Quantum Chemical Modeling of the Oxygen Evolution Reaction on Se-Doped TiO_2 (101)

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Developing clean, renewable, and affordable energy sources is crucial for meeting increasing energy demands in an environmentally sustainable manner. The water splitting is one of the most promising energy conversion systems and consists of the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER). Of these two reactions, the OER plays a limiting role in the ability to convert water into hydrogen. Understanding the detailed mechanism and energetics of this reaction and improving catalytic activity are keys to developing advanced and effective catalysts for the OER. TiO_2 is one of the most popular and intensively studied catalysts for the photochemical water splitting in theoretical and experimental research. Despite this interest and potential, the influence of Se doping in modifying the electrocatalytic OER performance on TiO_2 has not been studied in detail. To address this gap in the literature, we have explored the effect of Se doping on TiO_2 anatase (101) surface for the electrocatalytic oxygen evolution using plane-wave density functional theory (DFT) calculations. In the seminar, we will discuss the energetics and electronic structures of species along the potential OER mechanisms on Se-doped TiO_2 anatase (101) surfaces. we will also discuss how replacing a range of O atoms in TiO_2 with Se affect the light absorption properties of this material with the goal of applying these insights to develop effective water splitting photocatalysts.