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Calculating polarons in TiO2

A talk by Peter Deak

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LOCATION: TU Wien, Seminarraum 138C (Freihaus, Turm B/yellow, 9. OG)

TiO2 is a model material, not only as reducable oxide in photocatalytic applications, but also for studying small polaron states, common in materials with strong electron phonon coupling. Interestingly, the two main polymorphs, rutile and anatase, behave quite differently in this respect, which poses a real challenge for electronic structure calculations. The screened hybrid functional HSE06 provides a total energy in TiO2 which is a correct piecewise linear function of the occupation numbers. Therefore, the band gap is well reproduced and the generalized Koopman’s theorem is satisfied. Consequently, HSE06 describes the localization of defect states very well, and provides also accurate gap levels in this material. Applying it to investigate carrier self-trapping in TiO2, I will show that, in rutile, electron polarons are favored with location in the bulk or subsurface. In anatase, hole polarons are strongly bond both in the bulk and on the surface, but electron polarons occur only on the surface. As I will discuss, this phenomenon gives rise to important differences between the two polymorphs in the doping properties of their bulk, as well as in the way photocatalysis works and oxygen vacancies behave on their surfaces. Finally, our study of the nature of the Nb dopant on the anatase surface will be described, using the Lany-Zunger polaron correction to GGA.