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Abstract for an Invited Paper
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First principles simulations of materials and processes in photo- and electro-catalysis

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I shall 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 $\text{O}_2 + \text{H}_2$, 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.