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Defects at the Nanoscale: The Role of Quantum Confinement and Dimensionality[1]

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One of the most challenging issues in materials physics is to predict the properties of defects in matter. Such defects play an important role in functionalizing materials for use in electronic devices. As the length scale for such devices approaches the nano-regime, the interplay of dimensionality, quantum confinement and defects can be complex. In particular, the usual rules for describing defects in bulk may be inoperative, *i.e.*, a shallow defect level in bulk may become a deep level at the nanoscale. The development of theoretical methods to describe the properties of nanoscale defects is a formidable challenge. Nanoscale systems may contain numerous electronic and nuclear degrees of freedom, and often possess little symmetry. My presentation will center on recent advances in this area based on new algorithms, which allow a solution of the Kohn-Sham eigenvalue problem without any explicit diagonalization. I will apply these algorithms to nanoscale systems, and present calculations for the structural and electronic properties of dopants (Li, Zn, B, P, Mn..) in semiconductor (Si, InP, ZnO, CdSe, ...) nanostructures. We will vary the size and dimensionality of these nanostructures, by considering nanocrystals, nanowires and nanofilms.

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