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Defect complexes in semiconductors and insulators[1] HANNES RAEBIGER, Yokohama National University, Yokohama, Japan — The interaction of isolated defects and impurities (concentration upto $\sim 10^{18}$ 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 ($\sim 10^{21}$ 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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