Polarons and excitons in insulators: insight from computer simulations
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Localization of electrons and holes as well as excitons in insulators is a ubiquitous phenomenon which controls carrier mobility, luminescence and radiation damage of many materials. When such localization takes place in a perfect lattice it is called self-trapping, however in many cases it is facilitated by perturbation induced by intrinsic defects and impurities. Whatever the mechanism, it is hard to prove experimentally and especially theoretically. I will first review briefly the established models of self-trapped polarons and excitons (STE) in alkali halides and cubic oxides and will demonstrate how they are linked to the mechanisms of photo-induced desorption of these materials [1]. I will then discuss the results of our modeling, which extend these models further to more complex oxides forming so called electrides – materials where electrons serve as anions [2], and to a qualitatively new type of electron trapping at grain boundaries in polycrystalline materials with negative electron affinity [3]. Combining periodic and embedded cluster methods we can explain and sometimes predict the properties of polarons and excitons in a range of insulators, such as amorphous SiO$_2$ [4], and polycrystalline HfO$_2$[5] and HfSiO$_4$. I will discuss the applicability of different techniques to studying localization problems in insulators and will compare the predictions of periodic plane wave and embedded cluster DFT calculations.


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