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Electron Counting Rules For The Stability Of Metal-Encapsulated Sin Cages ANIL KANDALAM, QIAN WANG, S. N. KHANNA, PURU JENA, Virginia Commonwealth University — The possibility of stabilizing silicon cages by encapsulating metal atoms has received wide attention due to their potential applications as building blocks for novel silicon based materials. It was earlier proposed that the stability of such cages could be reconciled within a simple model where each Si contributes one electron to the valence manifold. It was suggested that cages where the sum of the valence electrons from the metal and the contributed electrons from the Si is 18 exhibit enhanced stability. Recent experiments have suggested that cages with 20 valence electrons also exhibit enhanced stability. In this work, we will present preliminary results on a systematic theoretical study of 3d-TM doped Si cages containing a wide variety of transition metals to examine the applicability of these rules. Our studies, not only cover clusters with different number of Si atoms but we also vary charge on these clusters. The results will be compared with recent experiments on a wide variety of clusters.

[X] Prefer Oral Session
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