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Nearly Free Electron Gas in a Silicon Cage J. ULISES REVELES, SHIV KHANNA, Department of Physics, Virginia Commonwealth University, Richmond Va. 23284 — Theoretical investigations of the ground state geometries, electronic structure, spin magnetic moment and the stability of the metal encapsulated MSi_{12} (M= Sc, Ti, V, Cr, Mn, Fe, Co, Ni) clusters have been carried out within a gradient corrected density functional formalism. The ground state of most MSi_{12} clusters are shown to have the lowest spin multiplicity as opposed to the high spin multiplicity of free transition metal atoms. Consequently, a proper inclusion of the spin conservation rules is needed to understand the variation of the binding energy of M to Si_{12} clusters. Using such rules, $CrSi_{12}$ and $FeSi_{12}$ are found to exhibit the highest binding energy across the neutral while VSi_{12}^- has the highest binding energy across the anionic MSi_{12}^-series. It is shown that the variations in binding energy, electron affinity and ionization potential can be rationalized within an 18-electron sum rule commonly used to understand the stability of chemical complexes and shell filling in a confined free electron gas.

Shiv Khanna
Virginia Commonwealth University

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