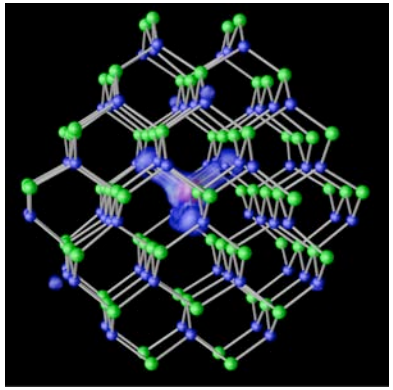
Institute for the Theory of Advanced Materials in Information Technology: James R. Chelikowsky (Texas), Yousef Saad and Renata Wentzcovitch (Minnesota), Steven Louie (UC Berkeley) and Efthimios Kaxiras (Harvard) (DMR- 0551195): Doping nanocrystals and self-purification

The properties of impurities in nanostructures can be very different from the precursor materials, sometimes even leading to novel phenomena. This usually is due to quantum confinement effects and to the reduced size of the system. In pure semiconductor nanocrystals, the most remarkable change is in their energy gap, that is blue-shifted from the bulk value as the size of the nanocrystal decreases. This leads to the possibility of tuning the band gap of the material in order to satisfy specific needs, providing a wide spread of applications such as solar cells, electroluminescent devices, and possible electronic devices. Bulk semiconductors need to be doped to build functional devices. In order to develop functional devices with semiconductor *nanocrystals*, they should also be doped. However, the doping process is difficult and not well understood within the nano-size regime. In particular, nanocrystals are thought to "self-purify" as dopants may easily diffuse to the surface of a nanocrystal. We have discovered that doping may also be energetically unfavorable as the size of the nanocrystal decreases. This is illustrated for Mn doped CdSe nanocrystals (top right) where the relative energy to create to insert the Mn atom increases dramatically for small nanocrystals (bottom right.)



Charge density plot of the impurity d levels in a Mn-doped CdSe nanocrystal with 1.7nm diameter.