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A first principles study of noble metal-doped silicon nanocrystals $Si_{n-1}M$ (n = 75 and 150 and M = Cu, Ag, Au) CEDRIC MAYFIELD, MUHAMMAD HUDA, Department of Physics, University of Texas Arlington — Silicon nano-structures can have important roles in many useful applications, such as in nano-scale energy conversion materials, as nano-detectors of gas particles or as thermoelectric materials. To achieve efficient performance of these nano-devices, electronically tailored nano-materials are needed. For this a thorough understanding of both doped and undoped nano-structures is essential. Here we will present results of our first principles spin polarized electronic structure calculations of noble metal atom doped silicon nanocrystals using a hybrid density functional theory method (B3LYP-DFT) and a LanL2DZ basis set. The nanocrystals are used here as a test group, and are based on three different isomers of bulk silicon: diamond, wurtzite, and BC8. Geometry optimizations of the pure Si_n nanocrystals were performed for spin magnetic moments of s=0 μ_B and s=2 μ_B for each isomer. Then the substitutional doping of M atom was done separately at the inside and at the surface of the nanocrystals. The doped nanocrystals' geometries were also optimized for spin magnetic moments s=1 μ_B and s=3 μ_B. For the bigger nanocrystals, the energy differences between the two spin states are very small. Binding energies and HOMO-LUMO gaps were calculated and a comparative analysis of the pure and doped silicon nanocrystals will be presented.

Cedric Mayfield
Department of Physics, University of Texas Arlington

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