Defect induced magnetism in semiconductor nanostructures

HYUNWOOK KWAK, University of Minnesota, TZU-LIANG CHAN, JAMES CHELIKOWSKY, University of Texas — It has been proposed that magnetic semiconductors can be designed by using non-magnetic defects, e.g., through the introduction of an extrinsic impurity atom that does not exhibit magnetism by itself (Phys. Rev. Lett. 99, 127201). In order to address such proposals, we have employed a real-space pseudopotential method based on the generalized gradient approximation to determine the magnetic properties of boron and aluminum doped silicon nanocrystals and nanowires. We will discuss theoretical evidence for defect induced magnetism as a function of the nanostructure size. We suggest that defect induced magnetism can be strongly enhanced by quantum confinement.

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