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Accuracy of defect formation energies from first-principles calculations: A study of vacancies in ZnO YIYANG SUN, National Renewable Energy Laboratory — Formation energy of point defects determines the concentration of the defects at thermal equilibrium. Accurately calculated formation energies can be used to pinpoint the type of the dominant defects at specific experimental conditions. First-principles calculations based on the density-functional theory and the supercell modeling of the point defects are the state-of-the-art approach to obtaining the formation energies. In this study, taking the O and Zn vacancies in ZnO as examples, we investigate the effects of supercell size on the accuracy of calculated formation energies. It is found that the 5x5x3 supercell is sufficient to reach the accuracy of about 0.06 eV in the formation energies, which means that the defect concentration can be evaluated with an accuracy in the magnitude of 10, considering k_BT is about 0.026 eV at room temperature. For charged defects, the shift of valence band maximum (VBM) is an additional factor which affects the accuracy of calculated formation energies. It is found that the 5x5x3 supercell is able to obtain the VBM shift at an accuracy of about 0.02 eV.

Yiyang Sun
National Renewable Energy Laboratory

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