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Does the 18-Electron Rule Apply to $CrSi_{12}$?[1] MARISSA BADDICK ABREU, VIKAS CHAUHAN, ARTHUR REBER, SHIV KHANNA, Virginia Commonwealth University — Understanding the bonding between silicon and transition metals is valuable for devising strategies for incorporating magnetic species into silicon. $CrSi_{12}$ is the standard example of a cluster whose apparent high stability has been explained by the 18-electron rule. We critically examine the bonding and nature of stability of $CrSi_{12}$ and show that its electronic structure does not conform to the 18-electron rule. Through theoretical studies we find that $CrSi_{12}$ has 16 effective valence electrons assigned to the Cr atom and an unoccupied $3d_z^2$ orbital. We demonstrate that the cluster's apparent stability is rooted in a crystal field-like splitting of the 3d orbitals analogous to that of square planar complexes. $CrSi_{14}$ is shown to follow the 18-electron rule and exhibits all the conventional markers characteristic of a magic cluster. We will also present results on the stability and electronic structure of $FeSi_n$ clusters and in particular examine the valence configuration of $FeSi_{12}$ since Fe has two additional valence electrons compared to Cr.

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