Imprints of the electronic structure in the photoelectron spectra of strong field-ionized triatomic molecules

M Paul and **S Gräfe**

Institut für Physikalische Chemie, Friedrich-Schiller-Universität Jena, 07743 Jena, Germany

We examine the strong-field ionization of a class of triatomic model systems interacting with few-cycle circularly polarized laser fields. The model systems are such parameterized that for all systems, the ionization potential is kept the same, while completely symmetric and asymmetric configurations can be directly compared, as well as short- and Coulomb-like potentials. [1,2] In order to characterize the ionization process, we employ a large toolset of methods, including quantum dynamical simulations, modified classical trajectory calculations, and extensions of the strong-field approximation (SFA). The aim is to disentangle the respective contributions of electronic excited states and the long-range character of the potential in different wavelength regions. [2,3]

We demonstrate how the symmetry and electronic structure of the system is imprinted into the photoelectron momentum distribution. Our analysis reveals that upon interaction with circularly polarized laser fields, the long-range character merely induces a small shift in the spectra, while the contribution of excited states is essential, in particular in near-infrared laser fields, compared to mid-infrared drivers, and for systems with larger internuclear distances, when excited electronic states are energetically closer.

We also discuss the effect of the carrier-envelope phase on the ionization dynamics, as well as the influence of molecular averaging. We could show that if we consider additionally that the laser pulses interact with an ensemble of randomly oriented molecules, many of the features in the strong-field photoelectron spectra which could be attributed to molecular properties average out and CEP effects dominate. [3]

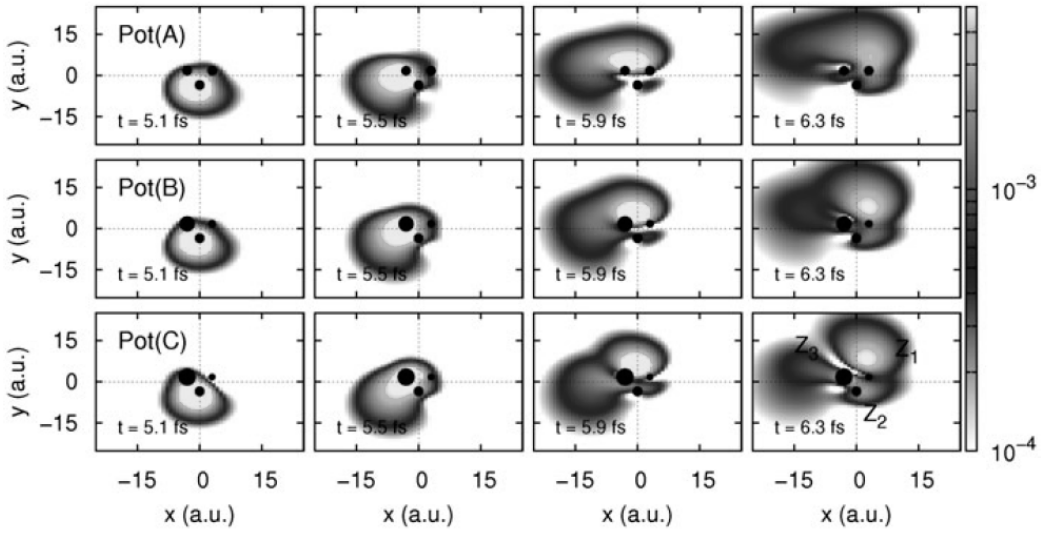

Figure 1: Exemplary snapshots of the strong-field ionization dynamics employing three different model potentials.

[1] Paul M, Yue L and Gräfe S. 2017 *J. Mod. Opt.* **64**, 1104.
[2] Paul M, Yue L and Gräfe S. 2018 *Phys. Rev. Lett.* **120** 233202
[3] Paul M and Gräfe S 2019 *Phys. Rev. A* **XXX** in press.