

Abstract Submitted
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Defect complexes in semiconductors and insulators¹ HANNES RAEBIGER, Yokohama National University, Yokohama, Japan — The interaction of isolated defects and impurities (concentration upto $\sim 10^{18} \text{ cm}^{-3}$) is usually rationalized as that of point charges in a dielectric medium, but as defect concentrations are in the order of atomic percent ($\sim 10^{21} \text{ cm}^{-3}$), the statistical probability for two or more defects to sit on neighboring sites, forming a cluster or complex, becomes significant [1]. The formation of such clusters changes the local chemical environment, which in turn affects the electronic (and optical and magnetic) properties of the constituent defects non-trivially. To understand these changes, I study a variety of bound defect complexes in wide-gap semiconductors, composed of both deep and shallow defects, focusing on the shifting of the gap levels caused by defect-defect chemical interactions. First the electronic structure is calculated from first principles calculations, and then I will outline a simple theory that describes the level shifts due to cluster formation qualitatively and semi-quantitatively in terms local atomic shielding constants derived from local charge self-regulation [2].

[1] R. Behringer, J. Chem. Phys. **29**, 537 (1958).

[2] H. Raebiger, S. Lany, and A. Zunger, Nature **453**, 763 (2008).

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Hannes Raebiger
Yokohama National University, Yokohama, Japan

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