



HAL
open science

Interatomic Coulombic decay in polyatomic rare-gas clusters

N Sisourat

► **To cite this version:**

N Sisourat. Interatomic Coulombic decay in polyatomic rare-gas clusters. Journal of Physics: Conference Series, 2015, 635 (11), pp.112022 10.1088/1742-6596/635/11/112022 . hal-01266921

HAL Id: hal-01266921

<https://hal.sorbonne-universite.fr/hal-01266921>

Submitted on 3 Feb 2016

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Distributed under a Creative Commons Attribution| 4.0 International License

Interatomic Coulombic decay in polyatomic rare-gas clusters

This content has been downloaded from IOPscience. Please scroll down to see the full text.

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

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

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 134.157.80.136

This content was downloaded on 03/02/2016 at 14:30

Please note that [terms and conditions apply](#).

Interatomic Coulombic decay in polyatomic rare-gas clusters.

N. Sisourat*¹

* Laboratoire de Chimie Physique - Matière et Rayonnement, Université Pierre et Marie Curie, Paris, France

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.

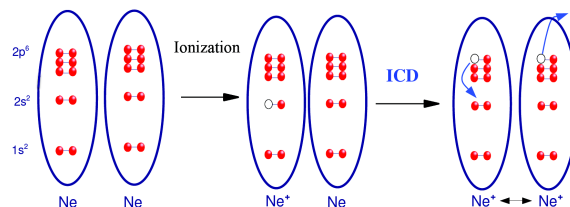


Figure 1. Scheme of the ICD process in Neon dimer.

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

¹E-mail: Nicolas.Sisourat@upmc.fr

