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93 ATOMIC AND MOLECULAR PHOTO PROCESSES

94 Role of multiphoton excitation and two-electron effects in high harmonic generation of H_2 : a TDDFT calculation* XI JI, PATRICK MEMOLI, *The University of Montana* Using different TDDFT methods, we study the role of electronically excited states and two-electron dynamics in high harmonic generation (HHG) of H_2 . The two methods produce slightly different ionic structures as reflected in the calculated ionization potentials. They nevertheless give similar HHG spectra. The difference between the two methods increases with the laser intensity, while predictions remain qualitatively consistent. Our results suggest that two-electron dynamics can extend the HHG cutoff. Specifically, such an extension depends on the internuclear distance and the laser intensity. We propose an ion excitation plus tunneling ionization mechanism to explain these extensions. The involvement of excited states is further revealed when we analyze each harmonic as a function of the internuclear distance. We see resonant peaks that are due to multiphoton excitation. These peaks exist above the ionization threshold as well.

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95 Numerical simulations of H_2^+ and H_3^{2+} in intense ultrashort laser pulses* DANIEL WEFLER, NORIO TAKEMOTO, BREAS BECKER, JILA and Department of Physics, University of Colorado, 440 UCB, Boulder, CO 80309-0440 We developed numerical simulation techniques to analyze H_2^+ and H_3^{2+} interacting with intense ultrashort laser fields based on the Crank-Nicholson method and the Born-Oppenheimer approximation. We present results for the ionization probabilities and photoelectron spectrum for molecular ions, and for circularly polarized light as well as linearly polarized light both on and off the molecular axis.

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96 Electric-field-induced dissociation of heavy Rydberg ion-pairs* CARLOS REINHOLD, *Oak Ridge National Laboratory* SHUHEI YOSHIDA, *Vienna University of Technology* HONGHAO WANG, BARRY DUNNING, *Rice University* A classical trajectory Monte Carlo approach is used to simulate the dissociation of H^+-F^- and K^+-Cl^- heavy-Rydberg ion pairs induced by a ramped electric field. Such field-induced dissociation has been observed experimentally to detect ion-pair states and analyze their binding energies. The simulations include the effects of the strong long-range repulsive interaction associated with ion-pair scattering. Their predictions are in good agreement with experimental results for Stark wavepackets probed by a ramped field, demonstrating that many of the characteristics of field-induced dissociation can be well described using a purely classical model. The data also show that states with a given value of principal quantum number (binding energy) can dissociate over a broad range of applied fields, the exact field being governed by the initial orbital angular momentum and orientation of the state.

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97 Free-free transitions in the presence of a Debye potential laser field at very low incident electron energies ANAND K. TIA, *NASA/Goddard Space Flight Center* We study the free-

free transition in electron-hydrogenic systems in the ground state and embedded in a Debye potential in the presence of an external laser field at very low incident electron energies. The laser field is treated classically while the collision dynamics is treated quantum mechanically. The laser field is chosen as monochromatic, linearly polarized and homogeneous. The incident electron is considered to be dressed by the laser field in a nonperturbative manner by choosing Volkov wave function for it. The scattering wave function for the incident electron on the target embedded in a Debye potential is solved numerically by taking into account the effect of electron exchange. We calculate the laser-assisted differential cross sections for free-free transition for absorption/emission of a single photon or no photon exchange. The results will be presented at the conference.

98 THE IRON PROJECT & THE RMAX PROJECT: Highly excited Core resonances in photoionization of Fe XVII and impact on plasma opacities, oscillator strengths of Fe XIV, and nebular abundance of O II* ANIL PRADHAN, *Ohio State University* SULTANA NAHAR, *Ohio State U* ETHAN PALAY, *Ohio State U* WERNER EISSNER, *Stuttgart U* The aims of the Iron Project and the Rmax Project are detailed study of radiative and collisional processes of astrophysically abundant atoms and ions, mainly iron and iron-peak elements, over a wide energy range, from infrared to X-rays. We will illustrate the dominance of high energy photoexcitation-of-core (PEC) resonances in photoionization of Fe XVII due to strong coupling effects on dipole transition arrays $2p^5 \rightarrow 2p^4 (3s, 3d)$ in the core and examine PEC and non-PEC resonance strengths for their expanded role to incorporate inner-shell excitations for improved opacities. Comparisons show that the currently available cross sections from the Opacity Project are considerably underestimated. For Fe XIV, we present preliminary results from a large scale computation where 747 fine structure levels with $n \leq 10$, $l \leq 9$, and $0.5 \leq J \leq 9.5$, and 71,407 electric dipole allowed fine structure transitions have been obtained. We will also demonstrate the fine structure effects on the collision strengths and in very low energy photoionization for in nebular oxygen abundance.

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L1 99 Optical field enhancement and strong-field effects at sharp metal tips SEBASTIAN THOMAS, MARKUS SCHENK, MICHAEL KRÜGER, PETER HOMMELHOFF, *Max Planck Institute of Quantum Optics* We are currently studying strong-field effects at a nanometric metal tip by illuminating it with few-cycle femtosecond laser oscillator pulses. In this setup, the electric field at the tip's surface is significantly enhanced. Local optical field enhancement in the vicinity of metal structures occurs due to geometrical effects and dynamical effects like plasmon resonances. Both are described by Maxwell's equations, which we solve numerically to simulate the electromagnetic field for our experimental configuration. In the simulation, we observe a strongly localized field enhancement that vanishes within a few tens of nanometers from the tip's surface. Furthermore, the enhancement is not symmetric with respect to the tip's axis, which underlines the significance of dynamical effects in our setup. Experimentally, we observe above-threshold photoemission and strong field effects* even at low pulse energies due to field enhancement. Electron spectra might yield insight into plasmon dynamics on the nanometer-(sub-)femtosecond scale. We report on the current status of simulation and experiment.

*M. Schenk, M. Krüger, P. Hommelhoff, PRL 105, 257601 (2010).