Chemical Physics Letters

Volume 284, Issues 1â€“2, 20 February 1998, Pages 71-77

An extended empirical valence bond model for describing proton transfer in $H^+(H_2O)_n$ clusters and liquid water

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https://doi.org/10.1016/S0009-2614(97)01365-1

Abstract

An extended empirical valence bond Hamiltonian for performing molecular dynamical simulations of an excess proton in water is proposed. This model includes an arbitrary number of valence states and allows for a consistent description of the delocalized electronic structure around the excess charge. The non-additive force field thus obtained was used to investigate equilibrium properties and finite temperature dynamics of small $H^+(H_2O)_n$ clusters, as well as proton transfer dynamics of an excess proton in liquid water.

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