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Effect of Iron(II) Ion Interactions on Silicon Nanoparticle Electronic Structure KEVIN MANTEY, MUNIR NAYFEH, University of Illinois, Urbana-Champaign — A better understanding of the interaction of silicon nanoparticles with ions can lead to diverse applications including biomedical sensing, filtering, and optoelectronics. Density functional theory is employed to investigate a simple ion test case, the interaction of an Iron(II) ion with a 1nm silicon nanoparticle (Si29H24). In the ground state the iron atom is found to sit below a six membered silicon ring on the particle surface. The effect on the molecular orbitals and charge distribution is presented, and time dependent density functional theory is used to investigate the excited state energy levels and oscillator strengths compared to the silicon nanoparticle alone. Absorption measurements of Iron(II) ions in solution with silicon nanoparticles are made for comparison.

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