7th Asian International Seminar on Atomic and Molecular Physics

 $4th$ to $7th$ December, 2006

Department of Physics

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Contents

Foreword

Asian physicists and chemists have made rich contributions to the growth of 'Atomic and Molecular Physics'. The initiatives since the earliest days of Japan-China meetings turned out to be very potent, fostering regional collaboration and productive science. The movement has grown much since, bringing other countries in the Asia-Pacific region actively engaged in sharing ideas and visions that have moved frontiers of science.

It is a great privilege to host the Asian International Seminar in Atomic and Molecular Physics, the seventh in the series, here in India. A significant community of young and senior atomic and molecular physicists would benefit from interacting with fellow scientists in the Asia-Pacific region through this dialogue; the benefits, we trust, will be mutual and open up a new vista for regional collaboration. The field of atomic and molecular physics is a vast one; choice of topics/themes is not easy in an area that is growing at extra-ordinary pace and inter-disciplinary contributions coming from world leaders cutting across traditional subject domains. Accommodating all interests in a '4 days' period was not easy – we are very disappointed that we failed to provide more time for many of our learned speakers from whom we all have much to gain. Worse, some prospective speakers simply could not be accommodated in the time-bound frame. We have to live with this frustration.

The academic program through the four days is dense; but the benefits will be very rewarding as we trust. A relaxed banquet evening on the third evening of the conference provides the only formal arrangement for relaxation, but we hope that on the day after the conference, the buses that would take delegates for an excursion will be full. We believe it will be an enjoyable, comfortable and very relaxed trip.

We shall consider the $7th$ AISAMP to be successful specially if some ideas discussed during the meeting lead to some new research problems and solutions, leading in the near future to some collaborative publications involving scientists coming from place far and wide. We strongly encourage such prospects. We are pleased to announce that the Institute of Physics will publish the proceedings of papers (both invited talks and poster presentations) in the electronic online publication *Journal of Physics: Conference Series*. Articles approved by the referees will be published after usual refereeing process. **Hard deadline for submission of complete manuscripts is January 15, 2007.**

We hope all participants find the atmosphere conducive for academic pursuits and for new ideas to blossom; for strengthening ties between peoples and countries and to nucleate new interactions. We hope you enjoy the conference; helped by many others, we have tried hard to provide for comprehensive facilities. Yet we know there must be shortfalls, perhaps some serious ones. We urge you to kindly condone the inconveniences and lapses, those that are brought to our notice will be rectified to the best of our ability and resources. *And yes, please do join the excursion on 8th!*

With our very best wishes, Sincerely,

Pranawa (in Chennai) and Purushottam (in Kolkata)

History of AISAMP

What follows is an article reproduced from Abstracts of AISAMP5 with the kind permission of the author and a note by Professor Matsuzawa augmenting the later development including AISAMP5.

Brief History of the Asian International Seminars on Atomic and Molecular Physics

Takayanagi, Kazuo *Institute of Space and Astronautical Science, Professor Emeritus University of Tokyo, Professor Emeritus.*

The first meeting of this series of Asian lnternationa1 Seminars on Atomic and Molecular Physics (AISAMP) was held in Tokyo in 1992. This meeting had another name, i.e., the Fourth China-Japan Joint Seminar on Atomic and Molecular Physics. This clearly indicates that the Asian Seminars are the continuation of the China-Japan Seminars.

In 1979, the 11th ICPEAC (International Conference on Physics of Electronic and Atomic Collisions) was held in Kyoto. It was the first big meeting held in Asia in the field of atomic and molecular physics. For the first time in the history of ICPEAC, scientists from the mainland China attended the meeting. Thus, communication started between scientists in China and those in Japan.

 The first China-Japan Seminar was organized by Professor Gou Qing-quan after exchanging some discussions by letters with Takayanagi in Japan. It was held in Chengdu in August 1985. Seven scientists from Japan attended the seminar

The Second China- Japan Seminar was held in Fuji-Yoshida at the northern foot of Mt. Fuji in October l 988. In addition to seven participants from the mainland China, there were two other Chinese, one from Korea and one from Germany, who were temporarily staying in Japan in some exchange programs. Number of Japanese participants was nearly30.

 The Third China-Japan Seminar was held in October 1990 in Taian near Mt. Taishan. Fifteen Japanese and twenty-eight Chinese scientists attended the meeting.

 The Fourth China-Japan Seminar was held in Tokyo in October 12-15,1992. The local organizing committee had intention to extend the China-Japan Seminar to an Asian Internationa1 Seminar. For some reasons, the title of the "Fourth China-Japan Seminar" was not removed, but the seminar had the second title, i.e., "The First Asian International Seminar on Atomic and Molecular Physics"(AISAMP). There were nine participants from the mainland China, one from Taiwan, two from Korea, and one from Singapore. In addition to these, there were also one from U.S.A., one from U. K., and one from Germany, who were staying in Japan for some other programs. The book of abstracts was printed in advance and distributed at the beginning of the seminar. During the meeting, an international committee was formed. They discussed and decided the name of the future seminars (Asian lnternationa1 Seminar on Atomic and Molecular Physics), purpose of the seminars, style of operation, and the site and the year of the next meeting (in Beijing in 1994), etc.

The Second AISAMP was held in Beijing, in October 24-28, 1994. More than 60 scientists attended the meeting. This number includes nine from Japan, nine from Korea, three from Taiwan and five from western countries. During the meeting, the International Advisory Committee was established. In the committee meeting, the Charter of this series of Seminars was written down and also it was decided that the next seminar would be held in Korea in 1996.

 The Third AISAMP was held in Pohang, Korea in October 7-10,1996. About one hundred scientists participated in the meeting. Excluding students from the local university, there were fortyseven Korean scientists, thirteen from the mainland China, two from India, fifteen from Japan, eight from Taiwan, seven from U.S.A. and one from Germany. There were about forty invited talks which were given orally and about eighty reports presented at two poster sessions. The proceedings of the Pohang meeting was published later (1998) in vol.32, No.3 of the Journal of the Korean Physical Society.

 At the Beijing meeting in 1994, it was decided by the International Advisory Committee that the Fourth Seminar would be held in 2000 and the following meetings should be held in every other years. A meeting in 1998 was avoided since there was a big international conference ICPEAC in 1999 in Sendai, Japan.

 The Committee met twice during the Pohang meeting and confirmed the schedule of the future meetings and Taipei was decided to be the site of the Fourth Seminar.

 The Fourth AISAMP was held in Taipei, Taiwan in October 13-18, 2000. Total number of participants was about 150. This includes 15 from the mainland China, two from Hong Kong, one from India, 23 from Japan, 10 from Korea, and one from Thailand. There were also three from Australia, 18 from U.S.A. and 11 from other (mainly European) countries. Most of the papers reported at the Seminar were later published in a special issue of the Journal of Chinese Chemical Society.

 Nature of the Seminars has been changed greatly since we started the China-Japan Seminar. At the beginning, we had in our mind something like US-Japan Seminar, That is, the number of participants was expected to be rather small (somewhere around 30). The Seminar was considered a meeting to exchange informally ideas and new-findings, to provide a chance to discuss on alreadypublished works, or to give review talks useful to many participants. It was not considered a formal meeting where original papers on completed works are presented. The name "Seminars" came from this idea. This is one of the reasons why the Seminar organizers in Japan do not plan to produce proceedings of the Seminars. However, local situation may be different from country to country where the Seminar is organized. Thus, the AISAMP Charter has flexibility and does not say anything definitely on, for instance, the proceedings of the Seminar. Now that the Seminar attracts one hundred or more participants each time, and the nature of AISAMP has been changing gradually, it may be better to change its name from "Seminar" to "Symposium" or "Conference", if most of the participants so desire.

NOTE ADDED by Professor Michio Matsuzawa

 The article shown above is the abstract of the talk on the history of AISAMP series given at the AISAMP5 (Nara, Japan, Oct.2002, Abstracts of AISAMP5 pp105-106) by K. Takayanagi who was one of the cofounders of the China-Japan Seminars on Atomic and Molecular Physics, i.e, the precursor of the AISAMP series. This article only covers the evolution of this series of the Seminars till the AISAMP4 (Taipei, 2000). Hence recent evolution after the AISAMP4 is briefly described in the following.

 The fifth AISAMP was held at Nara, Japan in October 2-5, 2002. Total number of the participants was about 120. About 40 invited talks were orally given at the AISAMP5; 4 from Australia, 5 from China, 4 from India, 15 from Japan, 5 from Korea, 5 from Taiwan, 1 from Vietnam and etc.

About 50 papers were also given at poster sessions. The current Charter of the Seminar was established by the International Advisory Committee during the AISAMP5 meeting at Nara. The sixth AISAMP was held in Beijing, China in September 20-23, 2004. Total number of participants was about 70 excluding local graduate students. More than 100 participants attended this meeting including local graduate students. 47 papers including invited talks were orally presented; 3 (3) from Australia, 20(9) from China, 5(5) from India, 7(5) from Japan, 6(4) from Korea, 3(2) from Taiwan etc. The numbers in parentheses denote the numbers of invited talks. About 30 papers were also given at poster sessions.

 Judging from these data, the AISAMP series is now evolving as a wide forum which enables Asian scientists in the field of atomic, molecular and optical sciences to exchange new scientific ideas freely and to get fruitful results. At the AISAMP6 (Beijing), the International Advisory Committee decided that the seventh AISAMP (2006) should go to Chennai, India. Table, shown below gives an overview of the evolution of the AISAMP series so far, namely, up to the AISAMP6.

Meeting site Dates Chairperson (Co-chairpersons)

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* The Fourth China-Japan Seminar was held simultaneously.

** Scientists from Australia and India began to participate in the AISAMP series.

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Program *7th AISAMP December 4-7, 2006* **VII AISAMP** - **Day 1:** Monday, December 4, 2006: IC & SR Auditorium, IIT-Madras **Session 1**

D1S1

- 09.05-09.10 : Welcome note, by P. C. Deshmukh
- 09.10-09.15 : Opening Remarks by Director, IIT-M.
- 09.15-10.05 : Key Note (KN) address (**Speaker from India :Kailash C. Rustagi**) **Atomic, Molecular and optical Physics in India -a Perspective**
- 10.00-10.10 : Q&A

- $11.00-11.05$: Q&A
- 11.05-11.10 : Vote of Thanks, by Purushottam Chakraborty

11.10-11.30 : Tea

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S2: Invited Talks: **Laser Cooling, Cold Traps for Atoms and Molecules Session 2**: **Chair : Robert Scholten**

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13.15-14.30 : Lunch

S3: Invited Talks: **Atomic and Molecular Collisions Session 3: Chair : Mark A. Buntine**

VII AISAMP - Day 2

Tuesday, December 5, 2006 : IC & SR Auditorium, IIT-Madras
Session 5 Chair \cdot F I Biocles

- *features* 10.30-10.35 : Q&A on T1
- 10.35-10.55 : **T2 Jung Bog Kim**
	- *Partial Storage and Retrieval of Light Pulse in Cs Atomic Vapors*

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- 10.55-11.00 : Q&A on T2
- -- 11.00-11.15 : Tea
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S7: Invited Talks **Atom and molecules in controlled laser fields Session 7: Chair : N Sathyamurthy**

- **--** D₂S₇
- 11.15-11.20 : Chairman's Remarks
- 11.20-11.40 : **T3 Deepak Mathur** *Matter in Intense Optical Fields: from molecules to living cells* 11.40-11.45 : Q&A on T3
- 11.45-12.05 : **T4 Robert Scholten**
	- *Atomic coherence ultracold plasma, and imaging*
- 12.05-12.10 : Q&A on T4
- 12.10-12.30 : **T5 Feng Lei Hong**
	- *Laser Frequency Control and Measurement with an Optical Comb*
- 12.30-12.35 : Q&A on T5
- 12.35-12.55 : **T6 S. Bhattacharyya** *Spin Currents from Helium in Intense-Field Photo ionization*
- 12.55-13.00 : Q&A on T6
- --

13.00-14.15 : Lunch

--- S8: Invited Talks **Atomic & Molecular Physics with Synchrotron Radiation Session 8**: **Chair : Naresh Chandra --** D2S8 14.15-14.20 : Chairman's Remarks 14.20-14.40 : **T7 Bhas Bapat** *Photo-triple-ionisation of CO2* 14.40-14.45 : Q&A on T7 14.45-15.05 : **T8 Jim J Lin** *Dynamics of Elementry Reactions studied by Crossed Molecular Beam technique combined with Ion Velocity Image or Synchrotron Radiation-exemplified by F+CH4 and F2+CH3SCH3 reactions* 15.05-15.10 : Q&A on T8 15.10-15.30 : **T9 G. S. Lodha** *Atomic and molecular research using vacuum ultra violet/soft x-ray reflectivity beamline on Indus-1* 15.30-15.35 : Q&A on T9 -- 15.35-15.50 : Tea 15.50-16.15 : *CONFERENECE PHOTOGRAPH* -- S9: Invited Talks **Atomic & Molecular Processes for Tests Of Fundamental Laws Session 9** : **Chair : Michio Matsuzawa --** D₂S₉ 16.15-16.20 : Chairman's Remarks 16.20-16.40 **: T10 Bhanu P Das** *Theory of Parity Nonconservation in Trapped Ions* 16.40-16.45 : Q&A on T10 16.45-17.05 **: T11 A I Jaman** *Millimeterwave Spectroscopy of Transient Molecules of Chemical and Astrophysical Interest* 17.05-17.10 : Q&A on T11 17.10-17.30 **: T12 T N Chang** *Core Excitation Effects on Atomic Transitions* 17.30-17.35 : Q&A on T12 17.35-17.55 **: T13 Ramesh Pai** *Mean Field Theory for Interacting Bosons on a Lattice* 17.55-18.00 : Q&A on T13

EVENING: IAC DINNER MEETING

VII AISAMP - **Day 3** Wednesday, December 6, 2006: IC & SR Auditorium, IIT-Madras **Session 10**: **Chair : T N Chang** D3S10 09.00-09.05 : Chairman's Remarks 09.05-09.55 : **Plenary Talk (PT3: Speaker from Korea: Sung Ho Suck Salk)** *Changes in physical properties from atomic to condensed matter state* $09.55-10.05$: Q&A -- S11: Invited Talks **BEC, Quantum Degenerate Gas Session 11**: **Chair : Jim Williams** D3S11 10.05-10.10 : Chairman's Remarks 10.10-10.30 : **T1 C S Unnikrishnan** *Atoms in cavities and near surfaces-New experiments in quantum electrodynamics with laser cooled atoms and Bose- Einstien condensates* 10.30-10.35 : Q&A on T1 10.35-10.55 : **T2 Dilip Angom** *Pairing in two component ultracold fermionic atoms* 10.55-11.00 : Q&A on T2 -- 11.00-11.15 : Tea -- S12: Invited Talks **Atomic & Molecular Spectroscopy Session 12**: **Chair : Lokesh Tribedi** D3S12 11.15-11.20 : Chairman's Remarks 11.20-11.40 **: T3 Hiroyuki Katsuki** *Visualizing and Controling Ultrafast Wave-Packet Interference in Diatomic Molecules* 11.40-11.45 : Q&A on T3 11.45-12.05 **: T4 Prem B. Bisht** *Time-Resolved Spectroscopy on Picosecond Time Scales- Laser induced transient grating and degenerate four wave mixing for studies of radiationless transitions in moleculer system* 12.05-12.10 : Q&A on T4 12.10-12.30 **: T5 Sonjoy Majumder** *Correlation Studies of Hyperfine Interactions in Atoms and Ions* 12.30-12.35 : Q&A on T5 12.35-12.55 **: T6 E. J. Bieske** *Probing the Interactions between Metal Cations and Molecular Hydrogen -infrared spectroscopy of mass selected Li⁺ -H2 and Al⁺ -H2 complexes* 12.55-13.00 : Q&A on T6

13.00-14.00 : Lunch

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S13: Invited Talks **Novel Techniques to Study Atom & Molecules-1 Chair: Keh-Ning Huang**

VII AISAMP - Day No. 4 Thursday, December 7, 2006: IC & SR Auditorium, IIT-Madras

Session 15

Chair : G Metha

S18: Invited Talks **Novel Techniques to Study Atom & Molecules-2**

Session 18: **Chair : B N Jagatap**

17.05-17.30 : 'Open' Session / Conference Closure.

"One must always do what one really cannot." Niels Bohr (1885-1962)

Abstracts *of* **Invited Talks**

D1/S1/KN Atomic, Molecular and Optical Physics in India: a Perspective

Kailash C. Rustagi

Physics Department, IIT Bombay, Mumbai400076, INDIA

Atomic and molecular physics has a profound impact on several areas of science such as astrophysics, nano-materials, optical physics , chemical engineering and surface science. In this talk, I will present a perspective review of the evolution of the Indian activities in this area with some emphasis on optical spectroscopy and nano materials. I will also discuss the impact of important experimental facilities that have become available or are expected to be available in near future in India.

D1/S1/PT1

Plenary Talk 1

Speaker from China: Mingsheng Zhan

 $D1/S2/T1$

Controlling the Translation of Molecules in Electric Fields: *Prospects for Infra-thermal Chemistry*

Y. Yamakita, 1,21 R. Takahashi,1 N. Hori,¹ K. Ohno,¹ S. R. Procter, ² A. L. Goodgame, ² T. P. Softley, ² and F. Merkt³

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Any atom or molecule in the Rydberg states shows the Stark effect with great magnitude due to its significant dipole moment (e.g., 1000 debye). Therefore a force can be exerted on neutral particles in inhomogeneous electric fields. This principle can be used to *decelerate* neutral molecules in a beam. By carefully applying the field it is also possible to *bunch* the translational temperature. Indeed, Meijer and coworkers [1] demonstrated both control for ND₃ molecules using fast-switched multi-stage inhomogeneous fields. Translational energy will be converted to electrostatic potential energy in the inhomogeneous field and dissipated when the field ramped down (or up). Their device, known as the "Stark decelerator", is applicable to any dipolar molecules in the ground state. However non-polar molecules, like the H_2 molecule, cannot be controlled in the ground state. In this paper we report on an alternative approach to control H_2 molecules by exciting them to the Rydberg states [2]. In fact, the large susceptibility of the Rydberg states realizes the observation of deflection and deceleration for H_2 molecules.

The Rydberg states are accessed by two-photon, two-color (VUV+UV) excitation including a selected ro-vibrational transition to the B¹ Σ ⁺ (*J*=1) intermediate sate. The VUV radiation ($\lambda \approx 110$ nm) is generated by non-resonant frequency tripling in a rare-gas cell with a frequency-doubled nanosecond dye laser [3]. An inhomogeneous electric field is applied with dipole rods with parallel orientation (for deflection) or perpendicular (for deceleration) to a supersonic molecular beam. The Rydberg H_2 molecules are deflected towards or away the dipole rods depending on the states excited, high-field-seeking or lowfield-seeking states, respectively. The time-of-flight distributions (detected by field ionization) are shifted towards longer arrival times in deceleration experiments.

We also perform numerical calculations aiming at slowing down the velocities of molecules completely. The molecules (or atoms) feel a force which is proportional to the gradient of the Stark effect and the spatial gradient of the electric filed $|E|$. 10,000 trajectories are simulated with the $4th$ order symplectic integrator based on experimentally determined Stark shifts [3,4]. The possibility of Stark slowing down to temperature less than $1 K$ has been demonstrated numerically for H_2 and He in the highest Stark sub-levels of Rydberg states *n*=16 or 15. Although the Rydberg-Stark deceleration has been demonstrated experimentally or theoretically for H_2 , Ar, and Na, the complete deceleration is yet to be realized. If a very low laboratory-frame temperature is realized for any ensemble, it leads to reduced Doppler linewidths, large collisional cross-sections, and significant de Broglie wavelengths.

References

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Optical Control of a Magneto-optical Trap

B. N. Jagatap*

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A magneto-optical trap (MOT) is a complex dynamical system that is rich in atom-field and atom-atom interaction processes [1]. Application of a near-resonant auxiliary laser beam can either enhance or suppress these basic processes and thereby provide an optical control over the number of trapped atoms (N) . Such studies are useful for various experiments in quantum optics, cold collisions, precision measurements etc., and also for understanding of the MOT dynamics. They also hold promise for development of deterministic atom sources that have gained much importance in very recent years [2]. Optical shielding is one such strategy where a near-resonant 'catalysis' laser is used to modify collision dynamics of ultra-cold atoms trapped in a MOT and to yield an optical control over the inelastic collisions responsible for the trap loss [3]. Recently we have demonstrated an interesting way of enhancing *N* by applying a blue detuned control laser beam to the capture region of a MOT [4]. Enhanced loading in these experiments is caused by increase in the capture rate that arises from the removal of the Zeeman inaccessibility. A systematic investigation of this phenomenon reveals that in general the control laser can be used to enhance as well as suppress *N* by a proper choice of frequency, intensity and position of the control laser beam. The overall result is to provide an ability to optically control the number of trapped atoms without changing the parameters of the trap. In this talk we discuss the details of these experiments, the mechanisms responsible for enhancement and suppression and the implications of this work in experiments based on laser cooled atoms.

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Quantum Optics Experiments with a Single-Atom Trap

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 The technique of single-atom trapping based on a microscopic magneto-optical trap and a micron-size dipole trap enables us to perform various quantum optics experiments of fundamental interest. In our single-atom trap, the atom number, monitored in real time, can be precisely controlled by a feedback on the magnetic-field gradient with an occupation probability as high as 99% [1]. Using this trap, we have measured the second-order coherence of resonance fluorescence, exhibiting photon antibunching, for various laser-atom detunings and Rabi frequencies. The spectrum of resonance fluorescence has also been measured by using the heterodyne second-order correlation spectroscopy. The connection between the second order coherence and the observed spectrum will be discussed. In addition, atom number statistics observed with and without the atom-number feedback will be presented.

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Coherent manipulation of ultracold atoms

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The realization of ultracold atomic ensembles creates a new area of cold atomic and molecular physics. One of the important topics in the blossoming area is how to manipulate the ultracold atomic ensembles for different applications. In this work, we report several methods to coherently control the matter waves of ultracold atoms by laser fields for studying the quantum dynamics of atoms in ultracold regime.

Electron Excitation of Initially Excited Alkaline Earth Atoms and Noble Gases: A Fully Relativistic Approach

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 There has been little work, either experimental or theoretical, on electron impact transitions between excited states of atoms. Sufficiently large populations of excited states can be produced by laser irradiation to allow for the measurement of inelastic and superelastic scattering processes. Pioneering measurements on such transitions were carried out by Johnson et al [1] for barium and by Boffard et al [2] for inert gases.

 We have previously applied fully relativistic distorted-wave (RDW) method to calculate electron excitation from the ground state of various atoms and obtained results, which gave good agreement with experiment and other theoretical work. In the present work we apply the RDW method to the inelastic and superelastic scattering of electrons from excited states of barium and inert gases in order to compare with the experimental and theoretical results.

 We have carried out relativistic distorted-wave calculations for inelastic electron scattering from the 6s5d $^{1,3}D_2$ and 6s6p $^{1}P_1$ excited states of barium in the energy range from 20 to 40 eV. Results are presented for the differential cross sections and electron impact coherence parameters and compared with experimental measurements and other theoretical calculations for these quantities [3].

 Very recently, we have also extended our RDW method to study the excitation from the initially excited metastable states of neon, argon, krypton and xenon (the $J = 0$, 2 levels of the $np^5(n+1)s$ configuration) to the ten higher-lying fine-structure levels of the $np^5(n+1)p$ configuration. We present and compare our results with experimental measurements of the integrated cross section at energies up to 400 eV and with other theoretical calculations for these cross sections [4].

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Spectroscopic Study of Multiply Charged Xenon and Tin Ions in Charge Exchanging Collisions

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 In semiconductor manufacturing, currently the wavelength used for lithography is 193 nm produced by an ArF excimer laser. In order to continue the progress according to Moore's Law, which states that the number of transistors on a chip doubles about every two years, development of 13.5 nm lithography is required. This wavelength is chosen to match the Mo/Si multilayer mirror, which have a maximum of the near-normal-incidence reflectivity around 13.5 nm. As candidates of the light sources, laser-produced and discharge-produced plasmas (LPPs and DPPs) of xenon and tin have been investigated in recent years [1]. Intimate spectroscopic data on multiply charged ions is necessary to understand the physics of the source plasmas. However, the available spectroscopic information on both xenon and tin ions is quite scarce at this moment in time.

 In this work, we have measured the EUV (extreme ultra-violet) emission spectra from excited multiply charged xenon and tin ions produced in charge-exchanging collisions of Xe^{q^+} ($q = 7 - 18$) and Sn^{q+} ($q = 5 - 15$) with rare gas targets to provide the fundamental spectroscopic data of xenon and tin ions. The multiply charged ions were produced in an ECR (electron cyclotron resonance) ion source with heating by microwave of 14.25 GHz. The ions were extracted with an electric potential of 20 kV and selected by a dipole magnet according to their charge-to-mass ratios. The ion beam was directed into a collision chamber, where it intersected an effusive beam of target gas. Optical radiation in the EUV region from the collision center was observed with a compact flat-field grazingincident spectrometer equipped with a liquid nitrogen cooled CCD camera.

 For Xe ions, emissions around 13.5 nm have been observed as a strong UTA (unresolved transition array) in the case of Xe^{11+} injection and also as weak UTAs with Xe^{10+} and Xe^{12+} injections. In collisions of multiply charged xenon ions with He, the single-electron capture and the transfer ionization have much larger cross sections than that of the double-electron capture [2]. Therefore we can guess that only Xe^{10+} has large contribution in the emission around 13.5 nm from xenon plasmas. On the other hand, the UTA emissions around 13.5 nm have been observed in collisions of various charge states of Sn^{q+} ions ($q = 11 - 15$), and weak emissions also have been observed with injections of $q = 7 - 9$. According to theoretical investigations, these UTAs are regarded as the 4d-4f transitions in both cases of xenon and tin ions. Not only the UTAs but also many emission lines have been observed and analyzed.

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D1/S3/T7

Secondary-ion Emission in grazing Collisions between Highly-charged Ions and Surfaces

- Coincidence Experiments with scattered Particles -

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Secondary-particle emission is one of the most important processes in collisions between highly-charged ions (HCIs) and solid surfaces because it gives rise to deformation of surface atoms [1]. The details of potential sputtering processes (PS), however, have not been cleared yet.

 We have studied the secondary-ion emission in grazing collisions between HCI and surface in order to make clear PS processes. The coincidence experiments with scattered neutral atoms were carried out. It was found in our previous study that topmost atoms belonged to substrate as well as hydrogen and hydrocarbon molecules adsorbed on the surface are preferentially desorbed in grazing collision with HCI. [2] When a HCI approaches to surface at grazing-incidence angle, many electrons are transferred into HCI from surface atoms along with ion trajectory. Actually the sputtering yields *Y* of protons ejected from GaN surface which was interacted with HCI increased rapidly with increase of charge state *q*, e.g. $Y \propto q^4$ [2].

We have developed a new experimental apparatus as shown in Fig. 1. This experimental setup allows us to detect secondary electrons and ions as well as scattered atoms and ions. The energy-loss of the scattered ions can be measured by a Wien-filter.

Fig. 1 A schematic illustration of the experimental setup

L, Lens; D, Deflection plates; WF, Wien filter (Velocity selector); CS, Charge-state separator; CEM, Channel-electron multipliers; MCP, Multi-channel plates; PSD, Position-sensitive detector; TOF-MS, Time-of-flight-mass spectrometer

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$D1/S3/T8$ Atomic Collision Experiment using Ultra-slow Antiproton Beams

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Antiproton, the antiparticle of proton, would be an interesting new probe for studies of atomic physics, both as a 'negative proton' and as a 'heavy electron', if it can be prepared either at rest or as a beam with a typical "atomic energy" in the eV to keV range. Antiprotons can be produced at accelerator facilities, but only at a huge energy in the GeV range. The Antiproton Decelerator (AD) at CERN, Geneva, is a unique facility which provides cooled low-energy antiprotons with MeV energies. There, the MUSASHI group of ASACUSA collaboration has been doing researches on development of an antiproton trap and production of ultra-slow antiproton beams. We have so far achieved efficient confinement of millions of antiprotons in a Multi-Ring electrode Trap (MRT) installed in a superconducting magnet of 2.5 T, by a sequential combination of the AD (down to 5.3 MeV), an RFQD (Radio-Frequency Quadrupole Decelerator; down to 50–120 keV) and the MRT [1]. Antiprotons, cooled to energies less than an electronvolt by preloaded electrons in the electromagnetic trap, was then extracted out of the magnetic field and transported along a 3-m beamline [2] as a monoenergetic beam of 10–500 eV.

 With this ultra-low-energy antiproton beam, we are now planning the first atomic collision experiments under single collision conditions, to measure ionization and atomic capture cross sections of antiprotons against helium atoms. An atomic gas-jet target of 10^{13} cm⁻³ density is prepared [3] and crossed with the antiproton beam. Antiprotons as well as electrons emitted during the reaction will be accelerated and detected by a microchannel plate (MCP) while the antiproton annihilation will be recognized by detection of annihilation products – mostly pions – by surrounding scintillation counters. When the antiproton is captured, it forms a neutral antiprotonic helium atom, some in a metastable state whose level structures have been well studied with spectroscopic methods by a group in the ASACUSA collaboration [4]. Some part of this exotic neutral atom will reach the MCP, but with a longer time-of-flight (TOF) interval after the collision, due to its neutrality and its heavier mass than a bare antiproton. The reaction cross section being of the order of 10^{-16} cm², the probability of atomic capture of antiprotons for a target thickness of 1 cm would be only 0.1%. Severe identification of particles and atoms plays an essential role in the design of the experiment, to distinguish the small number of reaction events out of a huge pile of background events. Details of the experiment will be presented in the talk.

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D1/S4A/T9A

Resonant Processes in Collisions of Highly Charged Ions with Electrons

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Resonant ionization and recombination are important processes in electron-ion interactions. In the interactions with highly charged ions (HCIs), a free electron is captured with a large probability and simultaneously a bound electron is excited to form a doubly excited state resonantly. This unstable intermediate state may decay by photon emission: Dielectronic Recombination (DR), or by emission of two electrons due to successive autoionization: Resonant Excitation/ Double Autoionization (REDA).

 In this paper, we present an observation of these resonant processes using the Tokyo electron beam ion trap (Tokyo-EBIT). An EBIT is suitable for studying such collision processes of HCIs with electrons because it has a mono-energetic and unidirectional electron beam interacting with trapped HCIs. The resonant processes can be studied by measuring charge state distribution inside an EBIT at the equilibrium [1]. In order to measure the charge state distribution, we observed the ions extracted from the EBIT while it can also be measured through the observation of emitted X-rays [2]. The Extracted ion measurements have the following advantage compared to the X-ray measurements.

- (1) The ion measurements have higher efficiency because the total (extraction and transport) efficiency is an order of 10% while the observation solid angle for X-ray measurements is usually less than 0.1%.
- (2) The charge state of extracted ions can be clearly separated by using an analyzing magnet while it is difficult to separate the charge state by X-ray observation with an ordinary solid state Ge detector.

With the advantage (1), one can study the process with small resonant strength. For example, we have succeeded to observe REDA in Li-like iodine which has never been observed for such highly charged heavy ions [3]. With the advantage (2), one can study the resonant processes for any charge state. For example, recently we have clearly observed *KLn* DR processes for various open shell system (e.g. Li- , Be-, B-, C-like ions) which is very difficult to be studied with the X-ray observation. As well as the results of these systematic studies of DR and REDA for highly charged heavy ions (up to Bi), the details of the experimental setup and procedure will be presented.

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D1/S4A/T10A Probing site Selective Fragmentation of Molecules using Velocity Map Imaging (VMI) for Hydroxyl group containing Compounds.

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Recently we discovered a novel aspect of dissociative electron attachment (DEA) process namely the functional group dependent site selective fragmentation of simple organic molecules^[1]. We showed that the DEA to simple organic compounds have similarity in the resonant energies in the H[–] channel depending on the functional group present in the molecule. Also these specific resonances were found to be the characteristic of the precursor molecules of the functional group under consideration i.e. H_2O for OH , NH_3 for amines and so on. The resonant energies for these channels are well indicative of the valance excited resonances playing crucial role in the process. In order to understand the dynamics of this process we carried out the angular distribution measurements of the H– ions from these molecules using velocity map imaging technique (VMI) adapted to work with the low energy electron beam experiments^[2]. The advantage of VMI is its ability to provide the angular distribution in the entire 2π angle with respect to the electron beam as well as the kinetic energies of the detected ions. The angular distribution measurements can provide a clear picture of the symmetries of the negative ion states that are involved and the kinetic energies provide the energetics and dynamics of the DEA process. We have carried out the angular distribution measurements for the hydride ion from acetic acid, methanol and water at various resonances in order to understand the dynamics of the DEA process that leads to site selective fragmentation. At the first resonance from all three molecules we found the angular distribution of hydride ions similar peaking at around 100° indicating the role of functional group as well as the orientation of the specific OH bond with respect to electron beam playing critical role in the site specificity observed. On comparison with the optical absorption spectrum of acetic acid we conclude that the site selectivity is achieved through the valence transition to the molecular orbital localized to the OH bond and having strong antibonding character. At third resonance, the kinetic energies in the hydride ions from CH site are found to peak at near zero energy with a tail extending up to 2eV (for acetic acid) whereas those from OH site have relatively large energy with narrow distribution indicating different mechanisms towards the DEA at different sites.

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D1/S4A/T11A Determining Conformational Preference for Molecules by Electron Momentum Spectroscopy

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Conformational phenomena exist in numerous molecules from simple inorganic compounds to large biomolecules. The relative stabilities of conformers (i.e. conformational preference) attract great interest both of theoretical and experimental studies due to the importance in stereo-chemistry. The enthalpy differences of conformers in gas, liquid, or solid phases as well as the relative abundances at various temperatures have been investigated extensively by means of NMR, Raman, infrared, microwave spectra, and various theoretical calculations. Most of these studies focused on determining totally energetic difference among the conformers. The conformational effects can also

be reflected by the variance of molecular electronic structures. The internal rotation of molecules can lead to different electron density distributions for certain molecular orbitals. Electron momentum spectroscopy (EMS) is an experimental technique which can effectively image the electron density distributions in momentum space for individual atomic and molecular orbitals.[1] By comparing the measured electron momentum profiles with the calculated ones for the conformers, it is possible to determine the Boltzmann-weighted abundances and thus to predict the relative stability for different conformers involved in the experiment. Our recent EMS studies of series molecules have shown that EMS is a feasible experimental method to study the conformational

preference of molecules. As an example shown in figure, 1-butene exists as a mixture of two stable conformers, the skew and the syn, in the gas phase. By comparing the experimental electron momentum profiles with the theoretical ones predicted by the B3LYP density functional method with 6-311++G** basis function, we find that skew-1-butene is more stable than syn-1-butene and their relative conformation abundances at room temperature are estimated to be $65\pm15\%$, $35\pm15\%$ respectively, which is different from the results of microwave spectra^[2] and infrared spectra^[3].

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D1/S4B/T9B Control of Interference of Molecular wavepacket and its Dynamics by using Delayed Ultrafast Pulses

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In molecules, selective excitation and de-excitation processes can be controlled by using phase locked delayed ultrafast pulses. Selectivity in the excitation and de-excitation processes can be achieved by designing a wave-packed of desired shape and position on the excited state by using two delayed ultrashort pulses and a suitable Franck-Condon region for excitation and de- excitation can be chosen by using a delayed ultrashort probe pulse. The interference of two excited wavepackets and its dynamics can be controlled by choosing the delay and the phase between two excitation pulses properly. Thus the dissociation and de-excitation (to a selective vibrational level) processes in molecules can be selectively enhanced or diminished. Phase locking of first two pulses gives rise to spectacular effects on dissociation depending on the vibrational period of the molecule.

Adiabatic Quantum Computation and Coherent Control

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Though attractive from scalability aspects, optical approaches to quantum computing are highly prone to decoherence and rapid population loss due to nonradiative processes such as vibrational redistribution. We show that such effects can be reduced by adiabatic coherent control, in which quantum interference between multiple excitation pathways is used to cancel coupling to the unwanted, non-radiative channels. We focus on experimentally demonstrated adiabatic controlled population transfer experiments [1] wherein the details on the coherence aspects have been minimally explored theoretically but are important for quantum computation. Such quantum computing schemes also form a back-action connection to coherent control developments [2]. We explain the counterintuitive coherence properties between resonant population transfer as compared to that in case of the adiabatic rapid passage.

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Plenary Talk 2

D2/S5/PT2 Molecular Frame (*e*,2*e*) Spectroscopy by (*e*, 2*e*+*M*) Triple Coincidence Study

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Binary (*e*,2*e*) spectroscopy or electron momentum spectroscopy(EMS) has been extensively applied to various atoms and molecules to look at individual electronic orbitals in momentum space [1]. For molecules, however, EMS has always been plagued by the fact that the experiments measure only averages over all orientations of gaseous targets; intrinsically anisotropic or three-dimensional character deteriorates into one-dimensional momentum distribution. If it were possible to fix a molecule in space, the experiment would remove ambiguities inherent in the analysis of the spherically averaged (*e*,2*e*) cross sections.

 Very recently, we have developed a multi-channel apparatus [2] to measure the (*e*,2*e*) cross section in the molecular frame by the use of ion fragmentation with axial recoil; if the molecular ion dissociates much faster than it rotates, the direction of fragment ion departure coincides with molecular orientation at the moment of the ionization. EMS experiments in conjunction with axial recoil fragmentation, which can be designated as the $(e, 2e+M)$ method, becomes possible by measurement of vector correlations between the two outgoing

electrons and the fragment ion by a triple coincidence technique.

We have carried out the first molecular frame (*e*,2*e*) cross section measurement on H_2 by a (*e*,2*e*+*M*) technique at an impact energy of 1200 eV[3]. Shown in Figure 1 are the molecular frame (*e*,2*e*) cross sections of the two transitions indicated. Theoretical calculations by the use of plane wave impulse approximation(PWIA) are also shown for comparison. Although the statistics of the data leave much to be desired, one can clearly see anisotropy that is peculiar to each transition; $2s\sigma g$ is rather isotropic while 2pσu is anisotropic. Discrepancy between experimental results and PWIA calculations will be discussed, and new experimental results at the impact energies of 2000 eV will be presented together with the design of an improved spectrometer.

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Fig.1 Experimental molecular frame (e,2e) cross sections of H_2

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Ionization of Molecules in Fast Ion Collisions: Special Features

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In recent years there has been a major development in the studies of ionization of molecules. The two center effect, electron capture in continuum, binary encounter and soft collisions are the main processes responsible for the continuum electron emission in fast ion collisions with a simple atom such as H , H_2 or He. For a molecular target (such as H_2) the additional mechanism of Young type interference effect is now proved to influence the shape of the electron spectrum. In more complicated molecule such as C_{60} the collective excitation mechanism has been shown to be a major process in single and multiple ionization. We study the single and multiple ionization of C60, in collisions with highly charged fast ($v_P \sim 10$ -15 a.u.) C, O, F and Si ions using time-of-flight technique. The charge-state dependence of single and double ionization is in sharp contrast to that expected in an ion-atom collision but well explained by the Giant dipole plasmon excitation (GDPE) model, which was originally proposed by the ANL group [1]. The GDPE model predicts a steep variation of the ionization cross sections as a function of projectile charge state, which was, however, not tested in earlier investigations [1-3]. For higher degrees of ionization (triple and quadruple ionization) the plasmon excitation as well as solid-like dynamical screening both play a major role based on the perturbation strength (q_P/v_P) . The present studies [4,5] along with our earlier investigation [6] on the solid-like effect in collisions with C_{60} by x-ray detections helps to bridge the gap between atoms and solids.

Since the two H-atoms in H_2 are indistinguishable, their contributions to the ionization add coherently and an interference effect in particle induced ionization of H2 has been reported recently in fast collisions [7,8]. We have studied this process by measuring the energy and angular distribution of low energy electron emission from H2 in collisions with bare C and F ions having energies 1-6 MeV/u, obtained from Pelletron accelerator, Mumbai. The electrons with energies of 1-1000 eV were detected for different emission angles. Oscillations due to interference are deduced by comparing the e-DDCS of H2 and atomic-H and therefore one has to depend on the theoretical calculations or complementary experimental data for H-cross sections. Very recently it has been shown [9] that the forward-backward asymmetry is also greatly influenced due to the interference and, therefore, one can get the evidence of interference effect based on the experimental data of H2-only from the angular asymmetry.

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Partial Storage and Retrieval of Light Pulse in Cs Atomic Vapors **Min Chae¹ , Fenglin Lee26, Xu Mei Su2 , Jung Bog Kim1***

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We are able to store and retrieve^{1,2} partially a pulse in Cs atomic vapors with λ -type EIT scheme. After saving information of a probe light pulse by cutting off a coupling field when the Gaussian light pulse of probe field was propagating through the vapor cell, then we were able to retrieve the pulse as the coupling field was turned on after the dark interval. Fig.1 shows a front part of the probe pulse was transmitted and a typical retrieved pulse after a dark interval. The retrieved signal was detected when the coupling field was turned on. From the figure we can see that the falling down line of the coupling field separates the probe field into two parts, the front part propagates very slowly in the cell, because of electronically induced transparency (E.I.T). When the coupling field is turned off, the coupling field will propagate in advance of the probe field by Δt . Thus, this delayed part of the probe field will be left behind and stored. If the delay of the probe is sufficiently long, the whole pulse will be mapped into the atomic coherence as shown in Fig.2, which is obtained theoretically. However, if the delay is insufficient, only a part of the pulse will be stored. We are able to show numerical agreement with experimental results by simulating the dynamics of partial light storage in the two-level degenerate atomic system considering the decay.

Fig.1 Temporal shapes of coupling field and probe field during storage and

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 $D2/S7/T3$

Matter in Intense Optical Fields: from Molecules to living Cells

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In this talk I shall describe result of recent adventures involve the interaction of intense laser light with matter in the form of isolated (single) molecules, atomic and molecular clusters, and living cells. When pulsed optical radiation is temporally compressed to durations of a few tens of femtoseconds, it becomes possible to attain peak electric fields whose magnitudes begin to match the Coulombic fields within atoms and molecules. Under such circumstances the irradiated matter is instantaneously multiply ionized and, in the case of molecules, is expected to dissociate under intense intra-molecular Coulombic forces. In other words, strong field molecular dynamics are expected to be governed solely by ultrafast bond breakages. However, contrary to expectations, I will describe the results of recent experiments that have shown that, counterintuitively, chemical reactions involving the *forming* of new bonds can also occur on ultrafast time scales that match the times scales of Coulomb explosion [1,2]. Possibilities of irradiating aggregates of atoms or molecules, in the form of large gaseous clusters, opens new vistas for unusual dynamics [3] and afford possible applications concerned with the development of table-top accelerators [4].

Interesting and unexpected dynamics also occur when laser radiation is not temporally but spatially compressed, by means of strong (tight) focusing over very short distances. Under such circumstances a strong gradient of electric field is created that acts as an attractor upon any dielectric material in its vicinity. This is the principle behind an optical trap, and I shall demonstrate some interesting and potentially useful dynamics involving optically trapped living cells. Examples of interest from a basic sciences viewpoint [5] and from the point of view of real and immediate applications [6] will be presented.

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 $D2/S7/T4$

Atomic Coherence, Ultracold Plasma, and Imaging

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Laser control of the *external* state of atoms has reinvigorated AMO physics in the last two decades, enabling many exciting new areas of endeavour including production of ultra-cold plasmas (UCPs) [1]. UCP is created by photo-ionisation of an ultra-cold atom cloud, and thus thermal energy can be weaker than Coulomb binding. Such strongly-coupled plasmas provide an interesting analogue for astrophysical systems including neutron stars and white dwarfs, and also potential direct applications.

 Control of the *internal* state of atoms has also leapt forward in recent years, particularly inducing superposition states of high coherence, leading to dramatic advances in non-linear optics, including EIT (electromagnetically induced transparency), slow and fast light, efficient frequency upconversion [2], and efficient quantum squeezing.

 Our groups are collaborating on development of an ultrabright electron source based on the very low electron emittance offered by an UCP [3], with future application to coherent x-ray production. We are exploiting control of both the external motion of the atoms to produce the ultracold plasma, and of the internal state of the atoms for imaging and feedback to define the electron distribution. We have developed a quantitative and robust diffraction contrast cold-atom imaging technique [4], and we are now combining that with atom coherence control [2] for application to ultracold plasma diagnostics.

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$D2/S7/T5$ Laser Frequency Control and Measurement with an Optical Comb

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Optical frequency standards are of great interest in relation to high-resolution spectroscopy, optical communications and testing of fundamental physics. It was recently demonstrated that modelocked femtosecond lasers can be used to measure the absolute frequency of an optical frequency standard using a Cs atomic clock as a frequency reference. A frequency comb obtained by injecting the light of a Kerr-lens mode-locked Ti:sapphire laser into a photonic crystal fiber (PCF) can cover more than one octave of optical frequencies, enabling the direct measurement of the carrier-envelope offset (CEO) frequency of the femtosecond comb. The frequency comb has been confirmed to be a reliable tool for optical frequency comparisons with an uncertainty of $\sim 10^{-19}$.

 In the present paper, we report the absolute frequency measurement of an iodine-stabilized Nd:YAG laser with an optical frequency comb based on a mode-locked Ti:sapphire laser [1]. We also report the laser frequency control and the frequency measurement in the experiment of an optical lattice clock, where cold atoms are confined in an optical lattice [2].

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Spin Currents from Helium in Intense-Field Photo-ionization **S. Bhattacharyya *1 , Mahua Mukherjee 1 , J. Chakraborty ¹ and**

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 Ionization of hydrogen atom by photon in strong fields has been investigated within the framework of Dirac theory in the past [1] by two of the authors, for the spin- resolved currents. We shall use the formalism in this paper to report on the result of analysis of spinflip probabilities and up-spin (u) and down-spin (d) currents from ionization by single photon of an ensemble of He-atoms subjected to intense circularly polarized laser (CPL) radiation. An intensity and frequency-dependent asymmetry between the spin up and down currents that varies according to the direction of electron emission is expected. Results of numerical calculations will be presented using the ground-state Dirac-Volkov wave function with no spin-orbit interaction in the final state. In the position of detection of the ionized electron there will be no electromagnetic field, eventually the final electron can be taken as a plane wave. The currents from spin-flip electrons is expected to exist with $u \rightarrow d$, but the current with $d \rightarrow u$ (du-current) may be identically zero. Thus the probability of a forbidden transition like the flip from $d \rightarrow u$ is supposed to exist. This occurs even when the spin-orbit interaction in the ground state is zero. This flip is a dynamical effect of intense laser field on a ionized spinning electron. Transformation properties of the up and down spin ionization amplitudes show that the sign of spin can be controlled by a change of helicity of the laser photons from outside.

The S-matrix series for the transition amplitude of single ionization by single photon is

$$
S_{s \to s'} = \int_{-\infty}^{\infty} \left\langle \psi_{1s}^{He^{+}(s'_{2})}(r', t) \psi_{\vec{p}}^{(s'_{1})}(r, t) \middle| \gamma^{\mu} A_{\mu} \middle| \psi_{1s}^{(s_{1}, s_{2})}(r, r' t) \right\rangle dt \tag{1}
$$

where the ground state wave function of He atom is

$$
\psi_{1s}^{(s_1,s_2)}(r,r',t) = \psi_{1s}^{s_1}(r,t)\psi_{1s}^{s_2}(r',t). \tag{2}
$$

Since the intensity of the laser field is high wave function of helium atom can be taken as the product of two hydrogen atom wave functions with spins

s and *s*['] respectively. Other terms are self-explanatory.

Elaborate computation and results will be presented at the conference. Reference:

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Photo-triple-ionisation of CO2

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The interaction of small molecules with photons is of interest not only to atomic and molecular physicists, but also to astrophysicists. Single photon absorption mainly leads to the formation of singly charged ions. The cross-section for double ionisation by single photon absorption is usually a copule of orders of magnitude weaker; triple ionization is even weaker. Doubly and triply charged molecular ions are usually unstable against dissociation. In a recent experiment, done at the Indus-1 synchrotron of the Centre for Advanced Technology, Indore, we have observed the formation of $CO³⁺₂$ by photoabsorption at various energies. The experimental technique is electron-ion-ion-ion four-fold coincidence measurement using a time-of-flight mass spectromter. The triple ionisation process is found to be non-resonant. The molecular ion is found to decay via three two-body and three-body break-up channels. These are analysed for kinematics. The kinetic energy released in a three-body break-up of CO^{3+} ₂ is measured and found to deviate from the Coulomb explosion model. On the basis of the kinematics, it is suggested that four electronic states of CO^{3+} ₂ contribute to the observed decay. This work was done as a collaboration between the Laboratory Astrophysics Group at PRL and the Synchrotron Utilisation Division at CAT.

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Several advances of reaction dynamics studies will be introduced. When a reaction forms two molecular products, the correlation between them provides very useful information, which may help us to unravel the complexity of a ployatomic reaction. If the internal energy and translational energy of one product can be measured coincidently, we can know the product pair correlation through the energy balance. Crossed molecular beam technique combined with ion velocity image is the method of choice. The resonance-enhanced multiphoton ionization probes a quantum state of the reaction product and the ion velocity image provides the measurement of its velocity. By energy and momentum conservation, the internal energy of the co-product can be deduced explicitly. We have developed a time-slicing technique which improves the conventional ion velocity image method by providing direct measurements of all three components of a velocity vector. Application of this novel method to a crossed molecular beam reaction of $F + CD_4$ will be demonstrated [1]. Also a unique reactive dynamical resonance has been discovered in the $F + CH_4$ reaction [2].

Fig. 1 (color) Product ion images of CH₃(0000) from \overline{F} + CH₄ crossed beam reaction at collision energies of 5.3, 2.7 and 0.5 kcal/mol, respectively. Behavior of reactive dynamical resonance is shown at the lowest collision energy.

Vacuum UV photoionization detection can provide both selectivity and universality. The soft ionization nature helps a lot in reducing backgrounds from dissociative ionization of scattered impurities in molecular beams. An intrigue reaction between two closed shell molecules, F_2 + CH3SCH3, has been studied using synchrotron radiation as the ionization light source. Reactive signals were detected even though the reaction cross section is much smaller than the inelastic scattering cross section. The photoionization efficiency spectra also provide important structure information of the reaction products [3].

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D2/S8/T9

Atomic and Molecular Research using Vacuum Ultra violet/ soft x-ray reflectivity Beamline on Indus-1

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The talk will give a brief introduction to Indus-1 synchrotron source (SR) and the various beamlines. In this talk, some of the research work carried out using a toroidal grating monochromator based beamline will be discussed. This is beamline operates in the wavelength range 40-1000 A with a moderate resolution of 500-800. This beamline has two interchangeable end stations, a reflectometer and a time of flight spectrometer. Using reflectometer end station some of the recent results on determination of optical constants of various materials near the absorption edges, surface/ interface studies in x-ray multilayers, soft x-ray damage in hydrated silicon nitride thin film will be presented. Time of flight station is used to carry out photo fragmentation studies on Ar, CO and $CO₂$. These results will be discussed in this talk.

A brief introduction to Indus-2 SR source (2.5 GeV) will also be given. This source is commissioned recently and various beamlines are under installation.

Theory of Parity Nonconservation in Trapped Ions

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Atomic parity nonconservation(PNC) arising from neutral weak currents has the potential to test the Standard Model(SM)of particle physics[1]. A proposal by Fortson to observe parity (PNC) in a single trapped and laser cooled ion marks a paradigm shift in this field[2].By combining the high precision results of the measurement of such an experiment and atomic calculation,it is possible to extract the nuclear weak charge and compare with its corresponding value in the SM.A discrepancy between these two values could be a possible signature of new physics beyond the SM. An experiment to measure PNC in the 6s-->5d 3/2 transition in Ba+ has been considered by Koerber and coworkers[3].Our work is concerne with a high precision calculation of this amplitude using the relativistic coupled-cluster theory.Considering,single,double and the leading triple excitations,we have achieved an accuracy of less than 1%[4]. If the accuracy of our calculation can be matched by that of the Ba+ PNC experiment,then the combination of the two results would provide an independent test of the Standard Model of particle physics.Some new directions in this line of research will also be proposed.

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Millimeterwave Spectroscopy of Transient Molecules of Chemical and Astrophysical Interest

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The discovery of many transient molecules in the interstellar space has evoked tremendous amount of research activity in the field of laboratory microwave and millimeterwave spectroscopy of transient species. Interstellar molecules having spectra in these frequency regions provide us with valuable information about the environment where the molecules exist. So far, more than 130 molecules have been identified in the interstellar space, majority of them are transient in nature e.g., molecular ions, free radicals etc. In general, transient molecules are chemically active and it is very difficult to produce them in high concentration in the laboratory.

Recently, we have assembled a millimeterwave spectrometer to produce and characterize stable and transient species of chemical and astrophysical interest. The recent trends of research activity in this important area will be reviewed in the present talk. Finally, the progress made, so far, in our laboratory will be presented.

Core Excitation Effects on Atomic Transitions

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By including explicitly the electronic configurations with three simultaneously excited electronic orbitals, we have successfully extended the BSCI (B-spline based configuration interaction) method [1,2] to estimate directly the effects of inner shell core excitation to atomic transitions. In particular, we are able to carry out detailed *ab initio* investigation on the core polarization effects without the need of using any parameterized model potential. In this talk, we will present explicitly the change in transition rates due to the core excitations, especially for transitions involving doubly excited states and transitions with small oscillator strengths. Our numerical results using length and velocity gauge typically agree to better than 1%.

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Mean Field Theory for Interacting Bosons on a Lattice

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Studies of ultracold atoms in optical lattices have opened up a new experimental window for the understanding of quantum phase transitions, quantum magnetism and Bose-Einstein condensation in confined, dilute atomic gases. The behaviour of such ultracold atoms in optical lattice can be described by generalized Bose-Hubbard models. We develop a simple mean-field theory for such models and obtain zero- and finite-temperature phase diagrams. We first apply our method to the spin-1 Bose-Hubbard model. The zero-temperature phase diagram comprises superfluid phase(SF) and Mottinsulator(MI) phases. We show that the superfluid phase is either polar or ferromagnetic depending upon the values of the scattering lengths in different angular-momentum channels. The polar-superfluid to Mott-insulator transition is first order if there are an even number of bosons per site because of the formation of singlets (this is quite different from the spin-0 case). However, at zero temperature all other superfluid to Mott-insulator transitions are continuous as in the spin-0 case. The degeneracies because of the spin degrees of freedom modify the nature of superfluid to Mott insulator transitions at finite temperatures. The SF-MI transition becomes first order at finite temperatures but eventually becomes continuous at higher temperatures via a tricritical point. We extend our study to the spin-2 Bose-Hubbard model and discuss the implications of our work for experiments.

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Plenary Talk 3

D3/S10/PT3

Changes in Physical Properties from Atomic to Condensed Matter State

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First we briefly review various physical properties for atoms (and molecules), atomic (molecular) clusters and bulks (condensed matters) with particular interest in electronic structures partially based on our earlier studies. Two different classes of phase transition involved with cluster to condensed matter states, namely the homogeneous and heterogeneous nucleation will be discussed. Similarities and dissimilarities in Bose-Einstein condensation (BEC) between atomic and bulk states will be discussed. BEC in high temperature superconductivity will be highlighted with emphasis on the importance of strongly correlated electrons and its associated classical phase transition as well as quantum phase transition. We find that there exists a remarkable one-to-one correspondence in bose condensation energy between the cluster and bulk states.

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D3/S11/T1

Atoms in Cavities and Near Surfaces – *New Experiments in Quantum Electrodynamics with Laser Cooled Atoms and Bose-Einstein Condensates*

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The study of the interaction of atoms with cavities, surfaces and other atoms have received a substantial boost due to advances in laser cooling of atoms. The interactions modifies the atomic properties and this can be probed by measuring spectral shifts in these atoms, modification of their dynamics and trajectories, and also phase shifts in atom interferometers, offering unprecedented flexibility in experimental studies. The coherence of a Bose-Einstein condensate offers new possibilities and several advantages in precision measurements of short range interactions in matterwave interferometers. Experiments on atom-surface interactions with ultra-cold atoms study aspects of quantum electrodynamics and the quantum vacuum, and can even probe hypothetical new shortrange interactions like modified gravity at small distances, motivated by higher dimensional theories.

 Apart from the short range interactions that affect the trajectory, spectrum and the phase of the atoms, quantum mechanical effects related to the presence of cavities and boundaries as well as the phenomenon of quantum reflection from tunable potentials can be studied in atom-optics experiments with ultra-cold atoms. The possibility of creating multiple potential wells using optical lattice adds an extra dimension to these studies.

I will review the various experimental possibilities and several results related the study of short range interactions between neutral atoms and Bose-Einstein condensates in cavities or near surfaces, with emphasis on the measurements related to cavity quantum electrodynamics and the measurement of van der Waals and Casimir forces.

Pairing in Two Component Ultracold Fermionic Atoms

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Cooper pairing in two-component degenerate fermionic gas with asymmetric density and mass exhibits very interesting phases. These are excellent systems to probe the physics of pairing in quark matter, high temperature superconductivity, etc. Following B. Deb et al[1], the gap equation has multiple solutions. For the degenerate mass case, we have explored the parameter space which supports the interior gap state.

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Visualizing and Controling Ultrafast Wave-Packet Interference in Diatomic Molecules

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Inteference of matter waves has been a focus topic in the quantum world, playing important roles in the studies on the quantum-classical boundary, quantum computations, quantum cryptography and so on. Here we demonstrate unprecedentedly high-resolution measurements and control of the interference of vibrational wave packets created in diatomic molecules [1-3].

 Recently we have observed transient interference of two counter-propagating vibrational wave-packets generated around the half-revival period on the *B*-state potential of the iodine molecule (I_2) [1]. 'Quantum ripples' appeared periodically only when the two wave packets cross each other, and their structures were measured successfully with a few picometers and \sim 100fs spatiotemporal resolutions (see Fig. 1).

Moreover, we have succeeded in tailoring such visualized spatiotemporal images (quantum tapestry). To the best of our knowledge, this is one of the finest manipulations within the molecules ever performed.

Fig. 1: (left) observed interferometric structure around half-revival period by pump-probe spectroscopy. (center) theoretical simulation of the pump-probe signal. Adopted from reference

Also, we have utilized these experimental techniques to read and write amplitude and phase information of the vibrational eigenstates within the wave packets.

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Time-Resolved Spectroscopy on Picosecond Time Scales– *Laser Induced transient Grating and Degenerate four wave mixing for Studies of Radiationless Transitions in Molecular Systems*

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The excited state fluorescence lifetimes of most of the molecular systems fall under time scales of a few nanoseconds (ns). Hence a picosecond (ps) pulse from a laser or a synchrotron source is suitable for time-resolved studies. It is not only that the time-scales are compatible but the spectral purity of ps pulses has an edge over that of the fs lasers which have broad bandwidth thereby restricting the studies of close lying spectral transition in UV-VISIBLE region. In frequency domain, the high-resolution spectra in gas phase or under supersonic free jet are best recorded by tunable ns lasers.

 The laser induced transient grating (LITG) technique with various geometries such as (i). self diffraction, (ii). degenerate four wave mixing, and (iii). Bragg diffraction of the probe beam as a function of the delay time, have been developed at IIT madras during last several years [1]. The parameters studied are the self diffraction efficiency, Bragg diffraction efficiency and higher order optical nonlinearities of organic and nanomaterials such as dyes and carbon nano tubes.

 The studies of the short lived entity 'the excited state' can be done with the help of its fluorescence intensity decay profile. The time-resolved fluorescence spectroscopy provides the information on the radiative and nonradiative decay channels. The information on pure nonradiative components, however, are limited. The LITG technique can provide a direct access to the nonradiative pathways of the excited state due to excited state grating and nonlinear optical effects.

 A brief account of the research work carried out on (i). orientational relaxation of dyes [1], (ii). Dipole-dipole induced long range energy transfer [2] and (iii). Third order optical nonlinearity of carbon nano tubes will be discussed in the present talk.

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Correlation Studies of Hyperfine Interactions *in* Atoms *and* Ions

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Hyperfine interactions (hfi) are the interactions of atomic and ionic electrons with electric and magnetic multipole fields of the nucleus. The famous '21 cm' line in radio astronomy arises due to hfi. The transition between ground state hyperfine levels of Cs has been used for atomic clocks. Accurate estimations of various interactions that determine the hyperfine constants corresponding to the inclusion of various multipole terms provide a test on the accuracy of the electronic wavefunctions especially in the region close to the nucleus. Determination of these parameters is extremely important to resolve many outstanding problems in physics, inclusive of parity nonconservation in atomic processes.

Different many-body correlation effects, like core correlation, core polarization and pair correlations have very different consequences for the hyperfine structure with regard to many low lying states of different atoms and ions. In this paper, we discuss the variation of these correlation effects for some light and heavy atoms and ions [1,2] using relativistic coupled cluster methods. Furthermore, variations with respect to nuclear charges are analyzed for each correlation effect in this work.

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Probing the Interactions between Metal Cations and Molecular Hydrogen – *Infrared Spectroscopy of Mass selected Li⁺ -H2 and Al⁺ -H2 Complexes*

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We report infrared photodissociation spectra of Li^{\dagger} -H₂, Li^{\dagger} -D₂ and Al⁺-H₂. The spectra, which feature full rotational resolution, provide critical information to test and refine potential energy surfaces describing the interaction between metal cations and molecular hydrogen. Complexes of metal cations and hydrogen molecules are interesting because of their relevance to molecular hydrogen adsorption at alkali cation sites in zeolites, their participation in astrophysical processes, and their suitability to accurate theoretical treatments. Despite their significance, there are no spectroscopic data on the alkali metal-hydrogen complexes, although there have been numerous theoretical studies.[1] The first direct observation of Li⁺-H₂ was by Clampitt and Jefferies who found that Li⁺ ions "solvated" by up to 6 H_2 molecules were ejected when a solid H_2 target was irradiated by a Li⁺ beam.[2] Subsequently the binding energy of H₂ to Li⁺ was estimated as 6.5±4.6 kcal/mol (2275) cm⁻¹) through appearance potential measurements of Li⁺-H₂.[3] Existing *ab initio* calculations agree that the Li⁺-H₂ complex has a T-shaped C_{2v} equilibrium structure with the Li⁺ ion loosely tethered to the H_2 molecule, a binding geometry favoured by the electrostatic interaction between the positive charge of the Li^+ and the H_2 quadrupole moment.

Infrared spectra of mass-selected Li^+ -H₂, Li^+ -D₂ and Al⁺-H₂ complexes were measured in the H-H or D-D stretch regions by monitoring production of metal cation photo-fragments. The complexes were generated in a supersonic expansion of H_2 or D_2 passing over a laser ablated metal alloy rod (10% Li/90% Al). As an example the $Li⁺-D₂$ spectrum is shown below. Spectral analysis confirms that the complexes have T-shaped structures and yields information on the intermolecular separations and bond strengths.

Fig 1. Infrared spectrum of Li⁺-D₂ in the D-D stretch region obtained by monitoring the Li⁺ *photofragment signal as the IR wavelength was scanned.*

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Progress at the Shanghai EBIT

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To promote Highly Charged Ion (HCI) related physics research in China the Shanghai Electron Beam Ion Trap, EBIT, project was launched in January of 2002. Since then the EBIT has made rapid progress to the situation in which it stands today. The design parameters of our EBIT put it well into the class of so-called super-EBITs, i.e. electron beam energies up to 200 keV at a current of 200-250 milliamps, compressed to a current density of around 5000 A/cm² by a magnetic field up to 5 Tesla. Presently the EBIT can be operated with a minimum of effort at electron beam energies spanning from 5 keV to 130 keV. The electron current depends on the beam energy, however at 130 keV the current has reached 160 milliamps. The performance of the Shanghai EBIT is steadily increasing towards the design parameters. Very recently a MEVVA ion source has been successfully installed for metal ion injection.

For spectroscopic experiments, the EBIT will be equipped with a number of instruments and detectors. Currently the EBIT ion plasma can be studied using a 1-meter normal incidence McPherson 225 instrument and a flat crystal spectrometer developed at Fudan University. The EBIT plasma is also viewed by a high purity Germanium detector. Other instruments are under development at Fudan to ensure wavelength coverage from $0.1 - 1000$ nm using only three instruments.

"Dirty Clusters": Adding Carbon to Control the Structure and Reactivity of Transition Metal Clusters

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In the early 1980s, Smalley developed the novel laser vapourisation method for producing bare metal clusters in the gas phase. It was quickly learnt that small metal clusters were unique species with chemical and physical properties that were strongly size-dependent and quite different from the bulk metal. Moreover, it has since been shown that substitution of one or more hetero-atoms into an otherwise pure cluster can also affect the electronic and geometric structure of the metal cluster, thus suggesting that each cluster's chemistry can be manipulated by both size and composition.

Excited States of Highly charged Ions after a Metallic Microcapillary

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When a highly charged ion (HCI) approaches a metallic surface, the ion resonantly captures target electrons into excited states. Such an atom (ion) with multiply excited electrons and inner shell vacancies is called a "hollow atom (ion)" [1]. For a few decades, the formation and relaxation dynamics of hollow atoms have been studied intensively with various measurements [2]. However, the hollow atom so formed then jumps into the target within a time interval of $\leq 10^{-13}$ s, because it has been accelerated towards the surface due to its own image charge, until it is completely neutralized. It is noted that physical quantities extractable from these measurements are those related to processes taking place mainly after the time interval (hollow atoms below the surface), and any transition with its lifetime longer than the time interval scarcely takes place above the surface.

In order to overcome this difficulty and to enable the study of the hollow atoms above the surface, we have developed technique using a thin metallic microcapillary foil [3]. When HCIs impinge on the microcapillay target parallel to the capillary axis, part of the hollow atoms formed in the capillary can pass through it before hitting the capillary wall and can be extracted in vacuum. The microcapillary used in our experiments is \sim 1 mm² in size with a thickness of \sim µm and a multitude of straight holes of ~100 nm in diameter.

 We have investigated the production and relaxation mechanism of the hollow atom employing the following techniques for free hollow atoms and related excited-ions [4]:

- 1: visible light measurements, which give information on Rydberg states produced with the first stage of the charge transfer from the capillary surface;
- 2: x-ray measurements in coincidence with final charge states, which reveal the lifetime of hollow atoms for different number of electrons transferred;
- 3: high-resolution x-ray measurements, which allow one to identify the core electron configurations of hollow atoms;
- 4: Auger electron measurements, which give us complement information to the x-ray measurements;
- 5: charge state and scattering angle measurements, which are expected to reflect the distance between the ion and the surface at the moment of the charge transfer.

I will review our research briefly and then explain the final stage of the decay processes of hollow atoms based on our recent results of x-ray and Auger electron measurements.

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Autoionization in O2 by High Harmonics

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Using the process of high harmonic generation (HHG) from few cycle laser pulses in the visible and near IR region, it has been possible to produce coherent XUV pulses in the attosecond time domain. The utility of these attosecond pulses in probing inner-shell dynamics of atoms has already been demonstrated [1, 2]. However, no such experiments have been undertaken in molecules. We have been conducting experiments to probe electron dynamics in the autoionization of O_2 using the XUV pulses. Our measurements using the high harmonic generated XUV in conjunction with a magnetic bottle time-of-flight electron spectrometer show vibrational intensity distribution in the O_2^+ $X^2\Pi_g$ state as expected from the autoionization process. Pump – probe measurements using XUV as the pump and IR as the probe have been carried out to study the dynamics of the autoionizing state. The results indicate definite changes in the autoionization process as a function of the probe delay.

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D3/S14A/T11A

Rotational Energy Distributions of Benzene Liberated from Aqueous Liquid Microjets: *a Comparison between Evaporation and Infrared Desorption*

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We have measured the rotational energy distribution of benzene molecules both evaporated and desorbed by an IR laser from a liquid microjet. [1] Analysis of the 6^1 vibronic band of benzene has shown that the benzene molecules evaporating from the liquid microjet surface have a rotational temperature of 157±7 K. In contrast, the rotational temperature of benzene molecules desorbed from the liquid microjet by a 1.9 μm laser pulse is 82±5 K. However, in both cases careful inspection of the spectral profiles shows that the experimental rotational distributions are non-Boltzmann, displaying an under population of high rotational states and a relative over population of the low rotational states. Vibrational temperatures are also determined that differ significantly from those of rotation. We will present our latest results of this study, highlighting differences between energy liberated in rotational and vibrational modes of the solute under each set of experimental conditions. The non-equilibrium evaporation and desorption spectral profiles are consistent with a model that involves transfer of internal energy into translation upon liberation from the condensed phase.[2]

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D3/S14A/T12A

Charge conductivity in Peptides: Dynamic simulations of a Bifunctional model supporting Experimental Data

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Our previous finding and the given mechanism of charge and electron transfer in polypeptides are here integrated in a bifunctional model involving electronic charge transfer coupled special internal rotations. Present molecular dynamics simulations that describe these motions in the chain result in the mean first passage times for the hopping process of an individual step. This "rest and fire" mechanism is formulated in detail-ie., individual amino acids are weakly coupled and must first undergo alignment to reach the special strong coupling. This bifunctional model contains the essential features demanded by our prior experiments. The molecular dynamics results yield a mean first passage time distribution peaked at about 140fs, in close agreement with our direct femtosecond measurements. In logic gate language this is a strongly conduction ON state resulting from small firing energies, the system otherwise being a quiescent OFF state. The observed time scale of about 200 fs provides confirmation of our simulations of transport, a model of extreme transduction efficiency. It explains the high efficiency of charge transport observed in polypeptides. We contend that the moderate speed of weak coupling is required in our model by the bifunctionlity of peptides. This bifunctional mechanism agrees with our data and contains valuable features for a general model of long-range conductivity, final reactivity, and binding at a long distance.

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Interaction of Low Energy Electrons with Biological Molecules

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It was generally believed that low energy electrons (LEE) i.e. electrons below 12eV, would play little role in radiation induced damage to biological molecules. However, Sanche [1] and coworkers showed that damage to DNA could occur at energies below the ionization energy. This was attributed to the interaction of LEE through the Negative ion resonant states. A recent review [2] on damage to bio-molecules, all the new studies that have been done on several molecules, are available. However, there are very few experiments on proteins. As part of our new program to study the interaction of LEE with biological molecules, we have studied DNA - plasmid pBR322 and protein - Translin.

 DNA (plasmid pBR322) and protein (Translin) were prepared using standard techniques and a thin layer was deposited on a tantalum surface and allowed to dry. The samples were then loaded to the UHV vacuum chamber and exposed to LEE. Electrons were generated using thermionic emission, accelerated to the required energy and guided to the target using a weak magnetic field. The exposed samples were recovered and analyzed using agarose gel electrophoresis technique for the DNA and SDS Polyacrylamide Gel Electrophoresis (SDS-PAGE) for the protein.

Our results indicate that Single Strand Break (SSB) occurs in plasmid pBR322 at 10eV, while no measurable damage takes place to the translin at the same energy. Changes in the conformation of DNA induced by counter cations to DNA appears to affect the damage caused by LEE.

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Modifying the Aggregation Behavior of Poly (N-isopropylacrylamide) Thermoreversible Gel by a Bile Salt

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Thermoreversible hydrogels which exhibit an LCST-type (lower critical solution temperature) discontinuous first order volume transition phenomenon are receiving increasing attention because of potential biomedical applications. The most widely studied thermoreversible gel, poly(Nisopropylacrylamide) (PNIPAM), is especially interesting as it exhibits the LCST at around 32 °C in pure water, which is close to the body temperature of homeothermic animals [1]. The importance of tailoring the gel-melting temperatures to suit a particular need has prompted much research interest recently [2]. One possible method of altering the CST of these gels is addition of surfactants. Because of the biological origin of bile salts, their inclusion in PNIPAM could lead to better biocompatibility when the materials are used for biomedical applications. This prompted us to study such systems.

Bile salts are surfactant molecules possessing 'facial polarity'. The gelling behavior of PINIPAM was studied at various concentrations: PINIPAM concentrations in the range of 1% to 12% (w/v) and NaC concentrations varied from 0 to 20 mM. The primary tool for the study was fluorescence spectroscopy using anilinonaphthalene sulphonate (ANS) as a fluorescent molecular probe. The choice of ANS as a probe was because it is an anionic fluorescent probe and is expected to have negligible interaction with the anionic bile salt – thus preferentially sensing the nanoenvironment of PINIPAM aggregates. In presence of PINIPAM and at the phase transition temperature, there was an increase in fluorescence intensity of ANS due to the decrease of nonradiative decay and a blue shift due to the increase in hydrophobic environment of the probe, clearly indicating the increased hydrophobicity of the aggregated gel environment. It was found that the presence of NaC the CST shifts to lower temperatures. This is an unusual observation since conventional surfactants are known to shift the CST to higher values, due to mutual solubilization. A study of fluorescence spectroscopic parameters like fluorescence anisotropy, spectral shift and intensity suggest that an NaC-induced aggregation could be responsible for this unusual observation.

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D3/S14B/T11B **Generation of Atomic Entangled and Cluster States in a Cavity**

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Although two-photon entangled states can commonly be produced using spontaneous parametric downconversion, there seems no easy way of generating entangled states of massive particles. In this talk we present two cavity qed schemes to generate entanglement in atoms trapped in cavities.

The first scheme[1] utilizes interaction between two three-level atoms in a cavity and the cavity field to generate maximally entangled states of the two atoms. The scheme is probabilistic, but, with the use of an automatic feedback, its success probability can be made to approach unity.

The second scheme[2] allows one to generate cluster states[3] among atoms each trapped in a different cavity. The basic building block for the scheme is a controlled phase gate that can be constructed based on the cavity input-output process. This gate, acting on an atom trapped in a cavity and a photon reflected from the cavity, can be repeatedly used to generate a cluster state among atoms that may be separated far in space.

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GENERATION AND CHARACTERIZATION OF PAIRS OF FLYING ELECTRONS WITH TUNABLE DEGREE OF ENTANGLEMENT

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Although, quantum information (QI) [1] has many unusual properties which are quite different from those of classical information; however, the most profound difference between these two is that the former, unlike the later, is encoded in non-local correlation between the different parts of a physical system. This non-local correlation has come to be known [1] as entanglement (E) . Two or more particles, possessing such non-local correlation, are known to be in an entangled state [1]. Many recent developments have shown [1] that E can be put to several important technological applications in QI. For these reasons, E is now considered to be a physical resource $[2]$, something that we must have available if we want to take advantages of newly developed $[1]$ quantum protocols.

Implementation of many (eg, quantum communication over remote distances [3], quantum teleporation and quantum cryptography [4], etc) of these protocols, however, requires bipartite, E states of 'flying qubits' [5]. (A qubit is a two level quantum system.) Parametric down conversion [6] in quantum optics has so far been the most successful and widely used methods for producing pairs of entangled photons. Photonic qubits can propagate long distances in fibers without absorption. Another qubit which can travel long distances in free space without absorption is electron. Furthermore, an electron can interact and be detected, unlike photons, without being destroved.

There are more than one simple processes in atomic and molecular physics which can produce two (or more) free electrons. Unlike in several other cases, E between these electrons needs not be imposed from outside, but arises naturally due to the interactions experienced by them inside an atom or molecule [7] and, hence, is least prone to harmful effects like decoherence and dissipation which take place due to the coupling of the E with the environment. Moreover, spin-entanglement generated between two electrons in these simple processes is tunable [7] and can be characterized, in certain cases [7a], without using any protocols $(eg, \underline{E}$ witness [8]) hitherto proposed in QI.

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Dynamics of certain Ion-Molecule Processes

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With the advent of high speed electronic computers with large memory and the developments in electronic structure theory, it has become possible to compute accurate ab initio potential energy surfaces and carry out time-dependent and time-independent quantum dynamical calculations for triatomic systems. It will be shown how an ab initio time-dependent quantum mechanical (TDQM) study of exchange in $(H(D), H_2(D_2))$ collisions could account for much of the experimentally observed results and could help in discriminating between two sets of experimental results [1]. Similarly, ab initio TDQM study of dissociation of CO_2^{2+} in its ground electronic state, following electron impact double ionization of $CO₂$ could account for the major portion of the experimentally observed kinetic energy release spectrum [2].

Low-Light-Level Cross-Phase Modulation Based on Stored Light Pulses

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The cross-phase modulation (XPM) refers to the phase of a photon pulse (probe pulse) modulated by another (signal pulse). If large Kerr nonlinearity is attainable in the XPM, the phase shift of the probe pulse will detect the photon number of the signal pulse in the quantum nondemolition measurement. Suppose that phase shifts of the order of π with single photons can be achieved in the XPM. One can utilize the signal and probe pulses as the control and target qubits to realize the controlled phase gate which is the basic and essential element in the quantum computation. It is also possible to generate entangled photon pairs from the outcomes of the XPM for quantum cryptograph and quantum teleportation.

We propose and experimentally demonstrate a low-light-level XPM scheme based on the light-storage technique in laser-cooled 87 Rb atoms [1]. A weak probe pulse and a coupling field form the three-level Λ-type configuration that gives rise to the effect of electromagnetically induced transparency. The probe pulse was stored in a sample by adiabatically switching off the coupling field [2]. During the storage, the ground-state coherence or the atomic spin excitation inherited the information of phase and amplitude of the probe pulse. A signal pulse applied to affect the phase evolution of the atomic spin excitation. This pulse drove the cycling transition. After the signal pulse was completed, we coherently converted the atomic spin excitation back to the light by adiabatically switching on the coupling field. The probe pulse acquired a phase shift which was induced by the signal pulse. Our XPM scheme is depicted in Fig. 1.

With the light-storage XPM, we obtained a phase shift of 44 \degree of the probe pulse by employing a 2-μs square signal pulse of the Rabi frequency of 0.32Γ. To achieve such phase shift, the energy transmission of the probe pulse due to the presence of the signal pulse is about 65% or the energy loss is less than e^{-1} . The phase shift and the energy loss of a probe pulse induced by a signal pulse are neither influenced by the coupling intensity nor by the atomic optical density. This scheme enhances the flexibility of the experiment and makes possible conditional phase shifts of the order of π with single photons.

Fig. 1 Scheme of the light-storage XPM.

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Symmetries in Atomic Collision Processes

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General kinematic analyses of various atomic collision processes by using the density-matrix and helicity formulations are reviewed. The rotation, parity, and time-reversal symmetries of the colliding systems are considered. In addition to polarization and angular correlations in each collision process, correspondences among different collision processes are also studied. As an example, the time-reversal symmetry between Photoionization and electron-capture fluorescence are demonstrated explicitly, and there is a one-to-one correspondence between angular correlation functions for the two processes. The symmetry study in atomic collisions provides a great deal of valuable information about the colliding systems and enhances our knowledge on the collision dynamics.

Laser Modified Collisions and Effect of Phase Control

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Laser aided collision processes have significant importance in the basic insight into atomic, molecular and solid state structures and they also find practical applications in a large number of different fields of research, such as plasma physics, astrophysics, astronomy, thermonuclear fusion, material science, holography, fiber optics, telecommunications and so on.

 In particular, laser assisted electron – ion collisions cross-sections are highly needed in the study of laser – induced plasma. Further, the influence of the radiation fields on collision processes and interactions is quite universal since all scattering processes take place in radiation fields even if it is only the thermal background. By virtue of the recent advances in laser physics and the availability of tunable lasers, it has now become possible to perform experiments on different collision processes in presence of external laser fields. Recently the effect of the coherent phase control on collision processes, i.e., the enhancement and reduction of the collision cross sections in presence of a two color laser field by controlling the phase difference between the two color fields has recently become a subject of particular interest both experimentally and theoretically.

 The talk will address some laser-assisted electron –ion excitation, ionization processes as well as some charge transfer processes involving anti-matters. The effect of the phase difference between the two color fields having frequencies, fundamental and its higher harmonics will also be focused.

$D4/S16/T2$ **Similarities and Differences between Electron and Positron Scatterings from Molecules**

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By comparing various processes resulting from positron and electron scattering from atoms and molecules, one can observe quite different features in cross sections in their behavior and characteristics in dynamics. However, one can also realize quite a similar behavior in some of inelastic cross sections as well. For vibrational excitation, for example, depending upon the vibrational mode, excitation cross sections for one mode for positron and electron are known to be nearly identical for a wide range of the energy, while for another, they differ by more than a few orders of magnitude. For other inelastic processes such as ionization and electronic excitation, differences and similarities in their cross sections have been also experimentally seen, although detailed theoretical interpretation still lacks. The interaction scheme between positron and electron with molecules are known to be quite different, that is, taking that the interaction is approximately described as a sum of static, exchange and correlation-polarization, then, the static interaction for positron is repulsive, but for electron, it is attractive, the correlation-polarization for both positron and electron is attractive, and the exchange interaction is believed to be attractive for electron but misses for positron. Hence, by adding all three terms, the total interaction for electron is strongly attractive, while for positron, it is very weak interaction. This difference for the interaction makes quite different scattering dynamics for each case. However, how these interaction schemes affect scattering dynamics and hence cross sections are not known at all. Furthermore, another interesting aspect of positron and electron scattering is their attachment. For positron and electron attachments, they should occupy different molecular spatial regions since positron is much attracted by negatively charged region of the molecule, while it may be, in some degree, opposite for electron. Consequently, the fragmentation dynamics for positron and electron should be different and resulting fragmented species thus produced are expected to be grossly different. We have carried out systematic investigations for inelastic processes, and, in particular, for fragmentation processes and the production of fragmented species between positron and electron impacts. This knowledge could be useful for applications particularly for plasma processing industries since some are considering to employ positron beams for the processing as well as diagnostic at the same site.

D4/S17/T3 Low-Energy Electron Collisions with Rare Gases and Biologically Relevant Molecules

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Low energy electron collision processes with atoms and molecules are fundamental to a complete understanding of the macroscopic phenomena ranging from low temperature plasmas to radiation damage of biomolecules.

The interaction of low energy electrons with rare gases has been one of the subjects studied in our group recently. In a paper by Cho *et al.* [1] absolute measurements of the differential cross section for elastic scattering from krypton and xenon at energies from 10 eV to 100 eV, and for scattering angles from 10[°] to 180[°], have been reported. A version of the magnetic-angle-changing device developed by Read and Channing has been used, in conjunction with a relative flow technique to measure the DCS at scattering angles up to 180°, where cross-section measurements are typically inaccessible due to the mechanical constraints of the electron spectrometer. The experimental results were compared with the theoretical studies at Australian National University group, and were in best agreement in the backward direction with the theoretical calculations which included absorption effects via a complex optical potential.

In the mean time, the past ten years have seen increasing interest in the interactions of low energy electrons with biomolecules. In particular, the observation that electrons of less than 10 eV can induce both single and double strand breaks in lyophilized plasmid DNA [2] has stimulated numerous experimental and theoretical studies of low energy electron interactions with DNA and related biomolecules.

To understand strand breaks, information must be obtained on low energy electron interactions with the sub-units of the DNA back-bone i.e., the phosphate group and the sugar ring. To this end, we studied, in collaboration with the University of Sherbrooke group, cross sections for electron capture processes occurring in condensed tetrahydrofuran (THF) for incident electron energies in the range 0 to 9 eV. Since THF may model of the furyl ring found in deoxyribose, these measurements may indicate the likely role of the furyl ring in either initiating or modulating strandbreak damage following exposure of DNA to ionizing radiation.

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Trapped Electrons in a novel Electron Recycling Spectrometer

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A revolutionary new type of electron spectrometer has been under development over the last 8 years. The spectrometer is a passive electron storage system conceived as a gas phase electron spectrometer with the aim of performing ultra-high energy resolution $(\sim 1 \text{ meV})$, low energy $(\sim 100 \text{ m})$ eV), electron scattering studies in atoms and molecules. It was specifically designed to avoid the factors limiting the energy resolution capabilities of conventional electron spectrometers and the more recent laser-light [1] and synchrotron-light based photoelectron sources [2].

The spectrometer is "desktop" sized and consists of two pairs of concentric hemispheres connected by two cylindrical lens stacks as shown schematically in figure 1. It is entirely electrostatic, with magnetic fields being excluded. A prototype has been constructed and is operating at the University of Windsor: current work consists of optimizing the performance of the prototype and comparing this performance with the theoretical models of the system.

Figure 1. The electron recycling spectrometer

 As design and development has progressed it has become clear that the device is likely to be useful for all types of charged particles e.g. positrons and ions, and offers the potential for not just ultra-high energy resolution beam production but also for storage of charged particles in which the conventional source strength is weak.

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Combustion and Other Studies with Tunable VUV Single-photon Ionization Technique **Fei Qi**

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I will introduce the tunable VUV single-photon ionization (TVUV SPI) technique and its applications in combustion and others studies. Molecular-beam mass spectrometry (MBMS) has been used to study combustion for over 40 years. Traditional mass spectrometers with electron impact ionization are limited in their utility by fragmentation, limited electron energy resolution, and low ionization cross-section at chemically interesting ionization thresholds (6-14 eV). Synchrotron radiation VUV single-photon ionization is a kind of "soft" process, which can overcome the difficulties that EI meets. Isomers can be distinguished by measurement of photoionization efficiency spectra. It is a *universal* and *selective* method for detecting both stable and radical species in flames. And it is potentially a powerful tool for the study of formation mechanisms of PAHs and soot in combustion¹⁻⁷

Recently we have developed this technique in various new applications successfully, i.e., plasma diagnostics, mechanism of material growth, catalysis reaction, oil analysis, cigarette smoke, drug analysis and discovery, and even biomolecules.

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D4/S18/T6 **Nonlinear optical processes in confined molecular clusters**

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Strong quantum confinement is known to bring about remarkable modifications in the electronic properties of molecular clusters making them very different from the corresponding bulk materials. One of the interesting features of such clusters is the observation of novel optical linear as well as nonlinear optical processes in them. The optical properties become size-dependent and the nonlinearity is often enhanced. Such phenomena have been observed in nanoclusters of several optical materials including metallic, semiconducting as well as insulating materials. This talk surveys the interesting optical properties of confined nanoclusters and focuses on nonlinear optical processes in strongly confined semiconductor nanolcusters with specific examples from recent results obtained in our laboratory.

Nanoclusters of CdS and PbS are obtained in the size range of a few nanometers by chemical routes of synthesis. These are prepared in a variety of physical forms such as free standing clusters, suspensions in organic solvents or embedded polymer films and their optical properties are investigated. The clusters of variable sizes can be prepared by a proper choice of the synthesis parameters thereby making it possible to study the size dependence of the optical properties systematically. Techniques of linear optical spectroscopy such as optical absorption, fluorescence and photoacoustic spectroscopy are used to probe the bandgap modification effects due to strong quantum confinement. The optical nonlinearity is studied by the standard techniques of optical phase conjugation and z scan which probe the effects arising from third order susceptibility.

Linear and nonlinear optical properties show a systematic dependence of the effective bandgap on the nanocluster size and features due to excitonic confinement are clearly visible even at room temperature. Evidence is also obtained for the occurrence of nonlinear absorption arising from multiphoton processes, free carrier absorption and saturable absorption mechanisms.

Short Electron Bunch generation by Laser-Accelerator for Ultra-short X-ray Sources

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Laser wake field accelerator (LWFA) can generated very short electron bunches. Using these short electron bunched femtosecond x-ray pulses can be generated. Femtosecond x-rays can be used to investigate the fast dynamics of material by pump probe type experiment. X-ray pulse can be generated by Thomson scattering process. If the electron beam duration and laser pulse duration is in femtosecond time scale, femtosecond x-ray pulse can be generated. For this purpose, short electron bunch is needed. But the conventional electron beam source, such as photocathode R.F. gun, the electron bunch length is in the order of ps time scale. This bunch length is not short enough to generate femtosecond x-rays. To generate short bunch length electron beam, laser wake field accelerator is a good candidate. Due to short acceleration region, electron bunch length can be as short as 10 fs. To generate short bunch length and monoenergetic electron beam, self modulated laser wake field acceleration and laser wake field acceleration with electron density gradients were studied. Using the 2 TW (energy 1.4 J, pulse duration 700 fs) Nd/Glass;Ti:sapphier hybrid laser system, multi-MeV quasi-monoenergetic electron beams were generated in the self-modulated laser wake field accelerator(SM-LWFA) regime. In the SM-LWFA regime, the electron beam has a very wide energy spectrum (energy spread $E/\Delta E \sim 100\%$). To make quasi-monoenergetic electron beams, a small pinhole was used as an energy collimator. Due to low divergence of high energy electron beam, we could get quasi-monoenergetic electron beams. Now a new experiment for *controllable* generation of quasi-monoenergetic electron beams is under way, where some background plasma electrons can be locally injected into the laser wake wave and a small energy spread is expected. Electrons at the sharp density gradient can be trapped in wake field. Due to this electron trapping process, we can generate high energy monoenergetic electron beam[1]. In this presentation, overview of x-ray generation by Thomson scattering and monoenergetic electron beam generation by LWFA will be given.

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(e, 2e) Triple Differential Cross section of Mg in Coplanar Symmetric Geometry

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Abstract:

Spin averaged static exchange potential and modified semiclassical exchange potential have been used in the Distorted Wave Born Approximation (DWBA) to calculate the triple differential cross

section of Mg $(3s^2)$ in the coplanar symmetric geometry. The calculations have been carried out at impact energies ranging from $(R=)$ 1.78 to 8.84 times above the first ionization potential for Mg. The effect of post collision interactions (PCI) has been included by making use of the Gamow factor introduced by Whelan et al. [Phys. Rev. A **50**, 4394 (1994)]. Present results have been compared with recent experiments of Murray [Phys.

Figure 1: Normalized triple differential cross section at the impact energy of 13.65 eV.

Rev. A **72**, 062711 (2005)] and found to be in excellent agreement with the same except for the lowest impact energy of 13.6 eV. These discrepancies between experiment and the theory with and without PCI at low impact energies are attributed to the nature of Gamova factor. Calculations with other forms of PCI are underway and will be discussed at the time of conference.

Experimental signature on selective high-lying Rydberg states: A possible origin of Radio Recombination lines in interstellar spaces

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Intensity plot of any transitions with time shows exponential decrease and the trend somewhat varies depending upon the complicated cascades and line-blending present in the experiment. However, appearance of a cusp-shaped structure, as normally observed in the forward scattered electron spectra in the ion-solid collisions, in the middle of a decay is beyond the current knowledge of physics. In the series of the experiments using the reliable experimental set up [1] we consistently observe such a structure. For example, the data of an experiment with Fe beam is shown in Figure 1. Origin of the cusp-shaped structure is found to be successive cascading from the specific high-lying Rydberg levels possibly populating from the interaction of electron in the continuum with the projectile ion and the free electron residing at the exit surface of the target foil. Experimental data have been analyzed in the light of a cascade model derived on the basis of ladder-like deexcitation chain and the Bethe and Salpeter hypothesis on the transition probabilities. Present observations may find important implications on the origin of radio recombination lines observed from intersteller spaces.

Figure 1: L: X-ray spectrum of 164 MeV Fe beam on C foil at 946 ps delay. R: X-ray photo peak intensity plot as a function of delay times: (a) the 6.65 keV peak intensity fitted with two-exponential function and (b) the 6.95 keV peak intensity fitted with the equation having two exponential and one Lorentzian terms. The Lorentzian term represents the cusp structure.

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Plenary Talk

Spin effects in electron scattering from atoms and surfaces.

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This paper concerns deductions about spin-dependent phenomena of free atoms and surfaces using incident photons or electrons in scattering experiments. Information on atomic structure and dynamics is deduced from conservation of momenta with measurement of polarization and detection of the number of emerging electrons, photons and ions. Maximum information can be obtained when the incident particles are polarized and the targets are state-selected both before and after scattering. Scattering amplitudes and their relative phases, as well as the parameters describing the electron charge cloud of the atomic target, as determined from recent experiments, have enabled significant advances of understanding of collision mechanisms and in quantum scattering theories.

For incident polarized electrons, electron exchange, through the Pauli principle and the relative orientation of the electron spins, affects the scattering probabilities. Also the spinorbit interaction for the target electrons may become large compared with the Coulomb electron-electron interactions. The nature of the spin effects is discussed for some examples to indicate recent advances, mostly from the work of others. The significant contributions to this field of the technology of time coincidence and spin production and detection are discussed.

The following four examples indicate the direction of the talk.

Electron correlations, particularly in the form of interchannel coupling, attracts much interest, particularly in the metallic atoms of Ca and Mg and Zn, and as shown recently in the spin polarization of photoelectrons, the angular distributions and cross sections for the Ne valence subshells [1].

Atomic fluorescence polarimetry for Xe 4d-1 5/26p ($J = 1$) photo-excitation indicates the Fano-like resonant behaviour of vector correlation parameters (the alignment and the orientation) of the photo-ion across an auto-ionizing resonance with universal values of the width and the energy shift [2].

In electron impact excitation processes, the polarization of the decay photons depends on the different LS-mixing properties of the intermediate coupled states; the triplet components may make exchange and spin-orbit interaction important while for states with a large singlet component the spin-orbit interaction may be dominant [3].

Correlation spectroscopy of two electrons, detected in time coincidence with momentum resolution after scattering from a surface, displays energy and angular paircorrelations from which electron-electron interactions are deduced. Electron exchange and the anisotropy of spin-orbit effects are clearly seen using polarized incident electrons for W(110), Co and Fe [4] surfaces. Here, the spin-orbit interaction couples the spin magnetic moment of a valence electron to the crystalline lattice and in ferromagnets this coupling often defines a direction for the macroscopic magnetic moment.

In summary, an overall view will be presented of aspects of spin-dependent phenomena of free atoms and surfaces.

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Program *for* Poster Presentations

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Linear Time of Flight Photoelectron Spectrometer for photodetachment studies

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Negative ions are of great interest as they aid in the understanding of electron-atom, electronmolecule and electron-electron interactions. Photo detachment spectroscopy has been prolific in throwing light on these aspects of negative ions. Kinetic energy and Angular distributions of the photoelectrons are the widely measured quantities in understanding the nature of negative ions. We have built a photodetachment experiment towards this. The experiment consists of a SNICS ion source, a wein filter for mass analysis and a linear time of flight photoelectron spectrometer. The setup has been optimized for reasonable ion beam current and mass resolution as well as optimum energy resolution for the photoelectrons and their angular distribution. We shall present the details of the experiment and the test results during the meeting.

S1/P02 Dynamics of E1 and E2 Photoionization Parameters of Atomic krypton

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 Atomic photoabsorption process is quite well described using the dipole approximation (E1) at low photon energies, up to ~5keV above the ionization threshold. With present advanced technology it is possible to observe higher order transitions even at low photon energies. In recent years studies have been carried out, both experimental and theoretical, to understand the dynamics of quadrupole (E2) transitions and the effects of electron correlations on photoionization parameters for some atoms, mainly the rare gas atoms [1, 2, 3]. In the present work we report E1 and E2 photoionization parameters for different subshells of atomic krypton using 'Relativistic Random Phase Approximation' (RRPA). We present in this work the first study of the Cooper minimum in E2 transition matrix elements for photoelectrons from n=4 and n=3 subshells of atomic krypton. The E2 photoionization parameters from 4p subshells go through two Cooper minima, as was found in the case of xenon 5p photoionization [4]. Correlation effects on the dynamics of the matrix elements and angular distribution of the photoelectrons are analyzed.

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S1/P03 Evaporative Cooling of Atoms to Quantum Degeneracy in an Optical Dipole Trap

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We discuss the process of forced evaporative cooling of cold rubidium $\binom{87}{8}$ h) atoms in an Optical Dipole Trap [1] to reach quantum degeneracy [2]. The atoms are first trapped and cooled in a magneto-optical trap (MOT) loaded from a continuous beam [3]. More than 10^{10} atoms are trapped in the MOT and then transferred to a Quasi-Electrostatic Trap (QUEST) formed by tightly focused $CO₂$ laser ($\lambda = 10.8 \mu m$) beams intersecting at the focus in orthogonal configuration. Before loading the atoms into the dipole trap, the phase-space density of the atomic ensemble was increased by making a temporal dark MOT by attenuating the repumper light.

 Since the atoms are trapped in the dipole trap irrespective of their magnetic sub-state, the condensate produced after evaporative cooling in the dipole trap is a spinor-condensate i.e. the condensate has all three spin components in $F = 1$ ground state. In a MOT the phase-space density of the atomic ensemble is six orders of magnitude less than what is required to achieve quantum degeneracy. After transferring atoms into the dipole trap efficiently, phase-space density increases by a factor of $10³$. Further increase in phase-space density to quantum degeneracy is achieved by forced evaporative cooling of atoms in the dipole trap.

 The evaporative cooling process involves ramping down the trapping laser intensity over several seconds so as to reduce the trap depth gradually. The temperature of the cold atomic cloud was measured by time-of-flight (TOF) technique. The spatial distribution of the atoms is measured using absorption imaging. We report results from comparative studies of cooling to quantum degeneracy in monotonic and temporally modulated evaporation schemes.

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Coplanar Doubly Symmetric (e, 2e) Process on Alkali Atoms

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 Recent experimental studies have focused on the (e, 2e) process on alkali and alkaline earth atoms [1, 2]. In the light of these experiments we have preformed theoretical calculations for triple differential cross section (TDCS) in doubly symmetric geometry and described the (e, 2e) process using distorted-wave Born approximation theory. Post collision interaction (PCI) is included by using effective charge model. The angular behaviour of TDCS and its variation with energy are compared with the experiment. We recently reported our calculations for the alkaline earth atoms viz. Be, Mg and Ca [3, 4]. In the present work we extend our calculation for the alkali atoms viz. sodium, potassium and rubidium. The details will be presented at the conference.

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Dissociation of Methanol and Acetylene by slow Highly Charged Ion Collision

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 Studies of the dynamics of formation and subsequent dissociation of multiply charged molecules produced by collisions of neutral molecules with highly charged atomic ions have been an active field of research during the last decade [1]. Here we report the results of dissociation of multiply charged methanol and acetylene molecules with 1.2 MeV Ar^{8+} projectiles. The experiment has been carried out in the Low Energy Ion Beam Facility of Inter-University Accelerator Centre, New Delhi, India. Ar^{8+} ions produced from the ECR ion source interacts with the CH₃OH and C₂H₂ molecules effusing from a needle at the centre of a differentially pumped chamber. The dissociated fragments are extracted from the interaction zone in the time-of-flight mass spectrometer (TOFMS) applying a uniform electric field perpendicular to both ion beam and gasjet. The dissociation products are finally detected by a position-sensitive MCP detector. Ejected electrons are extracted in the opposite direction to TOFMS and detected by a channeltron which gives the trigger for multihit coincidence data acquisition [2].

 From the TOF spectrum, we observed a wide range of dissociation products starting from undissociated molecular ions, fragments losing an hydrogen atom due to breakage of C-H and/or O-H bonds, to complete rupture of C-C and C-O skeletons. From the coincidence map of the fragments, we could separate out the different dissociation channels between C^{q+} (q=1-3) and O^{p+} (p=1-3) fragments as well as H⁺ formation pathways in coincidence with carbon and oxygen ions produced. Even complete dissociation events such as CH_3OH^{2+} CH_3^+ + OH^+ and $C_2H_2^{2+}$ CH^+ + CH^+ were observed along with incomplete ones where the missing fragments are either undetected neutrals or detected as a third or fourth hit in the MCP. The most striking feature in the coincidence map of CH₃OH breakup is the formation of H^+ , H_2^+ and H_3^+ due to cleavage of the C-H bonds. The shape of the islands gives further information about the fragmentation dynamics of complete and incomplete processes [3]. On careful study of the slopes of the islands we can deduce whether the fragmentation process is concerted or sequential. The kinetic energy release (KER) of the various dissociation pathways are calculated from the time spread of its coincidence peak. These measurements and their analysis revealing interesting facets about dissociation of these species will be presented.

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S1/P06 Large scale *ab-initio* Coupled Cluster calculations on allowed and Forbidden Transitions and Hyperfine constants of Doubly Ionized Thallium

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The possibility of observing parity violations in atoms is of great importance in present day research due to its table-top probing ability of the standard model of particle physics. Observation of electric dipole moments of atoms is another probe towards the same goal. Both of the physical estimations need precise inputs from atomic structure calculations. Tl III seems to be an ideal candidate for both cases [1]. The measured hyperfine structure [2] may serve as an important probe to determine different properties of nucleus, but only if the electronic structure is precisely described in atomic models. The observed abundances of ionized thallium in the evolved stars are important inputs for the characterization of different astronomical bodies [3]. The precise estimation of these abundances depends on the accuracy of transition probability calculations, especially for forbidden transitions where experimental measurements are difficult.

In this work, we report sophisticated calculations of allowed and forbidden transitions among ground to excited, excited to excited states of Tl III using coupled cluster method with single and double excitations (CCSD). We also present the estimation of hyperfine constant of different low lying states of this ion. Comparison has been made with different theoretical and experimental results, wherever available [4]. We obtain reasonably good agreement with them for most of the transitions. An attempt has been made to explain the discrepancies where they occur. To our knowledge many of these transitions are estimated for first time in literatures. Strong core-core and core-valence correlations are highlighted.

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Electron impact ionization of water molecules in liquid and ice phases

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Electron scattering processes in a solid like ice are important since icy matter is an important constituent in the astrophysical objects like comets, some of the planetary satellites, polar caps of Mars and even molecular clouds. Electron Collisions with free as well as condensed water molecules play an important role due to their abundance in these environments. A big gamut of phenomena takes place when these objects are exposed to charged particle flux (solar wind). The incident electrons ionize the H₂O (ice) and the H₂O (free) along with other molecular species, and their dissociation products, both neutral and charged, give rise to different channels of chemistry that eventually govern various properties οf the environment. We have addressed here the problem of electron scattering and ionization of H₂O in liquid and in ice about which scarce data exists [1] at present. In such problems where experiments are reasonably difficult, a theoretical estimate provides very useful inputs for bulk modeling.

Our present aim is to determine basically the total inelastic cross section, Q_{inel} , and hence total ionization cross section Q_{ion} together with a contribution of total electronic excitation TCS Q_{exc} , in a simple quantum mechanical formalism. We proceed by the complex (optical) potential method and invoke semi-empirical

Figure 1: Various total cross sections of electron incident on H₂O (ice)

arguments to deduce the total and the dissociative ionization cross sections $[2, 3]$. Bulk properties of the liquid or ice medium are included suitably in our scattering calculations. Results on cross sections and mean free paths, along with comparisons with other data as available [4], will be discussed in the conference. Figure 1 shows our sample results.

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Numerical Simulation of BEC Manipulation using Laser Pulses

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 BEC interferometers are expected to serve well for precision measurements. Splitting and merging of BEC in interferometers can be realized either using laser field or magnetic field or both. It is observed that manipulation of BEC by changing magnetic fields in atom chip turns out to be violent, leading to vortex creation [1]. Even in the experiments of laser manipulations, though less violent, dephasing is known to cause poor contrast and "thermalization due to scattering of atoms adds to degradation of fringes [2,3]. A rigorous theoritical and numerical study will be useful for understanding the underlying physics of such phenomena. There already exist theoretical attempts to this end, for example [4]. Our understanding of the physics of colliding BECs needs nevertheless to completed. Even a mean-field theory treatment of the problem over a wide range of experimental parameters will be useful before a rigorous treatment of the quantum fluctuations is expected.

 We simulate laser manipulation of BEC numerically using a two state model, starting with BEC in a two dimensional trap and splitting it into two by induced Raman transition and transporting and merging in the meanfield regime. Using experimental parameters even in the mean-field regime may help us gain solid understanding of the phenomena related to laser induced manipulation of BEC.

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S1/P09

Multiple Ionization and Fragmentation of C60 in Collisions with fast

highly Charged Si Ions and Giant Plasmon Excitation

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The fast highly charged ions has been proved to be an important probe to investigate the structural and collision aspects of molecules and clusters and in particular of C_{60} [1,2,3,4]. In particular it would be of interest to explore the effect of collective excitation such as giant dipole plasmon resonance (GDPR) on the multiple ionization [5]. We present results on the projectile charge state (q_p) dependence of various products, such as multiple ionization, evaporation and fragmentation products of C_{60} in collisions with fast moving heavy ion projectiles. The C_{60} molecules from a vapour source were bombarded with 2.33 MeV/u Si^{q+} (q=6-14) projectiles, obtained from the BARC-TIFR Pelletron accelerator facility at TIFR, Mumbai. The reaction products were detected using a Wiley- Mclaren type Time of Flight mass spectrometer combined with MCP+delay line detector. The charge state dependence of the multiple ionization yields of C_{60}^{r+} (r=1-4) were compared with GDPR^[1] model as well as the SED-LPA^[2] model. The relative yields of single and double ionization are in excellent agreement with the GDPR model showing an almost linear dependence with q_p , where as triple and quadruple ionization yields show better agreement with SED-LPA (statistical energy deposition-local plasma approximation) calculations with feeble dependence on 'qp'. This difference can be understood in terms of underlying assumptions of the two models. Indeed the results are in complete contrast with those for gaseous targets like Kr. which may indicate the different mechanisms of ionization processes for a gas-atom and C_{60} . A quantitative analysis of C_2 evaporated products C_{60-2m} ^{r+} (m=1-7) suggests that relaxation by evaporating stable C_2 fragments is a preferable process for higher recoil ion charge states. This indicates a strong coupling of electronic excitation to vibrational modes which are supposed to be responsible for C_2 evaporation. The relative yield of evaporation products to the parent recoil ion also shows q_p dependence similar to the ionization products. Relative fragmentation yields show a linear enhancement with q_p . The ratio of fragmentation yield to total reaction product seems to saturate for higher q_p. The signature of GDPR in large impact parameter collisions where C_{60} behaves as single entity as well as solid-like could be probed by a carefull study of the single, multiple ionization and fragmentation[1,2,3,4,5].

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S1/P10 New limits for the Parity and Time-reversal violating Coupling Constants from Hg Atomic Electric Dipole Moment

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Non-zero intrinsic electric dipole moment (EDMs) of a non-degenerate physical system is a direct signature of Parity (*P*) and Time-reversal (*T*) violating interactions. An atom can possess non-zero EDM due to Pb and b T violating interactions involving leptons and hadrons. Such EDMs are excellent probes of new physics beyond the Standard Model. The most accurate EDM experimental data comes from a measurement on Hg (Romalis et.al.,)(1). We focus on this atom for which the important EDM contributions come from the Tensor-pseudotensor (T-PT) electronnucleus interaction and the Nuclear Schiff moment (NSM). The coupling constants of these interactions are then determined by combining the experimental data with the atomic many-body calculations (Commins et.al.,)(2). We have developed a new many-body theory of EDMs of closed shell atoms to calculate these coupling constants which is the coupled-cluster method. This is equivalent to all order manybody perturbation theory that incorporates to all orders, the interplay of the short range *P* and *T* violating interaction and the long range Coulomb interaction. The present limits for the EDM of Hg atom induced by NSM are given by Dzuba *et al*., (3) and those of T-PT interaction are given by Martensson et.al., (4). Our present limit for the coupling constant of the T-PT interaction and the NSM for Hg can be used to improve constraints on the chromo electric dipole moments of quarks. Calculations using our new method when combined with the experimental data (Commins et.al.,) (2) improve the existing limits of P and T violating coupling constants at the elementary particle level, thereby providing valuable insights into the validity of the Standard Model of Particle Physics.

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New Autoionization Resonances in U I

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Study of autoionizing (AI) levels of heavy atomic systems is of considerable current interest owing to its importance in basic atomic physics and also in applications such as ultratrace elemental analysis $[1]$. Atomic uranium (U I) is a prototype of the heavy atomic systems, where the atomic structure is complicated by interaction of a large number of optically active electrons. There have been a number of investigations on AI levels of U I using various laser spectroscopic techniques that have resulted in identifying a large number of even and odd parity AI levels [1-3]. Despite this it is generally believed that the present survey of AI levels of U I is far from complete, particularly in the energy region > 1500 cm⁻¹ above the first continuum (49958.4 cm^{-f}). In this paper, we report our work on observation of new AI levels of U I in $51530 - 51700$ cm⁻¹ region using two-colour photoionization (PI) spectroscopy.

The basic experimental arrangement consists of two tunable dye lasers of wavelengths λ_1 and λ_2 that are temporally separated and spatially overlapped with a uranium atomic beam, and a time of flight mass spectrometer to detect the photo-ions. We choose $\overline{\lambda}_1 (= \lambda_1^{-1})$ =16900.38 cm⁻¹ and tune $\overline{\lambda}_2$ in the range 17730–17890 cm⁻¹ to generate a rich PI spectrum (spectrum-A), where each peak corresponds to a unique value of $n_1\overline{\lambda}_1 + n_2\overline{\lambda}_2$ where n_k is the number of photons of λ_k and $n_1 + n_2 = 3$. The dominant contributions arise from two distinct PI routes: (a) $n_1=1$, $n_2=2$ causing PI from resonant intermediate levels in 34630 - 34780 cm⁻¹ region and (b) $n_1=2$, $n_2=1$ involving excitation to a two-photon resonant level at 33801.05 cm⁻¹ and resulting in AI resonances in $51530 - 51700$ cm⁻¹ region. In order to distinguish between these two possibilities, an independent PI spectrum (spectrum-B) was obtained by fixing $\overline{\lambda}_1$ =16900.52 cm⁻¹ (at exact two-photon resonance) and scanning $\overline{\lambda}_2$ in the same wavelength region as before. PI peaks corresponding to the routes (a) and (b) are respectively suppressed and enhanced in the spectrum-B in comparison to the spectrum-A. PI routes have been further confirmed by studying the intensity dependence of the peaks in the PI spectrum. A systematic analysis of the experiments has resulted in identification of 23 AI levels of even parity in the region $51530 51700 \text{ cm}^3$, which includes 16 new levels. In addition the spectra have helped to confirm 6 high lying levels in the region $34630 - 34780$ cm⁻¹. Details of these investigations including the experimental configuration and data analysis will be presented.

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$S1/P12$ Two center Electron Emission in fast Collisions of Bare C and F Ions with He and H_2 and the CDW-EIS Model

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Electron spectroscopy is a very useful tool to explore the dynamics of ion-atom and ion-molecule collisions. The detection of low energy electrons emitted in atomic collisions provides crucial information on the various ionization-mechanisms. The double differential electron emission spectrum clearly identifies the different processes such as soft electrons (SE), electron capture in continuum (ECC) cusp and the binary encounter (BE) electron emission as well as the two center effect (TCE) [1]. Here we present the energy and angular distributions of DDCS of low energy electrons emitted in collisions of bare C and F ions with He and H2. The bare C ion of energy 72 MeV and F ions of energy 95 MeV were available from the BARC-TIFR Pelletron accelerator at TIFR. The experiments were carried using low pressure He and H_2 gas. The energy (between 1 and 500 eV) and angle resolved electrons were detected at several forward and backward angles between 20^0 and 160⁰. An e.s. hemispherical analyzer equipped with a CEM was used for this purpose. The first Born (B1) approximation fails to explain the doubly differential cross sections even at these high projectile velocities. The angular distribution of electron emission is known to be affected by the two center effect. The long range Coulomb interaction between the electron-target and electron-projectile in the final state influences the evolution of electron wave function and thereby the angular distribution. A large forward-backward asymmetry is caused due to such two-center effect which is included in the state of the art theoretical calculations like continuum distorted wave-eikonal initial state (CDW-EIS) approximation [2,3]. We show that although this model gives an overall very good agreement there are still some deviations from the measured data especially for the small forward and large backward angles.

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The role of relativistic many-body theory on electric dipole moment of electron

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Abstract

With an excellent progress in experimental techniques and the computational advancements in the recent years, it has now become possible to test the validity of many models of particle physics which question the very fundamental laws of physics. One such challenge for both theorists and experimentalists is the existence of parity and time reversal violating property called electric dipole moment (EDM) of an elementary particle like eletron. It is interesting for theorists because it is a direct proof of time reversal violation in nature and also it has serious consequencies ranging from sub-atomic physics to cosmology^[1]. For experimentalists, it will be a break through because it requires state of the art technology to achieve the best ever accuracy and precision till date.

An atom can have EDM even in the absence of any electromagnetic field due to an intrinsic EDM of any of its constituent particles like electrons, nucleons, quarks and also due to $P \& T$ violating electron-nucleus interactions. We mainly focus on the EDM of a heavy paramagnetic atom like Cesium and Thallium, wherein the electron EDM contribution to atomic EDM would be dominant. Therefore, we rather calculate a dimensionless quantity called enhancement factor which is the ratio of an atomic to electron EDM using a relativistic many-body theory known as coupled cluster theory. By combining the experimental measurement of atomic EDM and the enhancement factor calculated from theory we can deduce the electron EDM. The present best limit on the electron EDM obtained from Thallium EDM experiment done at Berkely is $< 1.7 \times 10^{-27}$ e-cm [2]. Many Non-Standard Models like Supersymmetric Model, Left-Right Symmetric Model etc. predict the EDM of electron to be almost in the same range, where as, Standard Model prediction is ten to twelve orders of magnitude less which is far off from the current experimental limits. If we can measure the EDM of an electron precisely, we can pick out the right model of particle physics which predicts the value of electron EDM in that range. Thus, the work on electron EDM has the potential to probe the physics beyond Standard Model.

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Expansion of Laser Cooled Atomic Clouds in Near-resonant Photon Field

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Studies on spatio-temporal expansion of a cloud of cooled and trapped atoms in a magnetooptical trap (MOT) are of considerable interest for characterization of the state of the cold cloud. Usually such studies are carried out on cold clouds that expand in vacuum after switching off the trapping laser beams. Here the expansion is completely determined by the internal energy of the cloud and the gravity, and as a consequence it provides a measure of the temperature of the lasercooled atoms [1]. The objective of this paper is to report new experimental observations on lasercooled cesium atomic clouds that are balanced against the gravity and expanding in near-resonant photon field. Dynamics of this expansion is expected to be complex and interesting since the photon field can alter the slow motion of the atoms by absorption and emission processes, analogous to the cold collisions that show significant dependence on these radiative processes [2].

The basic experimental set-up consists of a standard six beam $\sigma_{+} - \sigma_{-}$ MOT [3]. The cold cloud of cesium atoms trapped at the center of the MOT is allowed to expand in x direction by switching off the trapping laser beams along $\pm x$ axes while keeping other beams along $\pm y$, $\pm z$ axes on. The laser beams along the z-axis balance the cloud against the gravity. In this configuration we achieve 1-D expansion of the cloud devoid of the effect of gravity and in presence of an orthogonal 2-D laser field. The expanding cloud is imaged using an ICCD and the rms radii of the cloud ω_x and ω_z along x and z directions respectively are followed at $\Delta t = 0.5$ ms time interval up to t=20ms. During expansion ω_z remains constant and the expansion is fully characterized by the time variation of ω _x. Cloud temperature (*T*) is measured using the release and recapture method. Experiments are conducted on cold clouds of different number of atoms and temperatures in the range of 150-900 μ K. It is observed that the time variation of ω _x shows three distinctive regimes- contraction immediately after switching off $\pm x$ pair of trapping laser beams, ballistic expansion up to \sim 5 ms and damped expansion thereafter. The initial contraction is related to the reduction in the repulsive radiation trapping force [4] and is observed to be a dominant effect for large number of trapped atoms. In the ballistic regime ω _x grows as $\omega_x^2(t) = \omega_x^2(0) + (K_B T/M)t^2$ where K_B is the Boltzman constant and *M* is the mass of the atom. The damped behaviour appears to be a signature of the expansion in photon field. Details of the experiments and results will be presented.

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Low energy electron collisions with cometary's molecules CO, NO, HCN, and H₂CO

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Abstract:-

In this work we present theoretical study on electron collision with cometary molecules in the low energy range, we report, the rotationally excitation total and momentum transfer cross sections are calculated for electron collision with cometary's molecules CO, NO, HCN and H₂CO in the energy range (0.5-16.5 eV.) The Born Eikonal Series Approximation method and the hard sphere dipole interaction potential model are employed to present electron-molecule interaction. The results obtained are compared with experiment and theoretical data available in the literature.

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Study of Dissociation of N2 by Ar9+

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We report the results of the study of N₂ dissociation following collision with Ar^{9+} at a projectile velocity of approx 1a.u. The experiment is performed at the Low Energy Ion Beam Facility(LEIBF) of the Inter-University Accelerator Centre, New Delhi. At the centre of the experimental chamber, Ar^{9+} projectile ions produced from the Electron Cyclotron Resonance(ECR) ion source interacts with N_2 molecules effusing from a hypodermic needle. The dissociated fragments are extracted from the interaction zone in a time-of-flight mass spectrometer(TOFMS) on application of a uniform electric field perpendicular to both ion beam and gas jet. At the end of the TOFMS, the dissociation products are detected by a position-sensitive micro-channel plate(MCP) detector. Ejected electrons are extracted in the opposite direction to TOFMS and detected by a channel electron multiplier which gives the trigger for multi-hit coincidence data acquisition [1].

The TOF spectrum of N₂ shows fragment charge states upto N^{4+} and molecular charge state of upto N_2^{2+} . From the coincidence plot of the correlated charge state pairs we observe ion pairs of $(N^{1+} - N^{1+})$, $(N^{2+} - N^{2+})$, $(N^{3+} - N^{3+})$, $(N^{2+} - N^{1+})$, $(N^{3+} - N^{1+})$, $(N^{3+} - N^{2+})$, $(N^{4+} - N^{2+})$. The Kinetic Energy Release (KER) distributions for the various fragment charge states are extracted from the obtained data. From the relative yield of the fragments corresponding to one and the same parent molecular ion we find that the symmetric charge breakup channel is is preferred over asymmetric charge breakup. A signature of core excitation of the target followed by Auger emission is observed in one of the fragmentation channels and shall be presented.

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Absolute cross sections for Dissociative Electron Attachment to water and methane

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Electron-molecule collisions play an important part in various studies, including those of solar and planetary atmospheres, cometary bodies, large molecular cloud formations in deep space, radiation chemistry and radiation biology, amongst others. In recent times, there is a spurt in DEA studies for some simple organic molecules. These studies are motivated by the presence of organic molecules in astrophysical objects, and also by the realization that low energy electrons play an important role in radiation damage to biological molecules¹. Recent DEA studies in our laboratory² have led to a novel discovery of site specific fragmentation in some simple organic molecules. The site specificity in fragmentation is seen in the H channel depending on the functional group present in the molecule. It is expected that the electron attachment properties of a smaller sub-system would be retained also in the bigger molecular systems containing them. For example, any big molecule with O-H group should retain the electron attachment properties seen in water.

The present measurements are a part of an ongoing project to study the H channel in the DEA process to some organic molecules. It is pertinent to note here that such studies are difficult and not common, because of the difficulties faced in the analysis and detection of negative ions produced in this process, principally H, without any discrimination by their mass, kinetic energy and angular distribution. We have measured absolute cross sections for negative ions produced by DEA to water and methane. Both, water and methane are important molecules for various studies of planetary and space sciences. Also, while methane is the simplest of halocarbons in the chain of complex organic molecules, water is the most important constituent of biological molecules. In the present experiment a magnetically collimated and pulsed electron beam is collided, at right angles, with an effusive molecular beam generated by a capillary array. The negative ions produced in this interaction are lead into a Time of Flight (TOF) mass spectrometer, and the mass analyzed ions are then detected by a channel electron multiplier. The relative yields were put on an absolute scale using the Relative Flow Technique.

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$S1/P18$ Studies on Cold Atoms Trapped in a Quasi-Electrostatic Optical Dipole Trap

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 We discuss the results of measurements of temperature, density, state distribution and trap frequencies of cold Rubidium atoms trapped and cooled in an Optical Dipole trap formed by a 50 W $CO₂$ laser operating at 10.6 micro-meters.

 A Magneto-Optical Trap (MOT) in a spherical-square chamber is loaded fast (< 600 ms) from a cold, collimated and intense atomic beam of flux 2×10^{10} atoms/s produced using an elongated 2D⁺ Magneto-Optical Trap [1]. A large number of rubidium atoms ($> 10^{10}$) were trapped in the MOT and the number density of atoms are further increased by making a temporal dark-spot MOT to prevent light-assisted collisional losses of atoms at the trap centre. The phase-space density was further increased using molasses cooling technique by increasing the detuning and reducing the intensity of the cooling laser beams. The cold atoms were then transferred into a Quasi-Electrostatic trap (QUEST) [2] formed by focused high power 50 W $CO₂$ laser at the Magneto-Optical trap centre.

 Various measurements were done on the cold atoms trapped in the dipole trap. The atom number in the trap was measured by releasing the dipole trap and recapturing the atoms in the MOT and measuring the power of the emitted fluorescence using a calibrated photodiode. The temperature was determined by measuring the spatial density distribution of atoms in the dipole trap by absorption imaging method. The time-of-flight (TOF) method was also used for the temperature measurement. The vibration frequency of atoms in the trap was measured by modulating the laser intensity and driving parametric excitations of the atomic oscillations. The results from measurements are used to maximize the initial phase-space density prior to forced evaporative cooling to produce Bose-Einstein Condensate.

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Excitation of the Metastable States of the Noble Gases

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 We have used the relativistic distorted-wave approximation to study the excitation of the lowest metastable states of neon, argon, krypton and xenon (the $J = 0$, 2 levels of the $np^5(n+1)s$ configuration) to the ten higher-lying fine-structure levels of the $np^5(n+1)p$ configuration. We present and compare our results with experimental measurements of the integrated cross section at energies up to 400 eV and with other theoretical calculations for these cross sections.

Ergodicity properties of photon-added and multi-photon coherent states propagating in a nonlinear medium

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ABSTRACT

The dynamics of photon-added and multi-photon coherent states propagating in a nonlinear medium has potential applications in quantum information processing. We use a model nonlinear Hamiltonian to study the behavior of the time series represented by the quantum mechanical expectation value of a suitable quadrature variable. The ergodicity properties of this quantity, as deduced from the power spectrum corresponding to the time series data, are analyzed. We also examine the recurrence time statistics in a coarse-grained description of the dynamics, in the case of initial states that are, respectively, an ideal coherent state, an m -photon-added coherent state, and certain multi-photon coherent states. This helps distinguish between the precise nature of the ergodicity exhibited by these distinct initially-prepared states, that differ in the degree to which they depart from perfect coherence.

S1/P21 (e, 2e) Studies of Ca in Coplanar Symmetric Geometry at Low Impact Energies

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The triple differential cross section of Ca $(4s^2)$ at low impact energies in coplanar symmetric geometry has been calculated in the DWBA using a spin averaged static exchange potential and a modified semi classical exchange potential [1]. The impact energies range from 1.65 to 10.57 times the first ionization threshold for Ca. The effect of post collision interaction (PCI) has been studied using the Gamow factor [1].

The present results are in better agreement with experiment [2] in the intermediate angle region (35 \degree to 125 \degree) at low energies compared to an earlier study [3] in which PCI was accounted for using 'angle dependent effective charge' instead of the Gamow factor. At higher energies, however, both methods of including PCI show almost similar behavior, however, good agreement being restricted to lower angle region at some higher energies. It was suspected in an earlier study [3] that PCI was responsible for additional peaks in the TDCS; however, the present work shows that the multiple peak structure of the TDCS is independent of the PCI as predicted by the Convergent Close Coupling method [2]. Furthermore, it has been found that the only significant effect of PCI on the TDCS is to reduce it nearly to zero near 0° and 180° , which is what one expects considering the fact that the probability of the electrons to be scattered along the same direction is small.

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Siegert pseudostate representation of time-dependent quantum system – hydrogen atom under the ultrashort pulse Koudai Toyota¹, Toru Morishita¹, and Shinichi Watanabe¹

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Recent development of ultrafast physics enables us to understand electron dynamics in an atom or molecule such as mapping electron wavepacket motion onto high harmonic spectra [1], probing electron correlation in helium atom [2] and so on. In the poster we present hydrogen atom under the ultrashort pulse by exploiting time evolution method for Siegert pseudostate recently developed by Tolstikhin [3]. Siegert pseudostate(SPS) [4] is the solutions of Schrödinger equation which satisfies outgoing wave boundary condition. And when we plunge into time evolution of wavepacket, it can exclude unphysical reflection from the boundary.

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$S1/P23$

Non-linear Magneto Optical Effects in the Doppler- broadened Spectrum of Rb atoms.

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Doppler-broadened absorption spectrum of Rb $(^{87}Rb$ and ^{85}Rb) has been studied with the application of a magnetic field of intermediate strength, up to $5mT$. Earlier studies [1-3] have focused on magneto optical effects in low fields. Magneto optical effects have been observed for longitudinal and transverse magnetic fields. The horizontal and vertical polarization components of an absorption spectrum have been detected.

Magneto optical rotation was measured with the help of the absorption spectrum. The field dependent optical rotation clearly shows that deviation of linear effects occurs in intermediate fields. Other non-linear effects such as hole burning, polarization (σ_{+} , σ_{-} , π) dependent rotation and level crossing are also discussed.

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S1/P24 Theoretical Cross sections for Electron Induced Ionization of Si, SiO, SiO2, $SiH₄$, and $Si₂H₆$

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Electron impact ionizing collisions of molecules are of great interest in view of the applications of relevant cross sections in various fields of pure and applied Sciences. Silica $(SiO₂)$, silicates and other oxides are found to be the constituents of the interstellar dust and grains. Electron collision cross sections help to determine the density and reactivity of low-temperature technological plasmas. The targets listed in title are of great current interest in the modeling of chemical vapor deposition and plasma enhanced chemical vapor deposition of semiconductors. Silane (SiH₄) and disilane (Si₂H₆) are widely used for plasma assisted deposition of silicon and silicon dihydride films.

In this paper we report electron impact total ionization cross sections (TICS) calculated for these targets at incident energies from threshold to 2000 eV. Our calculation is based on Complex Scattering Potential approach, as developed by us [1, 2]. This leads basically to total inelastic cross sections, from which the total *ionization* cross-sections are extracted by reasonable physical arguments on ionization contribution. Sufficient comparisons are made here with the previous theoretical and experimental data. The present results are found satisfactory for all these molecules, for which the data is available. It is of interest to examine the contribution of TICS detailed results will be presented at the conference.

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in the total (complete) Cross Sections as a function of incident energy. This is a maiden attempt for the molecules like SiO and $SiO₂$ since no experimental or theoretical comparisons are available for these targets. The figure below indicates present results of e-SiH4 calculations. The

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Ionization using CBOA in Ps-Atom Scattering

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In positronium (Ps) and atom scattering, Ps-ionization channels open only at 6.8 eV [1-4]. Depending on the ionization potential of the target, targetionization channels open at below or above 6.8 eV. At this energy region the effect of exchange between the target and the projectile electrons are highly important. In our previous studies [5-6] on target-elastic Ps-ionization cross section using a Coulomb-Born-Oppenheimer approximation (CBOA) for Ps-H and Ps-He scattering, we have established the importance of exchange at lower energy region below 70 eV. In the present article we are interested to present the effect of exchange on target-ionization on Ps-H and Ps-He scattering using the similar methodology. In addition we are also interested to present the differential cross sections [7-8] of Ps-ionization for which the experimental data [9] are available.

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Regulation of Extra cellular Response protein kinase (ERK1/2)nuclear translocation in living cells:

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Abstract

The signal path ways of extra cellular signal regulated kinase $(ERK 1/2)$ to the stimulation of membrane bound receptors regulates cellular processes $[1,2]$. These processes are based on the fundamental mechanism called phosphorylation in the living cells.

The $ERK(1/2)$ concentrates on the nucleus, when it activates some specific programmes. Through some of importance of these processes and their significant role are used to know the regulation in exchange of $ERK(1/2)$ between the nucleus and cytoplasm in living cells[3].

In the present study the time dependent two level perturbation is used to the ERK from cytoplasm to nucleus and its dynamical regulation has been analytically obtained .The experiment is also conducted by expressing low levels of fluorescent tagged $ERK(1/2)$ in living fibroblast observations so obtained from the experiment is compared with the analytical results, which is found to be in good agreement.

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Optical Properties of a Novel Porphyrin-polymer Nanocomposite Film

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 Porphyrins are known to be candidate materials for linear as well as nonlinear optical applications ranging from image processing photonic switching. These materials also provide great scope for molecular engineering as their optical properties can be tuned to large extent easily by structural modification [1]. The idea of embedding the porphyrins in stable polymeric hosts has been attracting recent attention as this rendered the prophyrin in a physical form that is very stable and device-friendly [2]. The ionomer Nafion is a good candidate material for embedding as porphyrins in view of its excellent mechanical, chemical and thermal stability as well as transparency in the visible region.

Nafion has structural pores of a few nanometer size in which the embedded material would be in the form of nanoclusters within the membrane.

 The material chosen for the present study is Cu(CN)4TPP, a tetraphenyl porphyrin with strong optical absorption in the ultraviolet and visible regions. The starting material is in the powder form and is dissolved in organic solvents such as chloroform or ethyl alcohol. The material is embedded in Nafion membrane by an ion-exchange reaction. The optical properties of the solution as well as the film are studied by optical absorption and photoacoustic spectroscopy. The spectra reveal characteristic features of porphyrins. Fig..Photoacoustic spectrum of Cu(CN)₄TPP

 The optical nonlinearity arising from local photothermal variation of the refractive index is studied using the z scan technique which is based on self focusing properties of the medium. The nonlinear refractive index is found to be reasonably large and the effect could be seen clearly even at low laser power levels obtainable from a helium neon laser. The results demonstrate that structure-modified porphyrins stabilized in solid polymer membranes hold promise as device-friendly media for low intensity applications in nonlinear optics.

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Dissociation Pathway of FCN and ClCN in a varying Temperature Region.

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 Dissociation pathway of FCN and ClCN in a varying temperature region of the stratosphere has been studied in detail using ab initio and density functional methods. In the varying temperature region there is a possibility to have the fragmented atoms both in their ground state as well in their metastable states. Various dissociation channels have been investigated and the minimum energy pathway for dissociation of FCN and ClCN has been predicted. The structural properties of FCN and ClCN have also been studied in detail. The isomerization of FCN and ClCN is an important part of this investigation.

S2/P29 Autoionization resonances in 6s photoionization of free and trapped atomic mercury

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 Below 5d thresholds, 6s E1 cross-section in atomic mercury has been found to go through a Cooper minimum [1]. The Cooper minimum is the energy region of the 5d to *np, nf* resonances. We report in this work a detailed study of 6s photoionization crosssection and angular distribution asymmetry parameter β in the autoionization region using the RMQDT [2]. Furthermore, we report the effect of endohedral confinement [3] of the mercury atom on the cross-section and angular distribution parameter for the 6s subshell in the autoionization region.

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$S2/P30$ Spectroscopic constants of ZnHe, ZnNe and ZnAr Van der Waals Molecules

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Spectroscopic constants and molecular properties of van der Waals ZnHe, ZnNe and ZnAr molecules have been studied using our newly developed method published recently [1] where we prescribed the way to calculate the spectroscopic properties of weakly bound molecules in Lennard-Jones potential. The basis set of Zn has been designed to calculate the spectroscopic properties of these Zn containing molecules. The equilibrium bond length, harmonic frequency, dissociation energy, anharmonicity constants, rotational constants, centrifugal distortion term and other spectroscopic constants have been studied in detail using ab initio and density functional methods. Most of the spectroscopic constants are first predicted and the rest agree very well with the existing experimental values.

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Photoionization of Two-Electron Atoms – toward the Double Ionization Threshold from Below

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 Photoionization cross section (PICS) of two-electron atoms in 1-dimensional collinear model is calculated up to the $N=52$ threshold energy by using the complex rotation method [1]. The energy spectrum of PICS has very complicate resonance structures with high irregularity as in typical chaotic scattering systems. However, a Fourier transform, i.e. the scaled action spectrum of PICS shows prominent peaks at the action values of the orbits which begin at and end with triple collision [2]. Employing the semiclassical Green's functions associated with those orbits and exploiting the scaling properties of the Coulomb system, we find an universal scaling law for the decay of amplitudes of oscillations in PICS as the energy approaches the three-body breakup threshold. And we develop a semiclassical approach to PICS which may be considered as an extension of closed-orbit theory [3] for one-electron atoms in external fields to a theory for two-electron atoms in free space, focusing on the matching of semiclassical and quantum Green's functions at the boundary of quantum regime around the nucleus.

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Spectroscopy of weakly Bound Molecule: A new Theoretical Approach

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A simple method has been developed to study the spectroscopic properties of weakly bound molecules in Lennard-Jones potential. This new method removes the major drawback of earlier calculations where the weakly bound molecules have been assumed to obey Morse potential. The method has been applied to the weakly bound molecules containing light atoms and predicted their spectroscopic properties accurately. Most of the spectroscopic properties are first predicted. The equilibrium bond length, harmonic frequency and dissociation energy agree very well with the experimental values. Application to various interesting weakly bound molecules is now under progress.

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Control of De-excitation to Selected Vibrational Levels in the Ground state of NaH Molecule using two Broadband Ultrashort Pulses

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We show that the de-excitation to different vibrational levels of the ground state in NaH molecule can be controlled by using two delayed ultrashort pulses (4 fs Gaussian). A vibrational wave packet generated on the excited $A_1\Sigma$ state by the first pulse is deexcited back to the ground state by a second pulse after a time delay. The cross section for de-excitation of the wave packet to different vibrational levels of the ground electronic state can be controlled by controlling the delay time between the two pulses as well as by choosing a pulse duration much shorter than the vibrational period of the molecule, such that the de-excited wave packet remains localized in the Franck-Condon region of a particular vibrational level of the ground state. Hence, the de-excitation to a particular vibrational level can be enhanced by suppressing that in others. In spite of the large bandwidth of the pulse which includes nine vibrational levels of the upper state and five vibrational levels of the ground state, one can selectively de-excite the molecule to any one or two vibrational levels of the ground state by carefully choosing the delay time between the pulses and the pulse duration. We are designing the wave packet in the ground state by two short pulses and selectively distributing the population in one or two levels at various values of the delay time. In light molecules having small vibrational period, this selectivity in de-excitation to one or two vibrational levels in the ground state can be achieved only by using ultrashort (4 fs) pulses in presence of which the localisation of the wave packet in the Franck-Condon region of the vibrational levels are particularly possible. It has been shown that the de-excitation cross section to a particular vibrational level oscillates with delay betweenthe pulses which can be realized as the time dependent quantum gate [1,2].

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$S2/P34$ Effects of Spontaneously Generated Coherence and Dynamically Induced Coherence in the closed Λ system.

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In a three level Λ system with two near-degenerate lower levels, there exists an additional coherence term -`**Spontaneously Generated Coherence**' due to the interaction with the vacuum of the radiation field [1,2]. We report the effects of spontaneously generated coherence on inversionless gain (LWI), in the closed probe-pump – Λ system with an incoherent pump. We investigate the effect of both SGC and dynamically induced coherence on the probe-pump response of a nearly generated Λ system. It is shown that, the contribution of SGC term to the inversionless gain and dispersion may be comparable to the dynamically induced coherence within suitable parameters region. Hence it is not always true that SGC term contributes more to the probe-pump response of Λ-system. We support our results by analytical explanation, which is consistent with the numerical results. The analytical calculations are done considering all orders of Rabi frequencies, incoherent pumping, detuning and unequal spontaneous decay rates i.e. no simplifications are done in calculating the polarizations. To our knowledge the analytical expressions of polarizations have not been calculated so far without any simplification. We also study the effect of relative phase between the two applied fields and find that LWI and EIA can transform mutually by adjusting the relative phase. This acts like an optical switch by which the medium gives LWI to EIA and vice versa.

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Electron impact ionization of NO, N_2O , NO₂, NO₃ & N_2O_5 - Theoretical total cross sections

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The oxide molecules of nitrogen viz. NO, N₂O, NO₂, NO₃ & N₂O₅ are known to exist in various concentrations at different altitudes in our Earth's atmosphere. Their importance is recognized as atmospheric pollutants and in connection with ozone depletion processes. Ionization of NO₂ plays an important role in plasma applications. Electron impact ionization of nitric oxide molecules has been investigated by several workers both in theory [1] and in laboratory [2], but there are discrepancies (>15%) among different results. Further there are no measurements of ionization cross section for reactive species NO_3 and N_2O_5 . This is the motivation in our present paper, wherein we will report our theoretical cross sections of electron impact (above 10 eV) on the nitrogen compounds listed in the title.

The theoretical method adopted presently is based on 'complex scattering potential ionization contribution' approach. discussed in our recent papers [3, 4]. This method simply predicts total ionization cross section as a reasonable energy dependent fraction of total inelastic cross sections of the electron-molecule system. The present calculations do not include rotational/vibrational cross sections which important below ~ 10 eV.

Figure 1: Various total cross sections of electrons incident on NO

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Derivation of chemical potential using second order iteration in modified Thomas-Fermi model for Bose-Einstein condensate

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We have derived an equation for the chemical potential (μ) analytically using second order iteration for density of particles in the Bose-Einstein condensate (BEC) within modified Thomas-Fermi (MTF) limit. Thomas-Fermi approach (proposed earlier in ref [1]) to the modified Gross-Pitaevskii (MGP) equation [2] gives MTF equation for the condensate of N bosons each with mass m confined in a trap potential V(r). We solve MTF equation following the second order iteration procedure and obtain

$$
n(r) = g^{-1}(\mu - V(r)) - \frac{4m^{3/2}}{3\pi^2\hbar^3}(\mu - V(r))^{3/2} \left[1 - \frac{16m^{1/2}a}{3\pi\hbar}(\mu - V(r))^{1/2}\right]^{3/2} \dots \dots \dots (1)
$$

where $g = 4\pi\hbar^2 a/m$, μ is chemical potential, a is the scattering length, ω is the angular frequency of spherical harmonic trap and $n(r)$ is the particle density and hence the equation for μ is obtained analytically as

$$
\sum_{j=1}^{j_{\text{max}}} C_j \mu^{j/2+2} = N \qquad \text{........... (2)} \qquad \text{[C}_j \text{ is are functions of a, m and } \omega\text{]}
$$

which is valid as long as $-1 < \frac{10m^{1/2}a}{3\pi\hbar} (\mu-V(r))^{1/2} < +1$ ------------ (3)

 J_{max} has been chosen to obtain convergence in the binomial series, which also depend on system parameters. Eq.(2) can be solved by the method of successive iteration with initial value of μ as μ_{TF} (value of μ in Thomas-Fermi limit) and continue the process to get the convergence in the final value of μ , denoted by $\mu_{MTF(2)}$.

We calculate $\mu_{MTF(2)}$ and $x_{pk,MTF(2)} = n(0)a^3$ for N=10⁴ Rb⁸⁵ atoms confined in a spherical trap with frequency $\omega/2\pi$ = 12.83 Hz by using eq.(2) and eq.(1) respectively The results alongwith the corresponding values of $\mu_{\text{MTF(1)}}$ (as obtained in ref[1]) and μ_{MGP} obtained by solving MGP equation numerically [2] are given in table-1. Table-1 (u) 's are in ho unit, a is given in Bohr radius of hydrogen atom an)

when $na^3 > 10^{-3}$, $\mu_{MTF(1)} > \mu_{MGP}$ but, $\mu_{MTF(2)} < \mu_{MGP}$ which shows the correct trend. $x_{pk, MTF(2)}$ increases with scattering length 'a' .Similar increase in $x_{pk, MGP}$ is obtained giving 4.12×10^{-2} for a=10000a₀ [2]. Whereas the values of $x_{\rm pk, MTF(1)}$ decreases with increasing 'a' after giving maximum at $a=5000$ ao and becomes -ve at $a=10000$ ao [2]. References:

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Effect of Ca²⁺ on Low Energy Electron Induced Damage to **Plasmid DNA**

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 The use of radiation for tumor treatment has been in practice for a long time. It was, until recently, believed that the cell death was caused by the irreparable damage to the DNA in the Cell nucleus by the irradiating photons and its secondary particles. The new revelation by Sanche and coworkers [1] in 2000 showed that Low Energy Electrons (LEE) damage DNA. The mechanism is attributed to the formation negative ion resonances which result in breaking of the sugar phosphate backbone of the DNA. It is known that the back bone of the DNA carries a negative charge. Therefore, it would normally be difficult for a LEE to move close to the back bone to form temporary negative ion. This means that the electron is likely to attach to a suitable functional group which then transfers the excess energy to break the back bone. Calcium ions (Ca^{2+}) bind to the phosphate backbone of DNA as well as to DNA bases leading to varying degrees of charge neutralization [2]. In this context, it is relevant to ask whether shielding of DNA backbone by counter cations have any effect on strand break propensities.

Figure 1. Relative Yield (%) of Relaxed DNA caused by LEE, with and without calcium

 The LEE irradiation setup consists of a homemade conventional electron gun housed in an Ultra High Vacuum (UHV) chamber pumped by turbo molecular pump. 1.5 µl of commercial plasmid DNA pBR322 of concentration 300 ng/µl was diluted to a final volume of 5 µl and spotted on Tantalum foil. The sample was irradiated with electrons of known energy for a predetermined period. Similar experiments were carried out with DNA to which varying concentrations of calcium chloride $(CaCl₂)$ (analar grade) was added.

 After exposure to the electron beam, the samples were retrieved using TE buffer and the strand breaks were evaluated by running it in a 1% agarose gel.

Gels were analyzed and quantified using Quantity One (BioRad). The results indicated that exposure of DNA to LEE led to the generation of nicked circular form of DNA, with a concomitant drop in the supercoiled form (see Figure 1), an evidence of the generation of SSB's. Interestingly, presence of Ca^{2+} ions in DNA led to a near complete protection of DNA towards SSBs by LEE. Moreover, Ca^{2+} effect was rendered by $CaCl₂$ as well as $Ca(NO₃)₂$ to an equal efficiency, pointing out that the protective effect was likely due to divalent cations (Ca^{2+}) rather than the anions. These results demonstrate the role of backbone shielding chemistry in the mechanism of SSB generation. Future experiments are focused on trying to unravel the basic mechanistic description of such backbone protective effects against impinging LEEs.

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Velocity Map Imaging of H– ions resulting from Dissociative Electron Attachment to H₂O

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Study of electron collision on water molecules is important from the point view of basic physics and various practical applications, including biological effects of radiation. Dissociative Electron Attachment (DEA) is one of the dominant processes leading to electron induced chemistry. In order to understand the dynamics of the process as well as identify the symmetry and structure of the negative ion resonances involved in the DEA process, it is necessary to measure angular distribution and kinetic energies of the fragment ions. We have made use of the Velocity Map Imaging (VMI) technique to study the formation of H ions resulting from electron collision on H2O molecules. It is known that water molecules resonantly attach electrons at energies 6.5, 8.5 and 12 eV respectively and the H_2O^- anion dissociates to give H⁻ ions. The VMI technique $^{(1)}$ provides angular distribution of H ions in the whole 2π range and also, the kinetic energy of these ions in one go. We present here the angular distribution of H ions obtained from H2O at the above mentioned resonant electron energies using our setup and compare it with the existing results/experimental data^{(2), (3)}. While the H⁻ angular distribution at 6.5 eV matches very well with previous measurements reported in literature, there is considerable disagreement at 8.5 eV and 12 eV. The kinetic energy information is obtained by looking at the radial distribution of the H- ions. The excess energy after the dissociation of the H_2O^- transient ion is distributed between H^- and OH fragment (which is left vibrationally excited). A lower H kinetic energy indicates more energy in the OH fragment and vice versa. We have determined the relative intensities of the vibration states of the OH fragment from the kinetic energy distribution of H^- ions at the 6.5 eV resonance.

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L_3 - subshell Alignment of Au induced by 18 MeV C^{4+} Ion via the Measurement of Angular Distribution of L-subshell X-rays

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The inner-shell vacancy with total angular momentum (*j*) greater than 1/2 is expected to align in the beam direction in ion-atom collisions [1]. However, the multiple ionization in heavy ion collisions provides additional complexity in the vacancy distributions and therefore in the angular distribution of x-rays. Several measurements have been done to study the L₃-subshell ($j=3/2$) alignment induced by light ions (such as proton, He) and data can be reasonably well described within the framework of direct ionization theories [2]. In the case of heavy ions, only a few measurements are available and mostly in low energy region [3]. Hitachi *et al.* [4] found that the Ll and Lα x-ray lines of Sn are isotropic whereas Jitschin *et al.* [2] showed an alignment in the Ll x-rays in heavy ion collisions. In the present work, the angular distribution of the L x-ray lines of thin solid targets of Au induced by 18 MeV C^{4+} ions has been measured. The x-rays were detected in the angular range 20^0 -90⁰ using semiconductor detector. The experiment was performed using BARC-TIFR Pelletron accelerator facility at Mumbai, India. The L xrays originate from the L_1 and L_2 subshells ($j=1/2$) and are expected to have isotropic emission [2]. Therefore the Ll, L α and L β x-rays yield were normalized to the L γ x-ray yield. This way of normalization is free from the uncertainties in the detector solid angles. The Lβ x-ray was found isotropic whereas Ll and Lα show non-isotropic emission. The anisotropy parameter (β) was obtained to be – 0.144 \pm 0.033 and - 0.059 \pm 0.034 for Ll and Lα respectively. The observed anisotropy is close to the prediction of the Coulomb ionization theoretical model based on perturbed stationary state approximation. The details will be presented.

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Development of Doppler Tuned Beam-Foil X-Ray Absorption Spectrometer , Anjan Dutta³, C. P. Safvan¹, T. Nandi¹ and A. Roy¹ ¹Inter University Accelerator Centre, JNU New Campus, New Delhi-110 067, India ² Department of Physics, Aligarh Muslim University, Aligarh, India ³ Department of Physics and Astrophysics, University of Delhi, New Delhi, India

 Since decades beam foil time of flight technique serves as a versatile tool to measure the lifetime of different energy levels, specially metastable, which can be applied in principle to any charge state. Due to limitation in resolution of available energy dispersive solid state detectors (resolution \sim 150 eV at 5.9 keV), this technique does suffer from inherent cascading and blending problems. Up to some extent cascading problem may be overcome by proper selection of beam energy, but intra-ion and inter-ion blending (satellite blending) could not be avoided. Recently beam-foil technique using single foil as well as two foil target by Nandi *et al* has shown that above mentioned complexity can be disentangled to a great extent and produced some good result [1]. But absence of high resolution proved to be a major constraint. In order to spectroscopically resolve the satellite blending, high resolution x-ray Doppler Tuned Spectrometer (DTS) [2] is being developed in general purpose scattering chamber (GPSC) at IUAC.

 In most beam-foil experiments, the Doppler effect produces unwanted distortion of emission spectra. But DTS utilizes the Doppler shift as a function of angle of emission from the beam as a dispersive element. When the foil-excited beam emits a photon of energy E_0 , will be Doppler shifted and appears at energy E_{AB} to a stationary detector (Relation given in equation given below). The relation between Doppler shifted energy E_{AB} and rest energy E_0 is as follows:

$$
E_{AB} = \gamma [1-(v/c)\cos(\theta)] E_0
$$
 Where $\gamma = 1/\sqrt{1-(v^2/c^2)}$

and v is the velocity of the post foil beam and θ = angle of detection of photon with the beam axis. An absorber foil is placed between target foil and the proportional counter, which has an absorption edge just below the Doppler shifted energy E_{AB} for proper choice of angle . As the Doppler shifted energy matches with the absorption edge of the absorber foil, a dip appears in the spectrum due to the absorption of x-ray by absorber foil. Differentiation of this spectra contains the high resolution feature. Resolution of DTS is given by $\Delta E_{AB} = \gamma E_0$ $(\nu/c) \sin(\theta)$ $\Delta \theta$. Since absorption edges typically have widths (ΔE_{AB}) about a fraction of an electron volt so a resolution ~ 0.1% is possible. One of the main component of DTS setup is the Position Sensitive Proportional Counter (PSPC), which has been tested. The developed PSPC has a position resolution of 350

m in the linearity range of 140 mm and the energy resolution of \sim 20% at 5.9 keV of Fe x-ray. This setup has been designed for achieving the the resolution of \sim 3 eV and hence expected to resolve satellite line from the parent line. Such high resolution spectroscopy will shed light on various structural as well as collisional properties of highly charge ions; Viz. lifetime of metastable states, hyperfine effects on atomic levels in He- and Lilike heavy ions and intra-shell transitions. Such a novel facility will be described along with preliminary results.

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Electron Impact Total and Ionisation Cross Sections for simple Molecules of Biological Interest

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 In recent years, electron interactions with biologically important molecules such as formaldehyde, formic acid, amino acids etc have gained attention. It is now considered

that the types of primary damage induced in DNA by ionizing radiation leading to the most significant biological effects are double strand breaks (DSB) and clustered lesions [1]. The ionization induced by the secondary electrons also plays a vital role in understanding the damages caused by the primary radiations.

In this paper we have reported the important scattering quantities viz., total cross section Q_T , total elastic cross section Q_{el} , and total ionization cross section Q_{ion} for H_2O , HCHO, HCOOH molecules and CHO radical on electron impact. The present calculations are based on the spherical complex optical potential formalism [2,3]. The present energy range is from ionization threshold of the target to 2 KeV. The total and elastic cross sections for HCHO, HCOOH and CHO radical are reported for the first time in the current energy range. We have employed the well-known spherical complex (optical) potential formalism (SCOP), which provides total elastic cross section Q_{el} and its inelastic counterpart Q_{inel} such that

$$
Q_T(E_i) = Q_{el} + Q_{inel} \tag{1}
$$

 Q_{inel} includes Q_{ion} and we have developed a method to extract ionization cross sections Q_{ion} from calculated inelastic cross-section Q_{inel} , by introducing a ratio function

$$
R(E_i) = \frac{Q_{ion}(E_i)}{Q_{inel}(E_i)}
$$
\n(2)

 The calculated cross sections are examined as functions of incident electron energy along with available comparison. Our results will be presented in the conference. *References*

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S2/P42

Young type Interference Effect in the Forward Backward Asymmetry of Electron Emission in Ionization of H2 by fast Heavy Ions.

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Low energy electron emission spectrum from the simplest diatomic molecule H_2 in fast ion collisions manifests yet another important aspect of ion-atom ionization besides the well known mechanisms i.e. the soft collision, two center effect, binary encounter and electron capture in continuum and post collision interaction. Since the two indistinguishable H-atoms may be termed as a coherent source of electrons in a large impact parameter collision with a fast projectile, their contributions to the ionization add coherently and an interference effect may be expected. Therefore, the electron emission from H_2 may be viewed as a natural system which is similar to the Young's double slit arrangement to study interference phenomenon. Since the double differential cross section (DDCS) varies over several orders of magnitudes in an energy range of few hundred eV, it becomes difficult to observe a small variation in the DDCS spectrum owing to such a steep variation in the cross section. Therefore, to enhance the visibility of the structure, the molecular cross sections are divided by the corresponding atomic cross sections, which are either obtained theoretically [1] or in an experiment with atomic H [2]. We have now demonstrated [3] an independent way of obtaining the interference structure by using the forward backward asymmetry parameter of electron DDCS which is independent of the theoretical model calculations and also does not require a complementary experiment with atomic H. The energetic bare C and F ions were available from the BARC-TIFR Pelletron accelerator at TIFR. The experiments were carried using low pressure H_2 gas. Energy and angle resolved electrons were detected at several forward and backward angles between 20^0 and 160^0 . The results obtained were compared with a model calculation based on peaking appriximation as well as with the continuum distorted wave-eikonal initial state (CDW-EIS) approximation [4].

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Phase Separation in two species Bose-Hubbard Model

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Quantum Phase Transitions (QPTs), have attracted much attention in recent years. These transitions occur at very low temperatures, where the quantum ground state of a system undergoes some fundamental change. This change is not due to the temperature but some parameter in the Hamiltonian of the system. The realization of trapped Bose-Einstein condensates of ultracold atoms in optical lattices has opened up the possibility of obtaining various quantum phases in a controlled manner. We study the ground state phase diagram of a mixture of two species of bosonic atoms in one dimensional optical lattice, which can be described by two species Bose-Hubbard model. Keeping only the on-site interactions between a given species as well as between the two different species, we have obtained the complete phase diagram using the finite-size density matrix renormalization group (FSDMRG). The phase diagram consists of superfluid(SF), Mott insulator(MI) and phase separated phases. The experimental verifications of our results will provide important insights into quantum phase transitions.

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S2/P44 Ab *initio* Calculation of *P,T*-odd Effects in YbF Molecule

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A fully-relativistic restricted active space (RAS) configuration interaction (CI) approach is employed to compute the *P*,*T*-odd interaction constant W_d of the ground $({}^{2}\Sigma)$ state of YbF. A series of increasingly sophisticated CI space yields a best estimate of $\overline{W_d}$ = -1.088 \times 10²⁵ Hz/e-cm. We emphasize that the present estimate of W_d lies in between the values reported by Parpia $(-1.20 \times 10^{25} \text{ Hz/e-cm.})$ [1] and Titov *et al.* $(-0.91 \times 10^{25} \text{ Hz/e-cm})$ [2]. The CI space that yields the best estimate of W_d is also used to compute other molecular properties, all of which are found to be in good agreement with experiment.

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Lγ**¹** ′ **satellites in X-Ray Emission Spectra of Middle-Z Elements**

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The X-ray satellite spectra arising due to $L_2M_x-M_xN_{4,5}$ (x = 1-5) transition array, in elements with $Z = 41$ to 51, have been calculated. The energies of various transitions of the array have been determined by using available Hartree-Fock-Slater (HFS) data on $K-L₂M_x$ and $L₂-M_xN_{4,5}$ Auger transition energies and their relative intensities have been estimated by considering cross - sections of singly ionized $2x^{-1}$ ($x \equiv s$, p) states and then of subsequent Coster-Kronig (CK) and shake off processes. In both these processes initial single hole creation is the prime phenomenon and electron bombardment has been the primary source of energy. The calculated spectra have been compared with the measured satellite energies in Ly_1 spectra. Their intense peaks have been identified as the observed satellite lines. The one to one correspondence between the peaks in calculated spectra and the satellites in measured spectra has been established on the basis of the agreement between the separations in the peak energies and those in the measured satellite energies. It has been established that the satellite observed in the Ly_1 region of the X-ray spectra of various elements and named Ly_1' in order of increasing energy are mainly emitted by L_2 - $M_xN_{4,5}$ transitions. It is observed that the satellite $L\gamma_1$ in all these spectra can be assigned to superposition of four intense transitions, $L_2M_1{}^1P_1-M_1N_4{}^1D_2$, $L_2M_3{}^1D_2$ - $M_3N_4^1F_3$, $L_2M_3^1D_2-M_3N_5^1D_2$ and $L_2M_1^3P_0-M_1N_4^3D_1$, in order of decreasing contribution of intensity. The possible contributions of other transitions of the L₂M_x-M_xN₄₅ (x = 1-5) array have intensities comparable with the above transitions, and the corresponding lines, which have not yet been observed, are also discussed.

S2/P46 *Synthesis and Electrical Properties of CuClO4.4BN Doped Polyaniline Conducting System*

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Abstract

Polyaniline (PANI) has been synthesized by chemical route as suggested by Mac-Diarmid [1]. Chemical doping in dimethylsulfoxide (DMSO) solvent is made with Copper perchlorate tetra benzonitrite (CuClO₄.4BN) to enhance the conductivity level of synthesized polyaniline. An effort has been made to see the effect of dopant by IR spectra. Conductivity and dielectric properties have been measured at 25, 35, and 45° C. It has been found that dopant (CuClO₄.4BN) plays a significant role in polyaniline chain doping. It has been also observed that dimethylsulfoxide solvent in polyaniline doping with CuClO4.4BN also promise to increase the conductivity of doped polyaniline.This indicates that the DMSO is suitable solvent for polyaniline doping with dopant [CuClO4.4BN]. Dielectric properties measurements of doped PANI also show the effects of dopant.The electrical and dielectric properties of doped polyaniline suggested their potential applications [2] in electronic devices such as conducting rechargeable battery and other electronic devices applications.

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S2/P47

$(n = 2, 3, \ldots, 7)$ States of He

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High precision calculations have been performed for the doubly excited 2pnp: ${}^{3}P^{e}$ (n $= 2, 3 ... 7$) states of He within variational framework using highly correlated Hylleraas type expansion of the basis sets involving inter-electronic coordinates. The position of the energy levels have been systematically analysed by changing step by step the expansion length of the basis sets. With an expansion length of 483 parameters the doubly excited energy levels converge to within 6^{th} place of decimals for cases n>2. Result for the 2p²: ${}^{3}P^{e}$ state is benchmark with 336 parameters [1]. Benchmark calculations for n>2 are in progress in this direction. Calculated energy levels have been displayed in figure 1.

Fig 1. Doubly excited energy levels of 2pnp: ${}^{3}P^{e}$ (n = 2, 3 ... 7)

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S2/P48 Effect of Electron Correlations on Cooper Minimum of the *ns* Subshell of Free and Confined Atoms

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Studies of atoms confined in an endohedral environment, denoted as \mathcal{A} , have aroused great interest in the past few years [1, 2]. We report our studies on photoionization of ω_{Mg} , ω_{Ca} , ω_{Zn} , ω_{Ba} and ω_{Sr} . The effect of confinement on electron probability density distributions in $(a)Ca$, $(a)Ba$ and $(a)Sr$ differs from what it is in the case of ω_{Mg} and ω_{Zn} . In ω_{Ca} , ω_{Ba} and ω_{Sr} , the attractive trapping potential sucks in probability density in the region where it is significant, while in the case of $@Zn$ and @Mg, the peak in the probability density distribution remains largely unaffected by the cage even if a small part of the charge is sucked in the region of the cage but only where the probability density is low. This difference is found to have significant consequences on photoionization parameters.

 We use Relativistic Random Phase Approximation [3] to determine the photoionization parameters. It is found that in the case of $@Ca$, $@Sr$ and $@Ba$, interchannel coupling of photoionization channels from the *ns* subshell with channels from inner subshells moves the position of the Cooper minimum [4] to a higher energy relative to that obtained without coupling channels from the inner subshells. In the case of free Ca, Sr and Ba, the effect of interchannel coupling on the position of Cooper minimum is just the opposite, i.e. the Cooper minimum is drawn closer to the threshold when interchannel coupling with channels from inner subshells is included. However, it is found in the case of ωMg and ωZn , the interchannel coupling shifts the positions of the Cooper minima to lower values of energy, as also in the case of free Mg and Zn. The differences in the case of Mg and Zn on one hand and of Ca, Sr and Ba on the other are discussed in terms of the effect of the confining potential on the outer ns electron probability density distribution.

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S2/P49

Stark-Induced Transitions Between 'Same Parity' Electronic States of Atoms

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Single-photon induced electric dipole transitions between atomic states having same parity states are forbidden. Nevertheless, the static electric field mixes states of opposite parity and induces transitions between states of same parity which are weak, but have non-zero amplitudes. These 'Stark-induced transitions' have been used in several frontier experiments of current interest, like atomic parity-non-conservation processes [1].

In this paper we present and analyze the dependence on electric intensity of 'Starkinduced transitions' for some experimentally important atomic states. First order effect is considered in this work to address multi-reference electronic states obtained from Multi-Configuration Dirac-Fock (MCDF) method.

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Effect of crystal field on Ce3+ energy levels in La or Gd codoped $Y_3Al_5O_{12}$

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 $Y_3A₁₅O₁₂(YAG)$: Ce shows an intense greenish-yellow emission originating from ${}^{2}T_{2g}(5d) - {}^{2}F_{7/2}$, ${}^{2}F_{5/2}$ (4f) transition of Ce³⁺ ion due to spin-orbit coupling under the influence of O_h crystal filed. The excited levels of Ce^{3+} ion (5d) are sensitive to the local crystal field because these are not screened by other orbital. The effect of crystal field on $Ce³⁺$ ions are shown by change in photoluminescence emission maxima. In this work, we report the co-doping of Gd or La in YAG:Ce, which shows significant peak shift from 535 nm (YAG:Ce) to 556 and 576 nm for Gd or La phosphor, respectively.

S2/P51

Projectile Z dependence of Multiple Ionization and fragmentation of C_{60} **in collisions with 2.33 MeV/u highly charged ions and giant plasmon resonance**

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Studies on C_{60} fullerene molecules in collisions with fast heavy ions reveal many interesting features intermediate between typical gaseous and solid targets, owing to the nanoscale size of fullerene molecule. Here we present results from ionization, fragmentation and evaporation of C_{60} molecule in collisions with heavy ions. We used 2.33 MeV/u Li^{q^+} , C^{q^+} and O^{q^+} ion beams as projectiles. Various ionization and fragmentation products were detected using time of flight mass spectrometer. The multiply charged C_{60}^{Q+} were detected for maximum $Q = 4+$. The projectile charge state (q_p) dependence of the single and multiple ionization cross sections is well reproduced with a model based on giant dipole plasmon resonance (GPDR) [1]. A comparison is also made with the local plasma approximation. The data suggests that the model works well in case of single and double ionization [2,3]. We studied the behavior of fragmentation products as a function of q_p for different projectiles, which shows a linear increase in fragmentation yield with projectile charge. Interestingly the fragmentation yields show no dependence on the projectile atomic number. Variation of relative yield of evaporation products of C_{60}^{2+} (i.e. C_{58}^{2+} , C_{56}^{2+} etc) and those for C_{60}^{3+} + (i.e. C_{58}^{3+} , C_{56}^{3+} etc) has also been investigated for various projectiles and the data will be presented here.

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Author Index

Addicoat, M. D3/S13/T8 Ahmad, Nissar S2/P40 Ahuja, R S1/P05 Alderman, A. D4/S17/T4 Ali, Vazid S2/P46 Anandavadivel, A. S2/P26 Angom, Dilip D3/S11/T2, S1/P10 An, Kyungwon D1/S2/T3 Aslanidis, J. D3/S13/T8 Balakrishnan, V. S1/P20 Banerjee, T S1/P02, S2/P29 Bapat, B. D2/S8/T7 Barna, D. D1/S3/T8 Bell, C. Simon D2/S7/T4 Beltram, F S2/P26 Bera, N. C. S2/P28, S2/P30 Bhargavaram, N. D1/S4/T10A, S1/P17 Bhattacharya, A S2/P33 Bhattacharyya, I. S2/P28, S2/P30 Bhattacharyya, S. D2/S7/T6, S2/P47 Bieske, E. J. D3/S12/T6 Birdsey, B. D4/S17/T4 Bisht, B. PremD3/S12/T4 Buntine, M. D3/S13/T8 Buntine, Mark A. D3/S14/T11A Byun, Chang Woo S2/P31 Cardarelli, F. S2/P26 Chae, Min D2/S6/T2 Chakraborty, J. D2/S7/T6 Chandra, N. D3/S14/T12B Chang, T. N. D2/S9/T12 Chaudhuri, Rajat K. S1/P10, S2/P44 Chaudhuri, Saptarishi S1/P03, S1/P18 Chauhan, Raj Kumar S1/P04 Chen, Xiangjun D1/S4/T11A Chen, Yong-Fan D3/S14/T14B Chen, Weidong D3/S13/T7 Cheng, Wen-Yu D4/S15 Chhaya, V. M. S1/P15

Aravind, G. D1/S4/T10A, S1/P01, S1/P17 S2/P38

Chiba, Hisashi D3/S12/T3 Cho, Hyuck D4/S17/T3 Cho, Jaevoon D3/S14/T11B Choi, Nark Nyul S2/P31 Costa, Moario S2/P26 CURRELL, Fred J. D1/S4/T9A Das, A. K S2/P28, S2/P30, S2/P32 De, Sankar $S1/P05$, $S1/P16$ Deshmukh, P. C. S1/P02, S1/P06, S1/P21, Dixit, Gopal S1/P06, S2/P49 Dutta, Anjan S2/P40 Dutta, Sulagna S2/P34 Dryza, V. D3/S13/T8 Emmeluth, C. D3/S12/T6 Faisal, F.H.M**.** D2/S7/T6 Fujioka, S. D1/S3/T6 Fu, Yunging D3/S13/T7 Gangopadhyay, Sumona S1/P07, S1/P24, S2/P35 Gascooke, J. D3/S13/T8, D3/S14/T11A Gentleman, A. D3/S13/T8 Ghosh, P. N. S1/P05 Girard, Bertrand D3/S12/T3 Goodgame, A. L. D1/S2/T1 Goswami, Debabrata D1/S4/T10B Govekar, Rekha S2/P37 Guo, Panlin D3/S13/T7 Gupta,Jyotsana S2/P27 Gupta, Moumita S2/P36 Gupta, Sumit K. S2/P37 Hammond, P. D4/S17/T4 He, Mianhong D3/S13/T7 Hong, Feng-Lei D2/S7/T5 Hori, M. D1/S3/T8 Hori, N. D1/S2/T1 Hosaka, Kouichi D3/S12/T3 Hu, Wei D3/S13/T7 Huang, Min D3/S13/T7 Huang, Keh-Ning D4/S15/PT4 Hur, M. D4/S18/T7 Hutton, Roger D3/S13/T7 Imano, Miki D1/S3/T7 Imao, H. D1/S3/T8 Imran, Tayyab D3/S13/T10

Das, B.P. D2/S9/T10, S1/P10, S1/P13, S2/P43 Dastidar, Krishna Rai D1/S4/T9B, S2/P33, S2/P34, S2/P36 S1/P23, S2/P29, S2/P48, S2/P49, S2/P27

Jaman, A. I. D2/S9/T11 Jang, J. D4/S18/T7 Kanai, Yasuyuki D3/S13/T9 Kang, Kyung Sik D3/S13/T10 Karn,, Ranjeet K. S2/P40 KATO, Daiji D1/S4/T9A Katsuki, Hiroyuki D3/S12/T3 KAVANAGH, Anthony P. D1/S4/T9A Khajuria, Yugal S1/P21, D2/S5 Kim, J. D4/S18/T7 Kim, Jung Bog D2/S6/T2 Kim, Kyung Taec D3/S13/T10 Kimura, Mineo D4/S16/T2 Kobelt, Sarah L. D3/S14/T11A Komaki, K. D1/S3/T8 Koukitu, Akinori D1/S3/T7 Kottaisamy, M. S2/P50 Krishnakumar, E. S1/P01, S1/P17, S2/P38, Krishna, G Gopi S1/P08 Kulagin, V. D4/S18/T7 Kumar, Anitha C. D3/S14/T14A Kumar, S. V. K. D3/S14/T13A, S2/P37 Kuroda, N. D1/S3/T8 Lakshmibala, S. S1/P20 Latha, K.V.P. $S1/P10$ Lee, Fenglin D2/S6/T2 Lee, Hai-Woong D3/S14/T11B Lee, Min-Ho S2/P31 LI, Yueming D1/S4/T9A Liljeby, Leif D3/S13/T7 Lin, Jim J. D2/S8/T8 Limbachiya, C. G. S1/P07, S2/P41 Liu, Yong D3/S13/T7
Lodha. G. S. D2/S8/T9 Lodha, G. S. Lu, Di D3/S13/T7 Luo, Yuxiang D2/S9/T12 Maffei, L. S2/P26 Manohar, K.G. S1/P11, S1/P14 Marathe, Asawari P. S1/P11

Jagatap, B. N. D1/S2/T2,S1/P11, S1/P14 Joshipura, K N S1/P07, S1/P24, S2/P35, S2/P41 Kadhane, U S1/P09, S1/P12, S2/P42, S2/P51 Kelkar, Aditya S1/P09, S1/P12, S2/P39, S2/P42, S2/P51 D1/S4/T10A, D3/S13/T10 Kumar, Ajay S1/P09, S1/P12, S2/P39, S2/P42 Majumder, Sonjoy D3/S12/T5, S1/P06, S2/P49

Marchi, M. S2/P26 Maselli, Olivia J. D3/S14/T11A Mason, Nigel S2/P41 Mathur, Deepak D2/S7/T3 Meier, Christoph D3/S12/T3 Merkt, F. D1/S2/T1 Metha, G. D3/S13/T8 Metha, Gregory F. D3/S14/T11A Mishra, A. K. D3/S14/T14A $Misra$, J $S2/P50$ Mishra, Tapan S2/P43 Mohri, A D1/S3/T8 Momeen M. Ummal S1/P23 Morishita, Toru S1/P22 Motohashi, Kenji D1/S3/T7 Mukherjee, Mahua D2/S7/T6 Mukherjee, P. K. S2/P47 Mukherjee, T. K S2/P47 Nagata, Y. D1/S3/T8 NAKAMURA, Nobuyuki D1/S4/T9A Nam, Chang Hee D3/S13/T10 Nandedkar, R.V. D2/S8/T9 Nandi, T. D4/S18/T9, S2/P40 Nataraj, H. S. S1/P13 Nayak, Malaya K. S2/P44 Niu, Y. D4/S17/T4 Nishihara, K. D1/S3/T6 Nishimura, H. D1/S3/T6 Ohashi, H. D1/S3/T6 Ohmori, Kenji D3/S12/T3 Ohno, K. D1/S2/T1 OHTANI, Shunsuke D1/S4/T9A Pai, Akshay S2/P37 Pai, Ramesh V. D2/S9/T13, S2/P43 Pandit, Rahul D2/S9/T13 Park, Mi Na D3/S13/T10 Parida, Manas Ranjan S2/P27 Pattabiraman, M. S1/P23 Poad, B. L. J. D3/S12/T6 Poonia, Surendra S2/P45 Pradhan, Gagan Bihari S2/P49 Pradhan, S. S1/P14 Procter, S. R. D1/S2/T1 Qi, Fei D4/S17/T5

Misra, Deepankar S1/P09, S1/P12, S2/P39, S2/P42 S2/P51 Prabhudesai, Vaibhav S. D1/S4/T10A, S1/P17, S2/P38

Rahman, A. S1/P17 Raiyani, J. G. S1/P15 Rajput, Jyoti S1/P05, S1/P16 Ram, Bhargava N S2/P38 Ram, Nibedita S1/P23 Rangarajan, G. S1/P23 Rao, B. J. S2/P37 Rao, M.S.Ramachandra S2/P50 Ratto, G. M. S2/P26 Ray, Hasi S1/P25 Read, FH D4/S17/T4 Reddish, TJ D4/S17/T4 Roy, Anushree S2/P26, S2/P40 Roy, Sanjukta S1/P03, S1/P18 Rustagi, Kailash C. D1/S1/KN Safvan, C. P. S1/P05, S1/P16, S2/P40 Sahoo, B. K. $S1/P13$ SAKAUE, Hiroyuki A. D1/S4/T9A Salk, Sung-Ho Suck D3/S10/PT3 Sasaki, A. D1/S3/T6 Sathiyamoorthy, K S2/P27 Sathyamurthy, N D3/S14/T13B. Scholten, Robert E. D2/S7/T4 Seccombe, DP D4/S17/T4 Shan, Xu D1/S4/T11A Sharma, Lalita S1/P19 Sharma, Saroj K S2/P46 Sheludko, David D2/S7/T4 Sheshadri, K D2/S9/T13 Shibata, M. D1/S3/T8 Sil, A. N. S2/P47 Sinha, Chandana D4/S16/T1 Softley, T. P. D1/S2/T1 Soni, S. N. S2/P45 Srivastava, M. K S1/P04 Stauffer, A. D. S1/P19 Sudheesh, C. S1/P20 Sunil Kumar, S. S1/P21 Su, Xu Mei D2/S6/T2 Suk, H. D4/S18/T7 Takahashi, Masahiko D2/S5 Takahashi, R. D1/S2/T1 Tanner, Gregor S2/P31 Tanuma, H. D1/S3/T6 Tessier, D. D4/S17/T4

Rawat, P. D1/S4/T10A, S1/P17, S2/P38 Srivastava, Rajesh D1/S3/T5, S1/P04, S1/P19

Thompson, C. D. $D3/S12/T6$ Tiwari, Brajesh S2/P50 TORII, Hiroyuki A. D1/S3/T8 Toyota, Koudai S1/P22 Tribedi, Lokesh C. D2/S6/T1, S1/P09, S1/P12, Tsurubuchi, Seiji D1/S3/T7 Udagawa, Yasuo D2/S5/PT2 Umesh, G. D3/S13/T10 Unnikrishnan, C. S. D3/S11/T1, S1/P03, S1/P18 Vaishnav, B. G. S1/P24, S2/P35 Varma, Hari R. S2/P29, S2/P48 Varentsov, V. L. D1/S3/T8 Vijayan, C. D4/S18/T6, S1/P23, S2/P27 Vinodkumar, Minaxi S1/P07, S2/P41 Visser, B. D3/S13/T8 Vredenbregt, Edgar D2/S7/T4 Wang, Chang-Yi D3/S14/T14B Wang, Shih-Hao D3/S14/T14B WATANABE, Hirofumi D1/S4/T9A Watanabe, Shinichi S1/P08, S1/P22 Watanabe, Noboru D2/S5 Weddle, G. D3/S12/T6 Williams, Jim D4/S19/PT5 Wu, Fang $D1/S4/T11A$ Wu, Shimin D3/S13/T7 Xu, Kezun D1/S4/T11A Yamakita, Y. D1/S2/T1 Yamazaki, Y. D1/S3/T8 Yang, Dah-Yen D3/S14/T12A Yoo, S. D4/S18/T7 Yu, Ite A. D3/S14/T14B Zhan, Mingsheng D1/S1/PT1 Zhang, Weiping D1/S2/T4 Zhang, Xuemei D3/S13/T7 Zhu, Changjun D3/S13/T10 Zou, Yaming D3/S13/T7

S2/P39, S2/P42, S2/P51

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