On the possibility of photocatalytic water splitting on rutile TiO2(110): a theoretical study

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Solar-based hydrogen production by photocatalytic water splitting offers a route towards the delivery of clean fuel. Semiconductor metal oxides have been typically employed to mediate the photon-induced catalytic process but a comprehensive description of the elementary reaction pathways and charge-carrier dynamics is largely lacking even for the widely used TiO2 [1]. We performed Ehrenfest molecular dynamics within the framework of time-dependent density functional theory to assess the possibility of water oxidation by photogenerated hole on rutile TiO2. We find that molecular water adsorbed on a clean TiO2(110) surface readily dissociates under extreme ultraviolet irradiation, and that dissociation on defect-containing surfaces could be thermally assisted under weaker excitation.

References

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