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2015 J. Phys.: Conf. Ser. 635 112022

(http://iopscience.iop.org/1742-6596/635/11/112022)

XXIX International Conference on Photonic, Electronic, and Atomic Collisions (ICPEAC2015) IOP Publishing
Journal of Physics: Conference Series **635** (2015) 112022 doi:10.1088/1742-6596/635/11/112022

Interatomic Coulombic decay in polyatomic rare-gas clusters.

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Synopsis A new method for a complete theoretical description of Interatomic Coulombic decay (ICD) in large polyatomic rare-gas clusters will be presented. This original method combines the projection-operator formalism of resonant scattering theory, the diatomics-in-molecules technique and a surface hopping algorithm. Such combined approach has fairly low computational costs and constitutes an efficient tool for studying ICD in polyatomic clusters. Benchmark examples will be given to illustrate the method. Results on ICD in large rare-gas clusters will finally be reported.

Interatomic (molecular) Coulombic decay (ICD) is an ultrafast non-radiative electronic decay process for excited atoms or molecules embedded in a chemical environment [1]. Via ICD, the excited system can get rid of the excess energy, which is transferred to one of the neighbors and ionize it. ICD produces two charged particles next to each other and thus leads to Coulomb explosion (see Fig.1).

In the last decade, ICD has attracted considerable and rising attention [2]. One of the reasons for the current broad interest in ICD is the possibility of analytical applications. For example, Auger effect is widely used to probe the atomic composition and the environment of the atoms of materials via Auger electron spectroscopy. ICD is clearly superior to the Auger effect in its sensitivity to the chemical environment. Indeed, here the decay itself is possible only due to the effect of the environment, even if the interaction of the ionized atom or molecule with the environment is very weak.

In order to develop such ICD spectroscopy a better knowledge of this effect in large polyatomic systems is necessary. From the theoretical point of view general quantum mechanical equations for describing the decay processes and the subsequent fragmentations are known but are only applicable for rather small systems. Approximate, but accurate, methods are therefore needed to go beyond benchmark systems.

To this end, an original approach for a complete theoretical description of ICD in polyatomic rare-gas clusters will be presented. This approach combines the projection-operator formalism of resonant scattering theory, the diatomics-in-molecules technique and a surface hopping algorithm. It thus involves a classical treatment for the nuclear motion while retaining a quantum description for the electron dynamics [3]. The potential energy and the decay widths surfaces are computing on-the-fly using the diatomics-in-molecules technique. Such combined approach has low computational costs and can be used to study much larger systems. Some examples to illustrate the method will be given. Results on ICD in large rare-gas clusters will finally be reported.

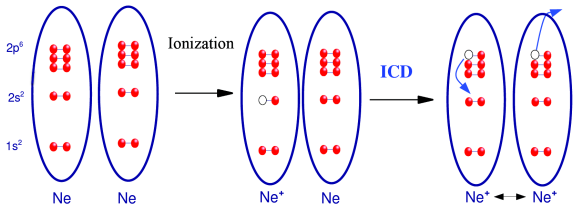

Figure 1. Scheme of the ICD process in Neon dimer.

References

[1] L. S. Cederbaum, J. Zobeley and F. Tarantelli 1997 *Phys. Rev. Lett.* **79** 4778

[2] see http://www.pci.uni-heidelberg.de/tc/usr /icd/ICD.refbase.html for a complete list of ICD publications

[3] N. Sisourat 2013 *J. Chem. Phys.* **139** 074111

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