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Electronic Counting Rules for the Stability of Metal-Silicon Clusters[1] JOSE ULISES REVELES, SHIV N. KHANNA, Department of Physics, Virginia Commonwealth University, Richmond, VA. 23284-2000, USA — Theoretical investigations of the ground state geometries, electronic structure, spin magnetic moment and the stability of the metal encapsulated neutral, cationic, and anionic MSi_{16} (M= Sc, Ti, V) clusters have been carried out within a gradient corrected density functional formalism. $ScSi_{16}^{-}$, $TiSi_{16}$, and VSi_{16}^{+} are found to be particularly stable in agreement with recent experiments. It is shown that the enhanced stability can be reconciled within a model where each Si atom coordinated to the metal contributes one electron to the valence pool. We propose the use of the bond critical points (BCP) from the topological analysis of the electronic density, in order to identify the Si sites that are bonded to the metal atom. Clusters where the total number of valence electrons obtained by summing one electron from each Si site coordinated to metal atom and the valence electrons of the metal attain 20 are found to be particularly stable. Combined with the earlier reported stability at 18 electrons, it is proposed that such valence pools might be looked upon as a nearly free electron gas inside a silicon cage.

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