Electron Dynamics of Solvated $Ti(OH)_4$

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Optimization of photocatalytic materials starts by understanding the properties of fundamental components that build such materials. Titania systems have shown promising results for alternative energy generation using photoelectrochemical processes.[1] Titanium dioxide nanostructures (nanorods, thin films, and quantum dots) are synthesized involving a form of Ti(IV).[2] We model $Ti(OH)_4$ in an explicit aqueous solution as an important step in understanding the mechanism of wet synthesis of TiO_2 nanostructures, according to laboratory procedure. Equilibrium geometry optimization and the finite temperature ab initio molecular dynamics are studied by DFT with PBE in VASP software. The radial distribution function, spin-polarized and non-spin polarized absorption spectra, and the non-adiabatic couplings are evaluated at different temperatures. Reduced density matrix theory, in the basis of Kohn-Sham orbitals is applied to explore non-radiative electron relaxation results.[3-5] The electron-hole relaxation rates show a non-linear dependence on temperature and were found to be near the same order of magnitude as electron-hole relaxation rates in bulk TiO_2 calculations. Observing the behavior of essential TiO_2 components complements knowledge of, bulk and nano, titania structure characteristics. The results can help to manipulate the synthesis of TiO_2 nanostructures toward a higher efficiency of harvesting, converting, and storing the energy from sun light.

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