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Onset of magnetism in supported transition metal encapsulated silicon cages[1] ROBERTO ROBLES, SHIV N. KHANNA, Dept. of Physics, Virginia Commonwealth University, Richmond, VA 23284 — In the past few years, silicon based clusters have attracted a lot of attention as building blocks of nanomaterials. Some of the most promising candidates are the transition metal encapsulated silicon cages, which have been shown to be specially stable, both experimentally and theoretically. However, for the use of these materials in fields like spintronics, it is not only necessary to be semiconductor based, but also that they present a finite magnetic moment. However, it has been shown that the magnetic moment of the transition metal atom encapsulated in silicon cages is quenched due to the hybridization with silicon. By performing density functional calculations in the generalized gradient approximation, we show that the magnetic moment of these clusters can be recovered by depositing then on a surface. Using $CrSi_{12}$ on Si(111) as an example, we have deposited the cluster in different orientations. The studies show that, for most of them, a finite magnetic moment is preserved in the system after a geometrical relaxation. The origin of this behavior is discussed in terms of hybridization, comparing to the unsupported situation.

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