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Hydrogen isotope dependence in dissociative electron attachment

Tuesday, 16 July 2024 13:55 (25 minutes)

In my talk, I will present a theoretical investigation on electron-D2 resonant collisions, via the low-lying and the Rydberg states of D2–. I will focus, in particular, on low-energy cross section calculations, vibrationally resolved, for the dissociative attachment process in the ground state, and two electronic excited states of D2. Isotopologue effect for H2 and D2 will be shown and transitions between electronic excited states will be considered.

The electronic structures of deuterium are obtained by using ab-initio quantum chemistry approaches implemented in computer codes like MOLPRO and UK–R-Matrix whereas the nuclear dynamics is studied within the theoretical models of Bardsley's local-complex-potential model.

Comparisons with cross sections present in the literature, where applicable, will be presented.

Primary author: Dr LAPORTA, Vincenzo (Istituto per la Scienza e Tecnologia dei Plasmi, CNR, Italy)

Presenter: Dr LAPORTA, Vincenzo (Istituto per la Scienza e Tecnologia dei Plasmi, CNR, Italy)

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