Computational methods for the prediction of vibrational spectra of oxygen-related defects in ZnO

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Zinc oxide is an n-type semiconductor that attracts interest from academic and industrial communities due to its wide-ranging applications. However, the nature of intrinsic point defects in ZnO is not yet established. Unexpectedly, computational studies consistently predict high formation energies for major intrinsic defects, which can be reconciled with experiment if either (i) formation of the intrinsic defects in the material is facilitated by heavy complexation or impurities, or (ii) defects are not in thermodynamic equilibrium within an infinite homogenous system, but are rather frozen in the material from synthesis or in dynamic equilibrium with environment or surface kinetics. In order to help resolve such uncertainties, we will present computational methods developed in the framework of hybrid QM/MM approaches to predict spectroscopic signatures of defects of interest, which we demonstrate for computational infrared and Raman vibrational spectra of oxygen defects in zinc oxide.