Computational modeling of catalytic materials for energy and environmental applications

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The development of renewable energy technologies is limited by the availability of novel materials that are abundant and that can efficiently promote the relevant fundamental chemical/physical processes. This is particularly important for technologies relying on materials that catalyze electrochemical reactions, which govern the conversion and storage of solar into chemical energy or the energy storage into batteries.

In my talk I will present an overview of how state-of-the-art ab-initio computational modeling can provide key guidelines for the rational design of superior molecular catalysts and composite materials designed with a bottom up approach and atomic control.

After a brief description of the methods, of their main predictive power and limitations, I will present recent results on novel catalytic materials for electrodes in solar-to-fuel and fuel cell technologies [1-6].

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