First principles simulations of materials and processes in photo- and electro-catalysis

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Environmental and energy-related issues have prompted considerable interest in photocatalysis and electrocatalysis over the last decade. In the search for new materials and processes capable of improving existing technologies, theoretical and computational modeling has proven a very useful tool which can provide microscopic insights sometimes difficult to obtain by experiment. In this talk I will discuss applications of electronic structure calculations and molecular dynamics simulations to understand materials properties and reaction mechanisms in photo- and electro-catalysis. Examples will include studies of the interface between water and titanium dioxide (TiO_2), a widely used photocatalyst capable of splitting water in O_2 + H_2, and the cycle of H_2 production from water by the active site of an enzyme of hydrogen-producing bacteria, the di-iron hydrogenase, linked to a pyrite electrode.

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