1.3. Data Acquisition System, LINAC Computer Control, and JRML Electronics Shop -- *Kevin Carnes*

#### 1.3.1. Data Acquisition

Our VME front-end data acquisition system has been in stable operation mode during the last three years. There have been no significant changes made to the system. We continue to have five independent data acquisition stations (VME front-end plus computer workstation) and five clustered offline analysis machines. All but one of the workstations are Compaq (formerly DEC) VAXStation 4000/96 color workstations with removable SCSI disks for data storage and 8mm tape for backup. As the VAXStations have aged, we have had to replace several of the large color monitors. Since these units are no longer in production, we have to purchase replacements on the used market.

Even though our data acquisition (DAQ) system is meeting our current needs, I have begun researching possible replacements. The real-time operating system used in the VME front-end computers is no longer available, even on the used market. Therefore, we are not able to expand the number of DAQ systems. As we increase the number of standalone experiments capable of simultaneous data acquisition, this becomes more of a limiting factor. The VAXStations themselves are also a limitation, as they are harder to replace and most incoming students have no experience with VMS, the VAX operating system. Currently I am investigating a Linux-based system used at several laboratories throughout the world, as well as a Labview system. Both run on commodity PC's, which should make upgrades and expansions much easier. We have recently received DOE supplemental equipment funds to build a prototype DAQ system.

I have provided leadership over the last several years to the KSU Physics Department computer committee. Our permanent departmental computer staff has done a good job of providing us with a stable, networked system of PC's. Currently, most machines have been converted to Windows XP, with large departmental servers running Windows 2000 Server to handle file, print, and application serving. Our users are doing more and more of their analysis with the program Origin, and the use of SIMION for detector and beam line design has increased as well. Vince Needham continues to supplement the departmental support we receive for our large number of PC's. Wireless access points will be installed in the laboratory this year to accommodate the increasing number of laptops. A departmental firewall was recently installed, which has greatly enhanced our security.

Vince Needham has implemented a computer security system, following discussions between Pat Richard, the Lab Director and Eric Rohlfing, DOE AMOP Program Officer. The Department of Energy maintains a service known as CIAC, or the "Computer Incident Advisory Capability" (<http://www.ciac.org/ciac/>). The mission of CIAC is to apply cyber security expertise to prevent, detect, react to, and recover from cyber incidents for DOE/NNSA and other national stakeholders. In pursuit of this mission, CIAC provides access to computer security software tools for DOE collaborators. Through CIAC, the James R. Macdonald Laboratory was able to obtain the "Internet Security Scanner" software package from Internet Security Systems. We have used this package to aggressively probe the KSU Physics Department's computer network for potential security vulnerabilities. Once identified, we can take the appropriate steps to correct these vulnerabilities and provide a safer, more productive computing environment for our researchers.

### 1.3.2. LINAC Computer Control

The new LINAC computer control system described in the last progress report was fully operational by March of 2001 and ran reliably for the remainder of that year. It proved to be much easier to use than the older system. We also installed an AmpTek MCA and associated software on the control PC, so that energy measurements using Rutherford scattering from a gold foil into a surface barrier detector could be made easily using the same PC. The control system is ready to use when the LINAC is restarted.

### 1.3.3. JRML Electronics Shop

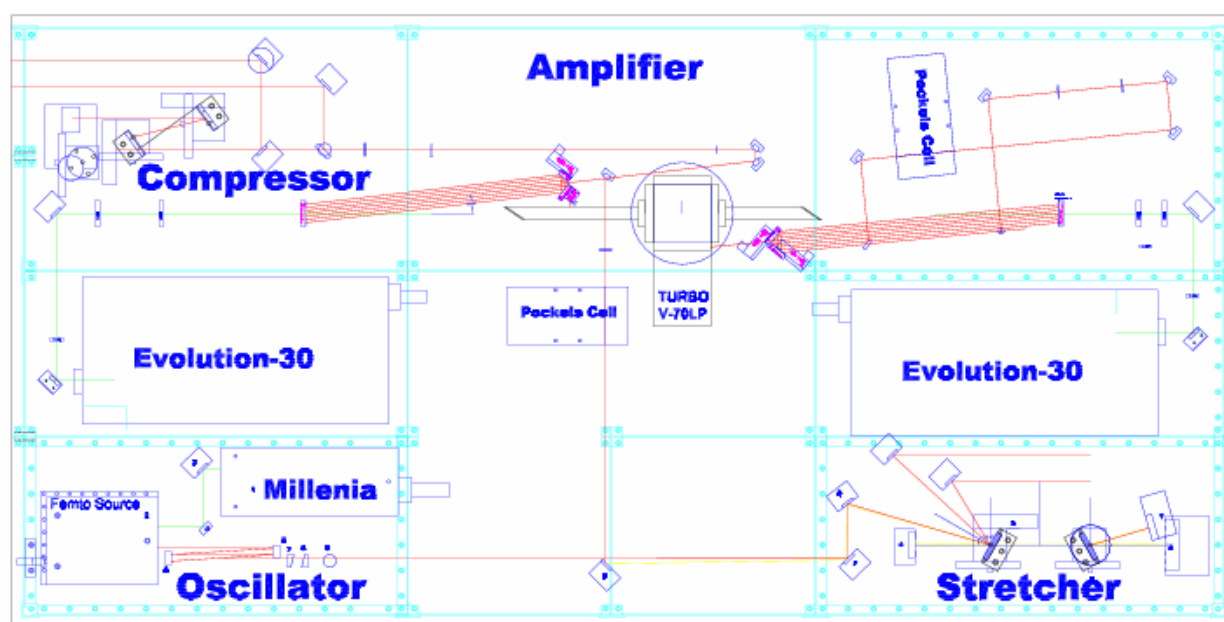
Scott Chainey has become an integral part of laboratory operations in the last three years as our electronics technologist. In addition to learning to repair many of our experimental electronics modules, he has laid out and constructed several circuit boards. A large fraction of his time recently has been spent on implementing a new laser safety interlock system. Since the laser beam has been transported to different target areas in the lab, those areas must have limited access to personnel while the beam is on, analogous to the situation we have experienced for years with radiation safety. Scott has implemented status panels, door interlocks, and bypasses that have greatly increased the safety of users. This is an ongoing project as additional laser experimental areas are being added. This was done in collaboration with Professor Brett DePaola, who is the JRM safety officer.

## 2. Laser Lab Operations Progress Report -- Zenghu Chang, Associate Professor

### 2.1. Development of the Kansas Light Source

During the last two years, the research direction of the Macdonald Laboratory has been significantly reshaped by the installation of a high intensity laser facility, the *Kansas Light Source*. Currently, the *Kansas Light Source* produces 4 mJ pulses with 25 fs duration at 1 kilohertz repetition rate. It also produces 8 fs pulses with 0.5 mJ energy, which was done by using a hollow fiber/chirped mirror pulse compressor.

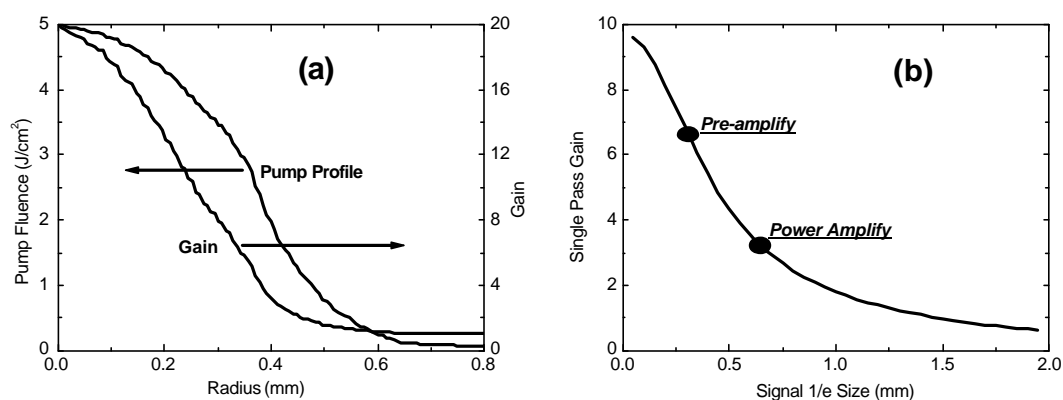
The layout of the portion of Kansas Light Source that generates the pulsed laser beam is shown in Fig. 2.1.1. It is a compact kilohertz system that is based on chirped pulse amplification. The difference between this laser and other similar systems is that the Kansas Light Source is the highest power kilohertz laser that uses only one stage of a multipass amplifier.



**Figure 2.1.1.** The layout of the Kansas Light Source.

Kilohertz lasers are becoming popular tools for high field atomic physics studies because of the short data taking time compared with low repetition rate lasers. Increasing the output power of kHz lasers will further expand their applications. High power kHz Ti: Sapphire laser systems have been developing rapidly in recent years. Typically 1~2 mJ pulse energy can be obtained from the system with a one-stage multi-pass amplifier. But in these systems the pump fluence is usually very high (close to the damage threshold). For even higher pulse energies, a multi-stage amplifier is required. In such systems, the preamplifier provides a high gain to bring the pulse energy from nJ to ~1 mJ with a high gain and relatively low efficiency, and the subsequent power amplifiers boost the pulse to the tens of mJ level with low gain and high efficiency (usually over 20%). Our laser system combines the advantages of pre- and power amplifiers, so that both high gain and high efficiency could be achieved with a one stage amplifier with a relatively low and safe pump level. This provides a feasible way to build reliable and compact laser systems with high efficiency and large pulse energy.

It is well known that the gain varies significantly in the radial direction of a gain medium. We take advantage of this variation in our system. Figure 2.1.2(a) illustrates the measured pump fluence at the laser crystal in our amplifier. Based on this spatial profile, the small signal gain is calculated and also illustrated in Fig. 2.1.2(a). As shown in the figure, the gain drops quickly along the radial dimension because of the very nonlinear relationship between the pump fluence and the gain. According to this distribution, we would expect a high gain for a small signal spot because the signal is localized in the center part of the pump. On the other hand, the large signal spot has a low gain as it spreads into the low gain area. Figure 2.1.2(b) shows the calculated small signal single pass gain versus signal beam dimension.



**Figure 2.1.2.** (a) Measured pump laser profile and calculated small signal gain; (b) calculated small signal single pass gain versus the signal beam size.

In our system, we employed a unique design so that the signal beam size can be changed in the laser amplifier. In the 14-pass amplifier, we first use a small beam size ( $\sim 0.3$  mm in the crystal) in the first 7 passes to amplify the signal to the tens of microjoule level. This process is similar to a pre-amplifier. Using the same size for further amplification would damage the laser crystal. Therefore, the amplified signal is released after the first 7 passes and changed to a bigger focus size,  $\sim 0.6$  mm, in the crystal. This beam with the large waist is amplified in the same pumped region for another seven passes like in a power amplifier. The final output is 6.5 mJ with a pump-to-signal efficiency of 26%. After a grating compressor, we obtain 25 fs pulses with 4 mJ of pulse energy. Since one amplifier is used, the laser system is compact and easy to operate.

## 2.2. Applications

At present, the laser is the busiest user facility in the Lab, running seven days a week, 10-15 hours a day. Most of the experimental faculty in the Macdonald Lab make frequent use of the laser. The following projects are being conducted using the Kansas Light Source:

- Dissociation of molecular ions, I. Ben-Itzhak
- High order harmonic generation from molecules, Z. Chang
- Ultrafast x-ray streak camera, Z. Chang, J. Wang (Argonne Lab)

## Facilities Report

- Dissociation of molecules, C. L. Cocke
- Ionization of alkali atoms , B. DePaola
- Ionization of molecules, P. Richard and Z. Chang
- Micromachining, S. Lei (Industrial Engineering Dept.) and Z. Chang

The laser beam has been split into 3 or 4 to serve 3 to 4 experiments at the same time. It has been operated by Dr. B. Shan who was my posdoc but is now an Assistant Research Professor, Dr. C. Wang and my students.



#### **IV. FINANCIAL REPORT**

It is anticipated that there will be no unexpended funds for the current funding period.

**V. JAMES R. MACDONALD LABORATORY  
PERSONNEL  
2000-2003**

**Senior Personnel:**

Ben-Itzhak, Itzhak	Professor of Physics
Bhalla, Chander	Professor Emeritus of Physics, 2001
Carnes, Kevin	Associate Research Professor Associate Director of Laboratory Operations, JRML, beginning February 2003
Chang, Zenghu	Associate Professor of Physics
Cocke, C. Lew	University Distinguished Professor of Physics Associate Director of Research, JRML
DePaola, Brett	Professor of Physics Safety Officer, JRML
Esry, Brett	Associate Professor of Physics
Fehrenbach, Charles	Assistant Research Professor
Gray, Tom	Professor of Physics; retired from KSU, July 2003 Associate Director of Laboratory Operations, JRML, Prior to February 2003
Hagmann, Siegbert	Professor of Physics, retired from KSU, July 2003
Lin, C. D.	Distinguished Professor of Physics Associate Director of Theory Research
Richard, Pat	Cortelyou-Rust Distinguished Professor of Physics Director, JRML
Shan, Bing	Assistant Research Professor
Thumm, Uwe	Professor of Physics
Tong, Xiao Min	Assistant Research Professor
Zouros, Theo	Adjunct Professor, KSU – Professor, University of Crete, Greece

**Technical/Laboratory Staff:**

Chainey, Scott	Electronics Technician
Eaton, Hilary	Assistant Scientist and JRML Safety Officer Resigned position 3/02
Gibson, Paul	Assistant Scientist; resigned position 7/01 Present Address: Oak Ridge National Lab, Spallation Neutron Source
Krause, Robert	Accelerator Engineer
Needham, Harold V.	Assistant Scientist
Peterson, Jane <sup>*</sup>	Senior Administrative Assistant
Rankin, Allan	Assistant Scientist
Regehr, Carol	Assistant Scientist
Richard, Dea	Administrative Assistant to Director
Wang, Chun	Assistant Scientist, resigned position 5/03
Wells, Mike <sup>1</sup>	Cryogenics Engineer

<sup>\*</sup>Part-time

<sup>1</sup>Supported by Kansas State University

**Research Associates/Long-Term Visiting Scientists:**

Ali, Imad	Present Address: Washington University Medical Center, St. Louis, Missouri
Bahrim, Bogdana	Present Address: Lamar University, Beaumont, Texas
Benis, Emmanouil	
Bredy, Richard	
Chakraborty, Himadri	
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Guo, Wei	Present Address: Charlotte, North Carolina
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Shi, Tingyun	
Sidky, Emil	Present Address: University of Chicago, Chicago, Illinois
Tawara, Hiro	Present Address: University of Heidelberg, Germany
Tseng, Hsiang-Chi	Present Address: Chung Yen University, ChungLi, Taiwan
Xia, Jiangfan	

**Graduate Research Assistants:**

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Camp, Howard

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Ghimire, Shambhu

Jahan, Quaji – transferred to engineering 8/01

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 Niederhausen, Thomas  
 Osipov, Timur  
 Prasai, Krishna – left Kansas State University  
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 Shakya, Mahendra  
 Smith, Mark  
 Unal, Ridvan, Ph.D. 2001  
     Present Address: Afyon Kocatepe University, Afyon, Turkey  
 Verzani, Chris, Ph.D. 2003  
     Present Address: NIST, Gaithersburg, MD  
 Woody, Nathan  
 Zamkov, Mikhail, Ph.D. 2003  
     Present Address: Kansas State University, Manhattan, KS  
 Zhao, Zengxiu

## **VISITORS/USERS:**

### **2000**

Theo Zouros, University of Crete, Greece  
 Chun-Yen Chen, Argonne National Laboratory  
 Jon Schauer, Concordia College  
 Steve Lundeen, Colorado State University  
 Tsuguhisa Sekioka, Himeji Institute, Japan  
 Mititake Terasawa, Himeji Institute, Japan  
 Claude Blieth, PANTECHNIK, France  
 S. Kitazawa, JAERI, Japan  
 Kazuhiko Oluno, Tokyo Metropolitan, Japan  
 Wania Wolff, UFRJ, Brazil  
 Hans Wolf, UFRJ, Brazil  
 Yasuyuki Kanai, RIKEN, Japan  
 Waldemar Mroz, Institute of Optoelectronics, Poland  
 A. Prokopiuk, Institute of Optoelectronics, Poland  
 Larry Lamm, Notre Dame, Indiana  
 Mike Stier, National Electrostatics  
 Chris Greene, JILA-CU  
 Leos Laska, Czech Academy of Sciences  
 Josef Krasa, Czech Academy of Sciences  
 Zach Miller, St. Olaf College  
 Ryan Holloman, University of Northern Colorado  
 Maria Herd, Bryn Mawr College  
 Kendal Clark, Central Methodist College  
 Kang Qian, Georgia Institute of Technology  
 Jonathan Columbia, Burknell University

Jesse Kinder, DePauw University  
Cheng Guan Koay, Berea College  
Carl Willis, Guilford College  
Brian Ispino, University of Central Florida  
Tasuo Kaneyasu, Tokyo Metropolitan, Japan  
Tomokazu Kitamura, Tokyo Metropolitan, Japan  
Akinori Igarishi, Miyazaki University  
Asad Hasan, Fort Hays State University  
Larry Wilson, Georgia Institute of Technology  
Ivan Chompalov, Georgia Institute of Technology  
Hajime Tanuma, Tokyo Metropolitan, Japan  
Christian Simm, Dresden Technical University, Germany  
Mike Schmidt, Dresden Technical University, Germany  
Harald Bräuning, Justus-Liebig University, Germany  
Tsuguhisu Sekioka, Himeji Institute, Japan  
Mititaka Terasawa, Himeji Institute, Japan  
John Tanis, Western Michigan University  
Allen Landers, Western Michigan University  
Ali Al-Naser, Western Michigan University  
Eric Wells, University of Virginia

## **2001**

Hossein Sadeghpour, ITAMP  
Manolis Benis, University of Crete, Greece  
Theo Zouros, University of Crete, Greece  
Steve Lundeen, Colorado State University  
Alina Gearba, Colorado State University  
Nobuyuki Toshima, Tsukuba, Japan  
Jim Burke, NIST  
George Makrakis, Technological Education Institution of Crete  
Toru Morishita, University of Electrocommunications, Tokyo  
Alejandro Gonzalez, Instituto Balseiro, S.C. de Bariloche, Rio Negro, Argentina  
Hiro Tawara, Toki, Japan  
K. R. Karim, University of Illinois  
Jason Morgan, San Luis Obispo, California  
Justin Zohner, Penokee, Kansas  
Jack Maseberg, Macksville, Kansas  
Maggie Stauffer, Eldorado, Kansas  
Matthew Horne, Camarillo, California  
Daniel Kost, Dresden Technical University, Germany  
Mike Schmidt, Dresden Technical University, Germany  
Yasuyuki Kanai, RIKEN, Japan  
Lokesh Tribedi, Tata Institute of Fundamental Research, India  
Ali Al-Naser, Western Michigan University  
Eric Wells, University of Virginia  
Allen Landers, Western Michigan University  
Mike Mendicino, Saint-Gobain Crystals & Detectors

Chris Jones, Saint-Gobain Crystals & Detectors  
Gerard Mourou, University of Michigan  
Eric Abraham, University of Oklahoma  
William (Greg) Sturru, Youngstown State University  
Jinyuan Liu, Argonne National Laboratory  
Andrew MacPhee, Lawrence-Berkeley Laboratories  
John Tanis, Western Michigan University  
Allen Landers, Western Michigan University  
Ali Al-Naser, Western Michigan University  
Sabbir Hossain, Western Michigan University  
Osama Abukaija, Western Michigan University  
Steve Ferguson, Western Michigan University

**2002**

Matthew Horne, California Polytechnic Institute  
Alix Preston, Colorado School of Mines  
Michael Litos, Michigan State University  
Jinyuan Liu, Argonne National Laboratory  
Jack Maseberg, Fort State University  
Sabbir Hossain, Western Michigan University  
Osama Abuhaija, Western Michigan University  
Andrew MacPhee, University of California, Berkeley  
Ottmar Jagutzki, University of Frankfurt, Germany  
William Sturru, Youngstown State University  
Robert Vacha, Charles University, Czechoslovakia  
Tom Gorczyca, Western Michigan University  
Mark Gealy, Concordia College  
Jin Yuan Liu, Argonne National Laboratory  
Steve Lundeen, Colorado State University  
Alina Gearba, Colorado State University  
Robert Kamara, Colorado State University  
John Tanis, Western Michigan University  
Allen Landers, Western Michigan University  
Ali Al-Naser, Western Michigan University  
Lutz Huwel, Wesleyan University  
Chunlei Guo, Los Alamos National Laboratory  
Paul Corkum, National Research Council, Canada  
Alex V. Hamza, Lawrence Livermore National Laboratory  
Klaus Bartschat, Drake University  
Jan Chaloupka, Brookhaven National Laboratory  
Eric Wells, University of Virginia  
Herman Batelaan, University of Nebraska  
Dan Otero, St. Francis Hospital, Topeka, Kansas  
Takaaki Awata, Naruto, Japan  
Wilhelm Becker, Max-Born-Institute, Berlin, Germany  
Alan Chin, UltraPhotonics  
Jason Jones, JILA

Henry Kapteyn, JILA  
Neal Lane, Rice University  
Tom Loftus, JILA  
Steve Lundeen, Colorado State University  
Margaret Murnane, JILA

**COLLOQUIA**  
**2000 – 2003**

**[Sponsored by KSU Department of Physics]**

- 1) Michael Cherney, Creighton University  
“First Collisions at STAR, the Solenoidal Tracker at RHIC”
- 2) Peter Gorham, JPL  
“The Moon as Detector for Ultra-High Energy Neutrinos: Fact, Fiction, or Lunacy?”
- 3) John Harton, Colorado State  
“Beauty Particle Decays”
- 4) Alexander Szalay, Johns Hopkins  
“The Sloan Digital Sky Survey”
- 5) John Hardy, Texas A & M University  
“Superallowed Beta Decay: a Nuclear Probe of the Electroweak Standard Model”
- 6) Pierre Sikivie, Florida  
“The Search for Axion Dark Matter”
- 7) Peter Nugent, LBL  
“Measurements of the Cosmological Parameters using Supernovae”
- 8) Martin Gaskell, U of Nebraska  
“The Environs of Supermassive Black Holes”
- 9) Phillip Gould, U of Connecticut  
“Ultracold Collisions: The Influences of Laser Light”
- 10) Beth Ann Thacker, Texas Tech  
“A Study of the Nature of Students’ Models of Microscopic Processes in Modern Physics and Quantum Mechanics”
- 11) Ira Wasserman, Cornell  
“The Expansion of the Universe”
- 12) Arnold Honig, Syracuse  
“Large, Portable, WORKING High Spin Polarized Solid HD Targets”
- 13) Amy Liu, Georgetown  
“Topics in Condensed Matter”
- 14) Andrew Rappe, U of Pennsylvania  
“Topics in Condensed Matter”
- 15) John Delos, William & Mary  
“Topics in Atomic Physics Theory”
- 16) Sergei Nagaitsev, Fermilab  
“Physics of Electron Cooling”

- 17) M. Dobrowolska-Furdyna, Notre Dame  
“Side Gap Semiconductor Quantum Dots-Fabrication, Carrier Localization and Optics”
- 18) Jeffrey Peterson, CMU  
“The Flat Universe”
- 19) Ken Shih, Texas  
“Quantum Engineering of Metallic Thin Films”
- 20) Michael Turner, U of Chicago  
“The Dark Side of the Universe”
- 21) Gary Wysin, KSU  
“Spin Waves and Nonlinearity in Magnets”
- 22) Robert Jones, U of Virginia  
“Using Short Electromagnetic Pulses to Manipulate Electronic Wavefunctions”
- 23) Stephen Reucroft, Northeastern  
“What is Mass?”
- 24) Bharat Ratra, KSU  
“Is the Universe Flat or Open?”
- 25) Robert Beichner, N. Carolina State  
“Scale-up: Student Centered Activities for Large Enrollment University Physics”
- 26) Stephen McGuire, SUBR  
“LIGO, Material Science, and Education”
- 27) Uwe Thumm, KSU  
“How to Deal with Nanostructures in Femtoseconds”
- 28) Suzanne Franks, KSU  
“Women and Minorities in Engineering and Science”
- 29) Timothy Gay, Nebraska  
“Physics of Football”
- 30) Megan Donahue, STSCI  
“Distant Cluster Hunting: The Past and the Promise”
- 31) Robert Weinstock, Oberlin College  
“Inverse-Square Orbits, Uniform Circular Motion, and Newton’s Principia EXPOSED”
- 32) Sanjay Rebello, KSU  
“Adapting Research-Based Pedagogy: Lessons Learned”
- 33) Mel Sabella, University of Washington  
“The Role of Multiple Formats and Contexts in Systematic Investigations of Student Learning”
- 34) James Peebles, Princeton University  
“How I Learned to Love the Cold Dark Matter Model for Cosmic Structure Formation and Still Avoid Settling Bets on the Cosmological Tests”
- 35) Ken Wharton, Lawrence Livermore National Laboratory  
“Hot Electrons from Intense Laser-Solid Interactions”
- 36) Zenghu Chang, KSU  
“High Intensity Laser for Ultrafast X-Ray Science”
- 37) George Musser, Scientific American  
“Bridging Science and Journalism: The Inner Workings of Scientific American”



- 38) Kip Thorne, Caltech  
“LIGO and LISA: Opening the Gravitational Wave Window onto the Universe”
- 39) Chunlei Guo, Los Alamos National Laboratory  
“Cartoon Solutions of Multielectron Problems in Strong Laser Fields”
- 40) Michael O’Shea, KSU  
“Nanostructured Materials”
- 41) Yun Wang, University of Oklahoma  
“Probing Fundamental Physics with Cosmological Data”
- 42) Paul Corkum, National Research Council, Canada  
“Spinning Molecules Until They Break”
- 43) Klaus-Peter Bohnen, Karlsruhe, Germany  
“MgB<sub>2</sub> an Unconventional Superconductor?”
- 44) Uwe Thumm, KSU  
“Understanding Electronic Interactions of Atoms and Ions with Complex Targets: A Perspective for Nano Science?”
- 45) Bruce Margon, Space Telescope Science Institute  
“The Universe in 10 Terabytes: Results from the Sloan Digital Sky Survey”
- 46) Michael Barnett, LBL  
“Explaining Great Puzzles of Particle Physics”
- 47) Gerard Mourou, University of Michigan  
“High Intensity Lasers”
- 48) Jingyu Lin, KSU  
“III-Nitride Research at KSU – Physics: Growth, Fundamental Properties, and Applications”
- 49) Alex V. Hamza, Lawrence Livermore National Lab  
“Nanostructures Formed via Intense, Ultrafast Electronic Excitation Using Highly Charged Ions”
- 50) George Simonis, Army Research Lab  
“EO and Photonics”
- 51) Dan Green, Fermilab  
“CMS Experiment”
- 52) Trevor Weekes, Smithsonian  
“Astronomy with TeV Gamma Rays”
- 53) Klaus Bartschat, Drake University  
“Electron Collisions with Atoms and Ions: Recent Developments in Theory, Experiment, and Computer Simulations”
- 54) Roger Falcone, University of California Berkeley  
“Time-Resolved X-Ray Scattering from Excited Materials”
- 55) Dick Bond, Canadian Institute for Theoretical Astrophysics  
“The Parameters of Cosmic Structure Formation from Recent CMB Data,”
- 56) J. Chaloupka, Brookhaven National Lab  
“Double Ionization in an Intense Field”
- 57) E. Wells, University of Virginia  
“Laser-Molecule Interactions”

- 58) B. Esry, KSU  
“The Continuum in Atomic Physics: From Bose-Einstein to the Hubble Expansion”
- 59) R. Demina, KSU  
“On Beauty, Silicon and Light Without Mass”
- 60) Stuart Solin, NEC Res Institute  
“Extraordinary Magnetoresistance in Narrow-Gap Semi-Conductors: Fundamental Physics and Practical Applications”
- 61) K. Cummings, RPI  
“The Role of Conceptual Understanding in Problem Solving”
- 62) E. Von Toerne, University of Oklahoma  
“Recent CLEO Results on Rare Hadronic B Meson Decays”
- 63) Ron Sidwell, KSU  
“Finding Treasure at the Tevatron: Search for Supersymmetric Glue”
- 64) L. Babukhadia, Fermilab  
“Preons or PDFs? And what’s ahead?”
- 65) Owen Long, UCSB-SLAC  
“Recent Progress in CP Violation”
- 66) H. Batelaan, University of Nebraska  
“The Kapitza-Dirac Effect”
- 67) Harald Fox, Fermilab  
“Higgs Physics at the DO Experiment”
- 68) Anne M. Chaka, NIST  
“Quantum Mechanics and the Automobile”
- 69) Steve Bernasek, Princeton  
“Probing Internal State Effects in Heterogeneous Reactions”
- 70) F. Goldberg, San Diego State  
“How Computer Simulators Can Help Provide a Bridge Between Students’ Initial Models and Target Instructional Models of Physics Phenomena”
- 71) Maria Tamargo, City College of CUNY  
“Wide Bandgap II-VI Compounds for Red-Green-Blue LEDS and other Devices”
- 72) Justin Peatross, Brigham Young University  
“Gruppengeschwindigkeit and the Homer Simpson Effect”
- 73) X. Pan, University of Chicago  
“How Does Tomographic Imaging Work?”
- 74) Bill Porter, KSU Graduate and Founder of E-Trade  
“Applying Physics for the Betterment of Humankind”
- 75) M. Murnane, U of Colorado  
“Multiphoton Photonics”
- 76) Ruth Howes, Ball State University  
“Their Day in the Sun: Women Physicists and the Manhattan Project”
- 77) Hyuk Pak, Pusan National University  
“Physics of Granular Materials Under Vibration”
- 78) Neal Lane, Rice University  
“Physics Through Different Lenses – Differing Perspectives of Scientists, Policy Makers, and the Public”

- 79) C. Holbrow, Colgate University  
“Photon Quantum Mechanics for Undergraduates”
- 80) Jun Ye, Colorado  
“Control of Coherent Light: Time Meets Frequency”
- 81) Shanalyn Kemme, Sandia National Lab  
“Resonant Subwavelength Gratings: Ideal vs. Realizable Optical Components”
- 82) Lijun Wang, NEC  
“Superluminal Light Pulse Propagation, Causality and Quantum Fluctuation”
- 83) Kristan Corwin, NIST  
“Origin and Impact of Noise on Supercontinuum Generation”
- 84) Mark Robbins, Johns Hopkins  
“Where Does Friction Come From?”
- 85) Shin Inouye, JILA & CU-Boulder  
“Ultracold Dilute Gas Fermions – Recent Experiments at JILA”
- 86) Zenghu Chang, KSU  
“Kansas Light Source, A Powerful Laser for Studying and Teaching AMO Physics”
- 87) Eric Cornell, Nobel Laureate- NIST & JILA  
“Rotating the Irrotatable: Quantized Vortices in a Supergas”  
and public lecture:  
“Stone Cold Science: Bose-Einstein Condensation and the Weird World of Physics a Millionth of a Degree from Absolute Zero”
- 88) Valerie Milner, Queens College of CUNY  
“Optical Billiards: Controlling the Dynamics of Atoms and Photons”
- 89) Igor Litvinyuk, Steacie Institute for Molecular Sciences & NRC-Canada  
“Molecules in Strong Laser Field”
- 90) Wolfgang Theobald, University of Michigan  
“High Harmonics as a Diagnostic for Femtosecond Laser Produced Plasmas”
- 91) John Womersley, Fermilab  
“Physics at the Fermilab Tevatron Collider”
- 92) Hitoshi Murayama, U.C. Berkeley  
“Big World of Small Neutrinos”
- 93) Roy Gephart, Pacific Northwest National Labs  
“Containment Legacy and Cleanup Challenge Facing the Hanford Nuclear Waste Site”

## VI. PUBLICATIONS

J. R. MACDONALD LABORATORY – KANSAS STATE UNIVERSITY

DOE Grant # DE-FG02-86ER13491

2000 – 2003

1. “Linear –Least-Squares Fitting Method for the Solution of the Time-Dependent Schrödinger Equation: Applications to Atoms in Intense Laser Fields,”  
Xiaoxin Zhou and C. D. Lin  
Phys. Rev. A **61**, 053411-1 (2000)
2. “State-Selective K-K Electron Transfer and K Ionization Cross Sections for Ar and Kr in Collisions with Highly Charged C, O, F, S, and Cl Ions at Intermediate Velocities,”  
B. B. Dhal, Lokesh C. Tribedi, U. Tiwari, K. V. Thulasiram, P. N. Tandon, T. G. Lee, C. D. Lin, and L. Gulyás  
Phys. Rev. A **62**, 022714-1 (2000)
3. “Electron Yield Per Ion Charge-State Correction for an Ion Collector with Unsuppressed Secondary Electron Emission,”  
J. Krása, L. Láská, M. P. Stöckli, and D. Fry  
Czech. J. Phys. **50**, 797 (2000)
4. “Symmetry Breakdown in Ground State Dissociation of  $\text{HD}^+$ ,”  
I. Ben-Itzhak, E. Wells, K. D. Carnes, Vidhya Krishnamurthi, O. L. Weaver, and B. D. Esry  
Phys. Rev. Letters **85**, 58 (2000)
5. “Observation of a Quasimolecular Ionization Window in Low-to-Intermediate Impact Velocity Collisions of  $\text{He}^+$  Ions with  $\text{H}_2$  and He,”  
M. A. Abdallah, W. Wolff, H. E. Wolf, L.F.S. Coelho, C. L. Cocke, and M. Stöckli  
Phys. Rev. A **62**, 012711-1 (2000)
6. “Three-Body Effects in the Fragmentation of  $\text{D}_2$  by Slow, Highly-Charged Xenon,”  
R. D. DuBois, I. Ali, C. L. Cocke, C. R. Feeler, and R. E. Olson  
Phys. Rev. A **62**, 060701-1 (2000)
7. “Strong Double K-K Transfer Channel in Near Symmetric Collision of Si + Ar at Intermediate Velocity Range,”  
B. B. Dhal, L. C. Tribedi, U. Tiwari, P. N. Tandon, T. G. Lee, C. D. Lin, and L. Gulyás  
J. Phys. B: At. Mol. Opt. Phys. **33**, 1069 (2000)
8. “Evaluation of Antiproton-Impact Ionization of He Atoms Below 40 keV,”  
T. G. Lee, H. C. Tseng, and C. D. Lin  
Phys. Rev. A **61**, 062713-1 (2000)
9. “Charge Transfer in  $\text{H}^+ + \text{Ar}$  Collisions from 10 to 150 keV,”  
A. Amaya-Tapia, H. Martinez, R. Hernández-Lamonedá, and C. D. Lin  
Phys. Rev. A **62**, 052718-1 (2000)
10. “Electrons Ejected with Half the Projectile Velocity and the Saddle Point Mechanism in Ion-Atom Collisions,”  
Emil Y. Sidky, Clara Illescas, and C. D. Lin  
Phys. Rev. Lett. **85**, 1634 (2000)

11. “Hyperspherical Calculations of  $H(1s) + \mu^+$  Rearrangement Collision Cross Sections from Threshold to 2 eV,”  
Z. X. Zhao, A. Igarashi, and C. D. Lin  
Phys. Rev. A **62**, 042706-1 (2000)
12. “Charge Exchange in Slow  $H^+ + D(1s)$  Collisions,”  
B. D. Esry, H. R. Sadeghpour, E. Wells, and I. Ben-Itzhak  
J. Phys. B: At. Mol. Opt. Phys. **33**, 5329 (2000)
13. “Asymmetric Branching Ratio for the Dissociation of  $HD^+(1s\sigma)$ ,”  
E. Wells, B. D. Esry, K. D. Carnes, and I. Ben-Itzhak  
Phys. Rev. A **62**, 062707-1 (2000)
14. “Boundary-Free Propagation with the Time-Dependent Schrödinger Equation,”  
E. Y. Sidky and B. D. Esry  
Phys. Rev. Lett. **85**, 5086 (2000)
15. “Experimental Evidence of Transfer Excitation in  $Ar^{6+}$ -He Collisions  
E. Y. Kamber, M. A. Abdallah, C. L. Cocke, M. Stöckli, J. Wang and  
J. P. Hansen  
J. Phys. B: At. Mol. Opt. Phys. **33**, L171 (2000)
16. “Correlated Three-Electron Continuum States in Triple Ionization by Fast Heavy-Ion Impact,”  
M. Schulz, R. Moshhammer, W. Schmitt, H. Kollmus, R. Mann,  
S. Hagmann, R. E. Olson, and J. Ullrich  
Phys. Rev. A **61**, 022703-1 (2000)
17. “Electron Correlations Observed through Intensity Interferometry,”  
M. Schulz, R. Moshhammer, W. Schmitt, H. Kollmus, B. Feuerstein,  
R. Mann, S. Hagmann, and J. Ullrich  
Phys. Rev. Lett. **84**, 863 (2000)
18. “Total and State-Selective Electron Capture Cross Sections for  $B^{4+} + H$  Collisions,”  
H. C. Tseng and C. D. Lin  
Phys. Rev. A **61**, 034701 (2000)
19. “Kinematically Complete Investigation of Momentum Transfer for Single Ionization in Fast Proton-Helium Collisions,”  
Th Weber, Kh Khayyat, R. Dörner, V. Mergel, O. Jagutzki, L. Schmidt,  
F. Afaneh, A. Gonzalez, C. L. Cocke, A. L. Landers and H. Schmidt-  
Böcking  
J. Phys. B: At. Mol. Opt. Phys. **33**, 3331 (2000)
20. “Polarization Spectroscopy of  $O^{5+}(1s^23p)$  States Produced in the Collisions of  $O^{6+}$  with He and  $H_2$ ,”  
H. Tanuma, T. Hayakawa, C. Verzani, H. Kano, H. Watanabe,  
B. D. DePaola, and N. Kobayashi  
J. Phys. B: At. Mol. Opt. Phys. **33**, 5091 (2000)
21. “Electron Capture from Elliptic Rydberg States: Impact Perpendicular to the Minor Axis,”  
L. Kristensen, T. Bové, B. D. DePaola, T. Ehrenreich, E. Horsdal-  
Pedersen and O. E. Povlsen  
J. Phys. B: At. Mol. Opt. Phys. **33**, 1103 (2000)

22. “Low-Lying  $^3P^0$  and  $^3S^e$  States of  $Rb^-$ ,  $Cs^-$  and  $Fr^-$ ,”  
C. Bahrim and U. Thumm  
Phys. Rev. A **61**, 022722 (2000)
23. “Electron-Capture Processes of Low-Energy  $Si^{3+}$ ,  $Si^{4+}$ , and  $Si^{5+}$  Ions in Collisions with Helium Atoms,”  
H. Tawara, K. Okuno, C. W. Fehrenbach, C. Verzani, M. P. Stöckli, B. D. DePaola, P. Richard, and P. C. Stancil  
Phys. Rev. A **63**, 062701-1 (2001)
24. “Two-Center Effect on Low-Energy Electron Emission in Collisions of 1-MeV/u Bare Ions with Atomic Hydrogen, Molecular Hydrogen, and Helium: I. Atomic Hydrogen,”  
Lokesh C. Tribedi, P. Richard, L. Gulyás, M. E. Rudd, and R. Moshhammer  
Phys. Rev. A **63**, 062723-1 (2001)
25. “Two-Center Effect on Low-Energy Electron Emission in Collisions of 1-MeV/u Bare Ions with Atomic Hydrogen, Molecular Hydrogen, and Helium: II.  $H_2$  and He,”  
Lokesh C. Tribedi, P. Richard, L. Gulyás, and M. E. Rudd  
Phys. Rev. A **63**, 062724-1 (2001)
26. “Stripping Energy Dependence of A  $B^{3+}(1s^2\ ^1S, 1s2s\ ^3S)$  Beam Metastable Fraction,”  
M. Zamkov, H. Aliabadi, E. P. Benis, P. Richard, H. Tawara, and T.J.M. Zouros  
Application of Accelerators in Research and Industry – XVIth Int’l Conf., ed. by J. L. Duggan and I. L. Morgan (American Institute of Physics, 2001) p. 149
27. “Zero-Degree Auger Electron spectroscopy of Quasi-Free Electrons Scattered by Highly Charged Ions,”  
Habib Aliabadi, Ridvan Unal, Mikhail Zamkov, Patrick Richard, Chander P. Bhalla, Hiro Tawara, Mark Gealy, and Asad T. Hasan  
Application of Accelerators in Research and Industry – XVIth Int’l Conf., ed. by J. L. Duggan and I. L. Morgan (American Institute of Physics, 2001) p. 172
28. “Dynamics of the Fragmentation of  $D_2$  by Fast Protons and Slow Highly Charged  $Xe^{26+}$ ,”  
I. Ali, R. D. DuBois, C. L. Cocke, S. Hagmann, C. R. Feeler, and R. E. Olson  
Phys. Rev. A **64**, 022712-1 (2001)
29. “Compton Profile of Multiply-Ionized Fluorine Atoms,”  
K. R. Karim and C. P. Bhalla  
Application of Accelerators in Research and Industry – XVIth Int’l Conf., ed. by J. L. Duggan and I. L. Morgan (American Institute of Physics, 2001) p. 201
30. “Electron Elastic Scattering Resonances in the Collision of Fast Hydrogenic Ions with Molecular Hydrogen,”  
G. Toth, P. Zavodszky, C. P. Bhalla, P. Richard, S. Grabbe and H. Aliabadi  
Physica Scripta **T92**, 272 (2001)
31. “Angle-Differential and Momentum-Transfer Cross Sections for  $e^- + Rb$ ,  $Cs$ , and  $Fr$  Collisions at Low Energies:  $^3F^0$  Shape Resonances in  $Rb^-$ ,  $Cs^-$ , and  $Fr^-$  Ions,”  
C. Bahrim and U. Thumm  
Phys. Rev. A **64**, 022716-1 (2001)

32. “Transfer Ionization to Single Capture Ratio for Fast Multiply Charged Ions on He,”  
R. Ünal, P. Richard, H. Aliabadi, H. Tawara, C. L. Cocke, I. Ben-Itzhak,  
M. J. Singh, and A. T. Hasan  
Application of Accelerators in Research and Industry – XVIth Int’l Conf., ed. by  
J. L. Duggan and I. L. Morgan (American Institute of Physics, 2001) p. 36
33. “Velocity Dependence of Electron Removal and Fragmentation of Water Molecules  
Caused by Fast Proton Impact,”  
A. M. Sayler, E. Wells, K. D. Carnes, and I. Ben-Itzhak  
Application of Accelerators in Research and Industry – XVIth Int’l Conf., ed. by  
J. L. Duggan and I. L. Morgan (American Institute of Physics, 2001) p. 33
34. “Secondary-Electron Yield from Au Induced by Highly Charged Ta Ions,”  
J. Krása, L. Láska, M. P. Stöckli, and D. Fry  
Nucl. Instrum. and Methods in Phys. Res. B **173**, 281 (2001)
35. “Superelastic Scattering of Electrons from Highly Charged Ions with Inner Shell  
Vacancies,”  
P. A. Zavodszky, H. Aliabadi, C. P. Bhalla, P. Richard, G. Toth, and  
J. A. Tanis, Phys. Rev. Letters **87**, 033202 (2001)
36. “Electron-Momentum Distributions in Singly Ionizing  $C^{6+}$ -He Collisions at  
Intermediate Velocities,”  
M. A. Abdallah, C. L. Cocke, W. Wolff, H. E. Wolf, and M. Stöckli  
Phys. Rev. A **63**, 024702-1 (2001)
37. “Studies of Charge Exchange in Symmetric Ion-Ion Collisions,”  
C. Y. Chen, C. L. Cocke, J. P. Giese, F. Melchert, I. Reiser,  
M. Stöckli, E. Sidky and C. D. Lin  
J. Phys. B: At. Mol. Opt. Phys. **34**, 469 (2001)
38. “Charge Transfer in Collisions of  $H_2^+$  Ions with  $He^{2+}$  and  $Ar^{2+}$ ,”  
H. Brauning, I. Reiser, A. Diehl, A. Theiss, E. Sidky, C. L. Cocke,  
and E. Salzborn  
J. Phys. B: At. Mol. Opt. Phys. **34**, L321 (2001)
39. “Comment on “Importance of Electron Time-of-Flight Measurements in  
Momentum Imaging of Saddle-Point Electron Emission,”  
M. A. Abdallah and C. L. Cocke  
Phys. Rev. A **63**, 056701-1 (2001)
40. “Photoelectron Diffraction Mapping: Molecules Illuminated from Within,”  
A. Landers, Th. Weber, I. Ali, A. Cassimi, M. Hattass, O. Jagutzki,  
A. Nauert, T. Osipov, A. Staudte, M. H. Prior, H. Schmidt-Böcking,  
C. L. Cocke, and R. Dörner  
Phys. Rev. Lett. **87**, 013002-1 (2001)
41. “Kinematically Complete Charge Exchange Experiment in the  $Cs^+ + Rb$   
Collision System Using a MOT Target,”  
X. Flechard, H. Nguyen, E. Wells, I. Ben-Itzhak, and B. D. DePaola  
Phys. Rev. Lett. **87**, 123203-1 (2001)
42. “Boundary Conditions for the Pauli Equation: Application to Photo-  
detachment of  $Cs^-$ ,”  
C. Bahrim, I. I. Fabrikant, and U. Thumm  
Phys. Rev. Lett. **87**, 123003-1 (2001)

43. "The Helium Trimer has no Bound Rotational Excited States,"  
T. G. Lee, B. D. Esry, Bing-Cong Gou, and C. D. Lin  
J. of Phys. B: At. Mol. Opt. Phys. **34**, L203 (2001)
44. "Radiative Decay of Helium Doubly Excited States,"  
Chien-Nan Liu, Ming-Keh Chen, and C. D. Lin  
Phys. Rev. A **64**, 010501-1 (2001)
45. "Cross Sections and Collision Dynamics of the Excitation of  $(1snp) \ ^1P^o$  Levels of Helium,  $n = 2-5$ , by Intermediate- and High-Velocity Electron, Proton, and Molecular-Ion ( $H_2^+$  and  $H_3^+$ ) Impact,"  
H. Merabet, M. Bailey, R. Bruch, J. Hanni, S. Bliman, D. V. Fursa, I. Bray, K. Bartschat, H. C. Tseng, and C. D. Lin  
Phys. Rev. A **64**, 012712-1 (2001)
46. "The Role of the Potential Saddle in  $He^{2+} + H$  Impact Ionization,"  
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- 17a “Hyperspherical Close Coupling Calculations for Charge Transfer Cross Sections in  $S^{4+} + H(D)$  and  $Be^{4+} + H$  Collisions at Low Energies,”  
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## VII. INVITED TALKS BY JRML PERSONNEL

### 2000

#### **Esry, Brett**

Colloquium, University of Nebraska

Lincoln, Nebraska

“Solving the Time-Dependent Schrödinger Equation for Fun and Profit”

Seminar, University of Kentucky

Lexington, Kentucky

“Boundary Free Propagation of Quantum Wave Packets”

#### **Lin, Chii-Dong**

Spectroscopy and Collision Dynamics with HCI

Abisko, Sweden

“Electron Correlation in Multiply Excited States of Atoms”

Many-Particle Dynamics in Coulomb Systems

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“Saddle Point Mechanism for Ion Impact Ionization”

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Madrid, Spain

“Overview of Ion-Atom Collision Theory”

#### **Richard, Patrick**

16th International Conference on the Application of Accelerators in Research and Industry

Denton, Texas

“Two Electron Processes in Ion-Atom Collisions at High Velocity:

Transfer Ionization and Transfer Excitation”

#### **Thumm, Uwe**

Seminar, University of Freiburg

Freiburg, Germany

“Ion-Surface Collisions”

Special Seminar of the SFB-276, University of Freiburg

Freiburg, Germany

“Interactions of Highly Charged Ions with Metal and Insulator Surfaces”

Seminar, University of Paris-Sud

Orsay, France

“Charge Exchange and Electron Emission during Ion-Surface Interactions”

Seminar, University of Kassel

Kassel, Germany

“Charge Exchange and Electron Emission during Ion-Surface Interactions”

Sequence of four seminars, University of Freiburg

Freiburg, Germany

“Ion-Surface and Ion-Cluster Interactions”

10th International Conference on the Physics of Highly Charged Ions (ICPEAC)

Berkeley, California

“Slow Collisions of Highly Charged Ions with Surfaces and C60-Clusters”  
Colloquium, Kansas State University  
Manhattan, Kansas  
“Physics at the Nano-Meter, Femto-Second Scales”

**Charles Fehrenbach**

16th International Conference on the Application of Accelerators in Research and Industry  
Denton, Texas  
“New Ion Beam Development at Kansas State University”

**Lew Cocke**

Workshop on Atomic Dynamics in Ion-Atom Physics  
Bonn, Germany  
“Capture and Ionization Processes Studied with COLTRIMS”  
DAMOP Meeting of American Physical Society  
Storrs, Connecticut  
“Application of Ion and Electron Momentum Imaging to Atomic Collisions”  
Institute for Theoretical Atomic and Molecular Physics  
Harvard-Smithsonian Observatory, Cambridge, Massachusetts  
“COLTRIMS: Cold Target Recoil Ion Momentum Spectroscopy”  
Colloquium, Manne Siegbahn Institute, University of Stockholm  
Stockholm, Sweden  
“COLTRIMS Studies of Charged-Particle and Photon Ionization”

**2001**

**Ben-Itzhak, Itzik**

DOE AMOP Research Meeting  
Granlibakken Conference Center, Lake Tahoe, Nevada  
“Ground State Dissociation (GSD) of HD<sup>+</sup>”  
Seminar, Physics Department, Technion  
Haifa, Israel  
“Re-Search for Long-Lived N<sup>-</sup>”  
Seminar, Physics Department, University of Virginia  
Charlottesville, Virginia  
“Imaging Dissociating Metastable He<sup>22+</sup>”  
Seminar, Chemistry Department, Ben-Gurion University  
Beer-Sheva, Israel  
“Charge Transfer and Elastic Scattering in Very Slow H<sup>+</sup> + D(1s) “half” Collisions”

**Esry, Brett**

Workshop on Few-Body Systems at Low and Moderate Energies: Open Questions  
Beyond Computational problems, European Centre for Theoretical Studies in Nuclear Physics  
and Related Areas (ECT\*)  
Trento, Italy  
“Antiproton Collisions with Hydrogen: Pn Formation”

**Lin, Chii-Dong**

DOE AMOP Research Meeting

Granlibakken Conference Center, Lake Tahoe, Nevada

“Vibrational Modes and Classification of Triply Excited States of Atoms”

**Thumm, Uwe**

XXII International Conference on Photonic, Electronic and Atomic Collisions (ICPEAC)

Santa Fe, New Mexico

“Ion-Surface Interactions”

Workshop on Atomic, Molecular and Optical Physics on Surfaces (ITAMP), Harvard

Cambridge, Massachusetts

“Interactions of Highly Charged Ions with Surfaces”

Colloquium, Kansas State University

Manhattan, Kansas

“Understanding Electronic Interactions of Atoms and Ions with Complex Targets: A Perspective for Nano-Science”

Colloquium, University of Nevada

Reno, Nevada

“Understanding Electronic Interactions of Atoms and Ions with Complex Targets: A Perspective for Nano-Science”

**Lew Cocke**

DOE AMOP Research Meeting

Granlibakken, Lake Tahoe, California

“X Rays from Molecules Fixed in Space: Illuminating Molecules from Within”

**2002****Ben-Itzhak, Itzik**

17th International Conference on the Application of Accelerators in Research and Industry (CAARI)

Denton, Texas

“Molecular Dissociation of Collision Induced Dissociation and Dissociative Capture in Slow  $H_2^+$ ”

**Esry, Brett**

Workshop on Cold Antimatter, ITAMP

Cambridge, Massachusetts

“Protonium Formation in Cold + H Collisions”

Colloquium, University of Missouri-Rolla

Rolla, Missouri

“Solving the Time-Dependent Schrödinger Equation for Fun and Profit”

**Lin, Chii-Dong**

Workshop on Multielectron Dynamics

Bad-Honnef, Germany

“Shakeoff Theory and Multiply Excited States of Atoms”

Resonances and Reflections: Profiles of Ugo Fano's physics and its Influences

ITAMP, Cambridge, Mass

“Multiply Excited States of Three- and Four-Electron Systems”

**Richard, Patrick**

Cecil and Ida Green Honors Chair In Physics, 2002

Texas Christian University, Waco, Texas

“Multiply Excited States of Ions and Atoms”

DOE AMOP Research Meeting

Airlie Conference Center, Warrenton, Virginia

“Triply Excited States in Three-Electron Ions”

**Thumm, Uwe**

Gaseous Electronics Conference

Minneapolis, Minnesota

“Almost Bound States of Heavy Negative Alkali Ions”

Workshop on Quantum Dynamics in Atomic and Molecular Physics

Dresden, Germany

“Freiburg’s Bobbele, John’s Gang, and Little Apple’s Wild Cat: Interactions between People, Electrons, atoms, Clusters, and Surfaces”

Max-Planck-Institute for Nuclear Physics

Heidelberg, Germany

“Fragmentation of  $H_2^+$  in Intense Laser Fields: Dissociation vs. Coulomb Explosion”

DOE AMOP Research Meeting

Airlie Conference Center, Virginia

“Dissociation and Coulomb Explosion of Model Molecular Hydrogen Ions by Intense Short Laser Pulses”

**Chang, Zenghu**

DOE AMOP Research Meeting

Airlie Conference Center, Virginia

“Kansas Light Source, a New Plug-in at the old Macdonald Lab”

17th International Conference on the Application of Accelerators in Research and Industry (CAARI)

Denton, Texas

“High Harmonic Generation from 02”

Wildcorn 2002, University of Nebraska

Lincoln, Nebraska

“Kansas Light Source”

Colloquium, Fudan University

Shanghai, China

“High Field Atomic Physics”  
Colloquium, Xianjaotong University  
Xi’an, China  
“High Field Atomic Physics”  
Colloquium, Institute of Physics, Chinese Academy of Sciences  
Beijing, China  
“High Field Atomic Physics”  
Colloquium, Xian Institute of Optics and Precision Mechanics, Chinese Academy of Sciences  
Beijing, China  
“High Field Atomic Physics”

## **2003**

### **Ben-Itzhak, Itzik**

Annual Division of Atomic, Molecular and Optical Physics (DAMOP Meeting of American Physical Society  
Boulder, Colorado  
“Molecular Dissociation Imaging of Slow Hydrogen Molecular Ions,”

### **Esry, Brett**

17th International IUPAP Conference on Few-Body Problems in Physics  
Durham, North Carolina  
“From Ultracold Collisions to Protonium Formation: Recent Applications of the Adiabatic Hyperspherical Representation”  
Division of Atomic, Molecular and Optical Physics (DAMOP)  
Boulder, Colorado  
“Adiabatic Floquet Representation for Atoms in an Intense Laser Field” - (Jesus Hernandez)

### **Thumm, Uwe**

Colloquium, California State University  
Sacramento, California  
“Fragmentation Mechanisms of Molecular Hydrogen Ions in Ultrashort, Intense Laser Pulses”  
XVIII International Symposium on Ionic and Atomic Collisions  
Stockholm, Sweden/Helsinki, Finland  
“Coherent Nuclear Dynamics of  $\text{H}_2^+$  and  $\text{D}_2^+$  in Intense Ultrashort Laser Pulses,”

### **Lew Cocke**

Colloquium, University of Kansas  
Lawrence, Kansas  
“Two Ways to Blow Apart Molecules with Photons”  
Plenary Talk, ICPEAC  
Stockholm, Sweden  
“Momentum Imaging in Atomic Collisions”