

Structure, dynamics and reactivity of the hydrated electron

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In this work, one of the products of ionization of water, namely the hydrated electron, has been investigated. The hydrated electron is a key-intermediate in aqueous radiation chemistry. Although known to exist for over 50 years, its structure remained elusive and under discussion up to the present day. We show in this work, that we can obtain a faithful picture of the hydrated electron, its equilibrium structure, dynamics after attachment to water, and its reactivity, using ab initio methods. To this end, small cluster models and extended bulk and slab geometries of water including an excess electron have been investigated.