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Describing ionization of small molecules with a Gaussian and B-Splines Mixed Basis (GABS)

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Synopsis An interface between quantum chemistry electronic structure and scattering electronic theory was developed for representing the ionization of molecules. This description is achieved by creating a mix of Gaussian and B-spline functions (GABS) for the ejected electron and standard multiconfigurational methodology for the remaining bounded ones

The extraordinary evolution of experiments with time resolution at atomistic level requires, in general, the use of two laser pulses in a pump-probe scheme [1]. Although it is possible to use fluorescence or stimulated emission to probe the time evolution of the system, it is more common to ionize the molecule. In this frame, the knowledge of the ionization channel is crucial to understand the experimental outcome. Moreover, the possibility to synthesize ultrashort light pulses [2], belonging to extreme UV and X-ray regimes, has opened the way to create the so-called autoionizing states where one electron is spontaneously emitted without a probe pulse.

The use of Gaussians as basis functions to describe electronic bound states using multiconfigurational methods is nowdays a well-established technique. However, ejected electrons are difficult to describe using his type of methodology. In our group, an alternative is presented using a mix of Gaussian and B-splines functions (GABS) to describe the electron ejected in the ionization process [3].

In this contribution we expand this methodology to be used in polielectronic system by dividing the system in two different parts. On the one hand, the method takes into account the neutral molecule and the cationic eigenfunctions using Complete Active Space Self Consistent (CASSCF) methodology [4] with Gaussian basis centered in the atoms. On the other hand the ejected electron is described using the GABS methodology. The interface between the electron in the continuum and the ones in the bound states is calculated using a modified version of the MOLCAS suite of programs [5, 6]. As a proof of principle, we show the first results in small molecules.

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