X-ray induced fragmentation dynamics of doubly charged L-alanine in gas phase

XXIX International Conference on Photonic, Electronic, and Atomic Collisions (ICPEAC2015) IOP Publishing
Journal of Physics: Conference Series **635** (2015) 112094 doi:10.1088/1742-6596/635/11/112094

X-ray induced fragmentation dynamics of doubly charged L-alanine in gas phase

Yang Wang[*,†,1], **Helena Levola**[§], **Estefanía Rossich**[*], **Dariusz Piekarski**[*], **Sergio Díaz-Tendero**[*], **Edwin Kukk**[§], **Manuel Alcamí**[*], **and Fernando Martín**[*,†,¶]

[*] Departamento de Química, Módulo 13, Universidad Autónoma de Madrid, 28049 Madrid, Spain
[†] Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA-Nanociencia), 28049 Madrid, Spain
[§] Department of Physics and Astronomy, University of Turku, FIN-20014 Turku, Finland
[¶] Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain

Synopsis The molecular fragmentation of doubly charged L-alanine in gas phase was studied in radiation synchrotron experiments. In this presentation, we summarize our theoretical study on the dynamics of this fragmentation, using various computational methods. We show that in practice the ground state MD simulations are able to statistically reproduce the experimental results of the photo-fragmentation initiated at the excited state.

The study of fragmentation dynamics of charged biomolecules is of great interest, aiming at helping us to better understand the processes of biological damage by irradiations. In recent experiments, L-alaline molecules were ionized into doubly charged excited states, as a result of the Auger decay induced by N 1s core photoionization. The excited molecules then dissociated into fragments. The Auger electron spectra were recorded in coincidence with time-of-flight mass spectra of the cationic fragments using the Auger Electron Photo-ion Photo-ion Coincidence (AEPIPICO) technique (see Fig. 1) [1]. The probabilities of various dissociation channels were also measured as functions of the kinetic energy of the Auger electron, which implied that the fragmentation of the parent dication would follow different mechanisms, depending strongly on the internal energy deposited on the molecule.

Here, we summarize our theoretical study on the fragmentation dynamics of doubly charged L-alaline molecule in gas phase by using various computational methods, including the time-dependent density functional theory (TD-DFT) Ehrenfest Molecular Dynamics (MD), the Born-Oppenheimer MD simulations, the Car-Parrinello MD, the self-consistent charge density functional tight-binding (SCC-DFTB) MD and the atom-centered density matrix propagation MD simulations. As one of the simplest amino acids, L-alanine is an excellent benchmark model to test the performance of these methods, By comparing with the experimental results, we show that the more accurate TD-DFT method for excited state dynamics is too time-consuming to afford a statistical study. In practice, one can apply ground state MD simulations by depositing the vibrational internal energy in place of the excitation energy onto the molecule. As shown in Fig. 1, the simulated AEPIPICO map by the SCC-DFTB method gives an overall agreement with experiment. We also show how the fragmentation dynamics depends on the spin state and the initial conformation of the molecule.

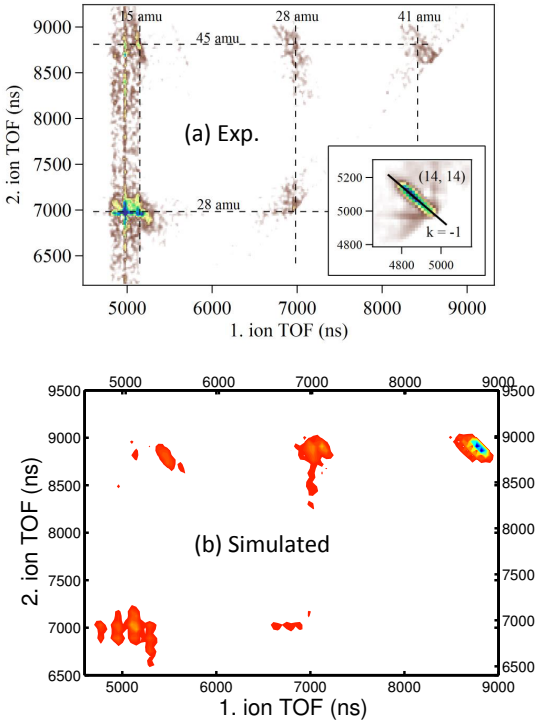

Figure 1. Comparison between (a) the experimental AEPIPICO map and (b) that obtained from the SCC-DFTB MD simulations.

References

[1] D. T. Ha *et al* 2014 *J. Phys. Chem. A* **118** 1374
[2] S. Maclot *et al* 2013 *J. Phys. Chem. Lett.* **4** 3903
[3] M. Capron *et al* 2012 *Chem. Eur. J.* **18** 9321

[1] E-mail: yang.wang@uam.es