

Dynamic Pathways in Multidimensional Landscapes



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Multidimensional Landscapes

Contribution ID : 6

Correlated non-adiabatic proton-hole motion after photoionization

Content :

The protonated water dimer irradiated with the free-electron laser FLASH at DESY (90 eV) undergoes Coulomb-explosion after losing one of its valence electrons via photoionization [1]. Because of the close-lying outer valence orbitals and various conical intersections, non-adiabatic effects are presumably important for the overall dynamics. Ab initio potential energy surfaces for the three lowest di-cationic states have been computed at the CASSCF level. A regularized diabaticization scheme is used to obtain a diabatic representation of the vibronic Hamiltonian [2]. The quantum dynamics of the photo-fragmentation has been investigated using the multi-configuration time-dependent Hartree (MCTDH) method [3]. We find that the correlation between the motion of the shared proton and the newly created hole builds up in less than five femtoseconds. The build up of the proton-hole correlation is a consequence of strong non-adiabatic effects [4,5].

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