Abstract:

In this talk I shall discuss applications of first principles electronic structure calculations and molecular dynamics simulations to understand materials properties and reaction mechanisms relevant to photocatalysis and energy applications. Examples will include studies of the surface properties of TiO$_2$, a widely used photocatalyst capable of splitting water in $\text{O}_2 + \text{H}_2$, and the spinel cobalt oxide Co$_3$O$_4$, a promising catalyst for low-temperature CO oxidation, water oxidation, and the oxygen reduction reaction.

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