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WG2 Expert Meeting on Biomolecules

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Institute of Physics Belgrade
University of Belgrade

Calculations of ionization probabilities for sodium in strong laser fields

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Ionization probabilities for sodium atom in strong laser fields are calculated for different ratios between the frequency and the field strength, covering both the quasistatic (tunneling/over-the-barrier) and the multiphoton ionization regimes. The probabilities are determined numerically using the wave-packet propagation technique [1] and the single electron model for alkali-metal atoms, where the valence electron moves in an effective core potential and the external field [2]. In the quasistatic regime (high-field-intensity/low-frequency) the ionization rate (probability per unit time) is obtained from the autocorrelation function, which is the overlap between the initial (here the ground) state $\psi(0)$ and the corresponding state $\psi(t)$ at a later time $t \geq 0$. The calculated values for the lowest state energies and ionization rates as functions of the field strength are in good agreement with the results obtained recently using other methods [2]. Additionally, the transition time from $t = 0$, when the external field is switched on, until the decaying (resonant) state becomes quasistationary (exponential decay) is estimated and the form of the final wave function is determined. The field ionization of sodium in the multiphoton regime (low-field-intensity/high-frequency) is studied for a linearly polarized laser pulse with the intensity profile of the electric field component $F \sin^2(\pi t/T_p)$ and the pulse duration T_p of a few femtoseconds. The ionization probability $P_{\text{ion}}(t)$ is determined by calculating the occupation probabilities $P_n(t)$ for each eigenstate of the valence electron as $P_{\text{ion}}(t) = 1 - \sum_n P_n(t)$ [3]. An example for the calculated probabilities as functions of time is shown in Fig. 1.

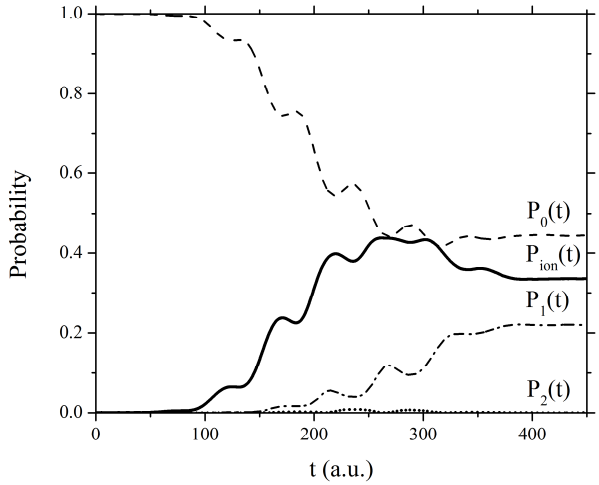

Fig.1. The occupation probabilities for the lowest three states as well as the related ionization probability for the sodium atom irradiated by the laser pulse of the wavelength λ = 760 nm, duration T_p = 10 fs (413.4 a.u.) and the peak intensity $1.72 \cdot 10^{12}$ W/cm^2 (F = 0.007 a.u.).

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WG2 Expert Meeting on Biomolecules is organized in the framework of the COST Action CM1204 ('XUV/X-ray Light and fast Ions for ultrafast Chemistry', XLIC). The project aims to better understand, to monitor and to control the complex ultrafast electronic and nuclear dynamics that occur in medium-sized and large molecules. Furthermore, new control strategies of reactions and a new generation of ultrafast spectroscopies combining attosecond temporal and sub-Angstrom spatial resolutions will be developed.

The WG2 Expert Meeting on Biomolecules will take place in Fruška gora (Serbia) from April 27th to April 30th, 2015. This meeting brings together experts from different disciplines (physics, chemistry), experiments and theory to discuss aspects on photon, ion and electron interaction with biomolecules, as well as properties of biomolecules, stability of highly excited and highly charged biological molecules in the gas phase and their reactivity.

We hope that this meeting will initiate new projects and collaborations, inspire new scientific achievements and help promotion of young researchers. We would like to thank the members of the Scientific Committee and Local Organizing Committee for their collaboration and the excellent work.

Paola Bolognesi and AleksandarMilosavljević
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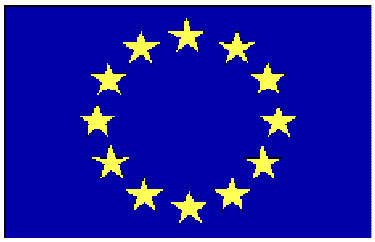

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