Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Transport properties of transition-metal-encapsulated Si cages[1]
LINGZHU KONG, University of Minnesota, JAMES R. CHELIKOWSKY, University of Texas at Austin — We performed density functional pseudopotential calculations of the spin dependent transport through transition-metal-atom-encapsulated Si cages $Si_{12}X$(X=Mn, Fe and Co). The effect of the metal atom on conductance is studied. Mn and Fe doped systems show highly spin polarized transmission whereas the magnetization in Co doped system is quenched. It is found that electrons are transferred from Si atoms into the minority d orbitals of the metal atoms. The conductance decreases as these electrons become localized around the encapsulated atoms.

[1]This work was supported in part by the National Science Foundation under DMR-0551195 and the Department of Energy under DE-FG02-06ER15760 and DE-FG02-06ER46286.

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Date submitted: 26 Nov 2007 Electronic form version 1.4