Theoretical Studies on the dynamics of Atoms and Molecules in Strong Laser Fields

Xiao-Min Tong
Center for Computational Sciences, University of Tsukuba

1. Project Purpose

a) to investigate the mechanism of the abnormal excitation probabilities of Ar atoms in ultra-short linearly polarized and elliptical polarized laser field and search an effective way to control the excitation probabilities by tuning the IR intensity, carrier-envelop phase and ellipticity.

b) to investigate the non-dipole effects on the tunneling ionization and study dynamics processes due to the retardation effect on the attosecond time domains.

c) to investigate the attosecond streaking of H_2 molecules in an elliptical polarized laser field by our time-dependent density functional theory with semi-empirical self-interaction corrections. Collaborating with the ongoing experiment, we focused on how the correlation affects the attosecond streaking.

2. Results

a) We investigated the abnormal excitation probabilities by solving the time-dependent Schrodinger equation with many different laser parameters and found that the abnormal excitation probabilities originate from the resonant excitation due to the AC stark shifts induced by laser field. Convoluting the laser focal volume intensity distributions, the simulation results are in good agreement with experiments in a linearly polarized laser field. The work was published in Physical Review A [**101**, 053402:1-6 (2020)] as an international collaboration achievement. Meanwhile the work on the elliptically polarized laser field was also published on Physical Review A [**102**, 013116:1-6 (2020)] and it may guide the future experiment work.

b) We investigated how the photon energy and momentum transfer to materials in the strong laser field and material interaction. In dipole approximation, momentum transfer is completely ignored, and we had to consider the non-dipole or high order approximation to study the momentum transfer. The non-dipole effect breaks the symmetry along the laser propagation direction, so the simulation was extremely difficult. In this work, we show that the subcycle-resolved linear momentum transfer can provide novel insights into the interplay between nonadiabatic and nondipole effects in strong-field ionization. This work paves the way towards the investigation of the so-far unexplored time-resolved

nondipole nonadiabatic tunneling dynamics. This work was published Physical Review Letters [125, 073202:1-7 (2020)] as an international collaboration achievement.

c) We calculated the momentum distribution of H2 molecules in attosecond streaking by an elliptically polarized laser field. The results were passed to our collaborators of the experiment group and the data are currently analyzed and we hope that the work can be published soon.

3. Roles of the MCRP and its significance

All the above works involved large scale numerical simulations and no one of them can be done even with a high-performance workstation. Without the support of MCRP, we could not do any meaningful research on the theoretic work on the laser materials interactions. With the MCRP support, we can also study macroscopic spectra of high-order harmonic generation, which is the source of next general X-ray laser.

4. Future plan

We will continue our present theoretical work on the laser material interactions, and mainly focus on the excitation processes, which were ignored in the most works. Meanwhile, we will also work on the exotic atoms like muon Fe, or the capture processes on pion by helium atoms motivated by the recent experimental advances.

5. Publications and conference presentations

(1) Journal papers

1) T Pauly, ABondy, KR Hamilton, N Douguet, XM Tong, D Chetty, and K. Bartschat, "Ellipticity Dependence of Excitation and Ionization of Argon Atoms by Short-Pulse Infrared Radiation", Phys. Rev. A **102**, 013116:1-6 (2020).

2) HC Ni, S Brennecke, X Gao, PL He, S Donsa, I Brezinova, F He, J Wu, M Lein, XM Tong, and J Burgdorfer, "Theory of Subcycle Linear Momentum Transfer in Strong-Field Tunneling Ionization", Phys. Rev. Lett. **125**, 073202:1-7 (2020).

3) GS Boltaev, RA Ganeev, NA Abbasi, M Iqbal, VV Kim, H Al-Harmi, XM Tong, and AS Alnaser, "Routes to Control Cooper Minimum in High Order Harmonics Generated in Argon Gas", New J. Phys. **22** 083031:1-9 (2020).

4) D Chetty, RD Glover, BA deHarak, XM Tong, H Xu, T Pauly, N Smith, KR Hamilton, K Bartschat, JP Ziegel, N Douguet, AN Luiten, PS Light, IV Litvinyuk, and RT Sang, "Observation of dynamic Stark resonances in strong-field excitation", Phys. Rev. A **101**, 053402:1-6 (2020).

(2) Presentations

(3) Others

Supercomputer	Use	Allocated resources*	
		Initial resources	Additional resources
Cygnus	Yes	4,000	
Oakforest-PACS	Yes	40,000	
*in units of node-hour product			