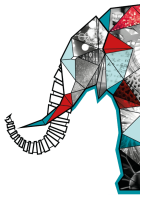
25e Congrès Général de la Société Française de Physique



ID de Contribution: **154** Type: **Orale**

COHERENT ELECTRON AND NUCLEAR DYNAMICS IN MOLECULES

mercredi 10 juillet 2019 14:30 (15 minutes)

Excitation or ionisation of a molecule with a short (attosecond) pulse leads to the coherent population of several electronic states, called an electronic wavepacket. The interference between electronic states in such a superposition, alternating between constructive and destructive, leads to oscillating motion of the electron cloud [1]. This purely quantum process relies on the coherence of the electronic wavepacket. A fundamental challenge is to understand to what extent the electronic wavepacket retains its coherence, i.e., how long the oscillations in the electron cloud survive, in the presence of interactions with the nuclei of the molecule [2,3]. To address this question, we have developed semi-classical and quantum mechanical methods [4,5] to simulate the dynamics upon ionisation of polyatomic molecules. The nuclear motion induced by an electronic wavepacket is also of interest in the context of attochemistry.

(1) Vacher, Mendive-Tapia, Bearpark, Robb, J. Chem. Phys. 2015, 142, 094105.
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(3) Vacher, Bearpark, Robb, Malhado, Phys. Rev. Lett. 2017, 118, 083001.
(4) Vacher, Mendive-Tapia, Bearpark, Robb, Theor. Chem. Acc. 2014, 133, 1505.
(5) Vacher, Bearpark, Robb, Theor. Chem. Acc. 2016, 135, 187.

Choix de session parallèle

4.4 Physique à l'échelle de l'atto-seconde

Auteur principal: VACHER, Morgane (Uppsala University)

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Classification de Session: Séance Parallèle