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Polarons and excitons in insulators: insight from computer simulations¹

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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 electriles – 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 SiO₂ [4], and polycrystalline HfO₂ [5] and HfSiO₄. 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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[3] K. P. McKenna and A. L. Shluger, Nature Materials, 7, 859 (2008)

[4] A. V. Kimmel, et al. J. Non-Cryst. Sol., 353, 599 (2007)

[5] D. Munoz Ramo, et al. Phys. Rev. Lett. 99, 155504 (2007)

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