Ab initio molecular dynamics of photovoltaic organic self-assembled monolayers adsorbed on metal surfaces

Researchers:

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Language Undefined

Description:

Proyecto asignado a través de la Red Española de Supercomputación [2].

Study of different properties of small carbon clusters, fullerenes, metal clusters and biomolecules. The main purpose is to understand the mechanism behind the collisions of these species with highly charged atomic ions and energetic photons. In carbon clusters, the project is focused on properties such as the electronic structure, geometrical properties and stability. For that it uses usual quantum chemistry methods (coupled cluster and multireference methods) as well as Density Functional Theory (DFT).

Study of the charge transfer and fragmentation in collisions of highly charged fullerenes, using a time-dependent close-coupling method developed in our group. The energy deposited leads to fragmentation, which we study using statistical methods also developed in our group.

Study of bigger systems, such as biomolecules (i.e. uracyl or adenine). Application of statistical methods and time-dependent DFT to study the fragmentation of such molecules after collisions with ions and photons.

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[1] https://www.uam.es [2] https://www.res.es/