

Signature of the neighbor's quantum nuclear dynamics in the electron transfer mediated decay spectra

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Abstract:

We computed fully quantum nuclear dynamics, which accompanies electron transfer mediated decay (ETMD) in weakly bound polyatomic clusters. We considered two HeLi₂ clusters – with Li₂ being either in the singlet electronic ground state or in the triplet first excited state – in which ETMD takes place after ionization of He. The electron transfer from Li₂ to He⁺ leads to the emission of another electron from Li₂ into the continuum. Due to the weak binding of He to Li₂ in the initial states of both clusters, the involved nuclear wave packets are very extended. This makes both the calculation of their evolution and the interpretation of the results difficult. We showed that despite the highly delocalized nature of the wave packets the nuclear dynamics in the decaying state is imprinted on the ETMD electron spectra. The analysis of the latter helps understanding the effect which electronic structure and binding strength in the cluster produce on the quantum motion of the nuclei in the decaying state. The results produce a detailed picture of this important charge transfer process in polyatomic systems.