Defect formation energies in FeO: A comparison of molecular statics and molecular dynamics

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Point defects affect various properties of crystals, for example, electrical conductivity, self-diffusion processes, and phase transition parameters depend on their concentration and mobility. The concentration of defects can be obtained directly from molecular dynamic calculation [1], but this method requires huge computational resources. At the same time concentration of point defects can be described in terms of the free energy of defect formation. Using the chemical potential, the concentration can be obtained from static calculations. However, the use of the chemical potential in multicomponent crystals raises the question of the choice of reference state. In this work, we use iron oxide FeO with a Tersoff potential [2] as a model of a two-component crystal, for it we obtain and compare the defect energies from both methods.

[1] Smirnov G S and Stegailov V V 2019 *J. Phys.: Condens. Matter* **31** 235704

[2] Byggmästar J, Nagel M, Albe K, Henriksson K O E and Nordlund K 2019 *J. Phys.: Condens. Matter* **31** 215401