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F Kossoski, M Barbatti. On-the-fly dynamics simulation of dissociative electron attachment to chloroethane. *Journal of Physics: Conference Series*, 2020, 1412 (17), pp.172010. 10.1088/1742-6596/1412/17/172010 . hal-03812068

HAL Id: hal-03812068

<https://hal-amu.archives-ouvertes.fr/hal-03812068>

Submitted on 12 Oct 2022

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On-the-fly dynamics simulation of dissociative electron attachment to chloroethane

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Synopsis We present a novel theoretical approach for describing dissociative electron attachment. It is based on classically propagating the nuclei on the potential surface of the resonant anion, which is described by bound state methods, while electron autodetachment is taken into account with an ad-hoc model built from scattering calculation results. As a first application, we considered the electron induced dissociation of chloroethane. Comparison to experimental data is very encouraging. The simulations reveal further details on the underlying dynamics of the dissociation.

Electron capture by a molecular target can give rise to a resonant anion, which decays either by detachment of the excess electron or by dissociation. The later process, dissociative electron attachment (DEA), plays key roles in radiation-induced biological damage, current and nascent technological applications, interstellar medium, among others [1].

Existing theoretical descriptions of DEA usually rely on propagating the nuclear wavepacket on complex potential energy surfaces, which are built from computationally demanding scattering calculations [2]. Despite being successful, most applications are limited to small molecules [3] or to models of reduced dimensionality [4]. Molecular dynamics simulations for the later stages of DEA are sometimes employed [5], after the anion becomes stable against autoionization. However, we are not aware of any current and feasible method capable of describing DEA to systems with more than a few vibrational degrees of freedom while considering for the finite lifetimes of the resonances.

We propose an alternative approach to the problem, where the resonant anions are described with bound state methods, nuclei are propagated classically, and electron autodetachment is accounted for by a model that requires few scattering calculations. This approach is benchmarked against quantum wavepacket propagation on model potential energy curves. Different curve steepness, magnitudes of the imaginary component and reduced mass were considered. We found a very similar overall behavior for the cases considered.

The very first application of the proposed ap-

proach concerns DEA to chloroethane, where the chloride ion is abstracted via formation of a σ^* resonance [6]. An ensemble of classical trajectories were propagated on potential surfaces computed on-the-fly at the Multireference configuration interaction with singles and doubles level of theory. The σ^* character of the anion state was confirmed with electron scattering calculations performed with the Schwinger multichannel method [7]. These later calculations further provided resonance widths, which were employed for modeling the autodetachment probability during the dynamics propagation.

The computed DEA cross section showed the same experimentally observed [6] displacement from the vertical resonance energy (~ 2.5 eV) to the maximum ion yield energy (~ 1.5 eV), as well as comparable magnitudes. This supports the adopted autodetachment model and the overall proposed strategy to the problem. We have also addressed the dependence of the DEA cross section on several components of the simulation: the accuracy of the autodetachment model, of the electronic structure and scattering calculations. Finally, the dynamics simulation provides a detailed time-dependent picture on the relaxation of the resonant anion.

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