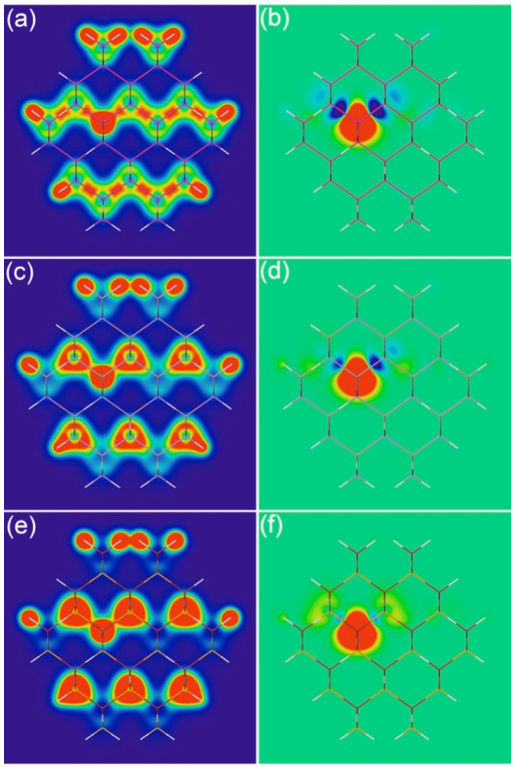
Institute for the Theory of Advanced Materials in Information Technology: James R. Chelikowsky (Texas), Yousef Saad and Renata Wentzcovitch (Minnesota), Steve Louie (UC Berkeley) and Efthimios Kaxiras (Harvard) (DMR- 0551195): Quantum Confinement in Spintronic Materials

A key area of ITAMIT's work is focused on magnetic dopants within the nanoscale regime, e.g., systems such as Mn in Ge, GaAs and ZnSe dots. These "spin in a box" systems can be used to examine the role of quantum confinement on magnetic systems. A central aspect of this work is to explore the strong role of the dot size on the coupling mechanism between magnetic dopants. we found a novel behavior of magnetically active dopants in semiconductor nanocrystals. Owing to the highly localized nature of the orbtials associated with Mn dopants, decreasing the size of the dot can change shallow holes to deep holes; this effect can profoundly change the magnetic coupling. For shallow dopants, the Zener picture is more appropriate; for deep donors, the double exchange is.

Ref. X. Huang, A. Makmal, J. R. Chelikowsky, and L. Kronik,Phys. Rev. Lett. **94**, 236801 (2005)



Total valence charge density (a),(c),(e) and spin density (b),(d),(f) for passivated $Ge_{81}Mn$, $Ga_{40}As_{41}Mn$, and $Zn_{40}Se_{41}Mn$ nanocrystals, respectively.