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Magnetic properties and stability of metalloinorganic clusters¹ ROBERTO ROBLES, SHIV KHANNA, Dept. of Physics, Virginia Commonwealth University, Richmond, VA 23284 — Theoretical studies on the structure, stability, electronic structure and magnetic properties of binary clusters Si_nTM_m (n=1-8, TM=Cr,Mn) have been carried out within a density functional formalism using the generalized gradient approximation. The stability of the clusters as a function size is analyzed in terms of several criteria, like the progression in bonding energy and HOMO-LUMO gap, with the ultimate objective of identifying the simple rules that can guide the search of stable species. The magnetic properties of the clusters are investigated by considering different ferromagnetic and antiferromagnetic arrangements of the local spin moments and optimizing the geometry and the spin state to determine the ground state including possible isomers. The possible use of these clusters as building blocks of cluster assemblies is discussed, and finally, the interest of these assemblies in the design of materials which could be used in the field of spintronics is briefly considered.

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