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A density functional theory investigation of the 3d, 4d, and 5d metals 13-atom clusters[1] PAULO PIQUINI, MAURICIO PIOTROWSKI, UFSM, JUAREZ DA SILVA, IFSC — In this work, we report a first-principles study based on density functional theory calculations of the atomic structure, binding energies, coordination numbers, average bond lengths, magnetic properties, and vibrational frequencies of 3d, 4d, and 5d metal clusters (30 elements) containing 13 atoms, M13. A set of lower energy local minimum structures were obtained by combining high-temperature first-principles molecular dynamics simulations with geometric optimizations at zero temperature for different spin configurations. The ground state structures for the M13 clusters show very clear features: (i) Compact icosahedral-like forms at the beginning of each metal series, (ii) more opened structures such as hexagonal bilayer-like and double cubic layer in the middle of each metal series, and (iii) structures with increasing average coordination number, e.g., icosahedron (Hg), for elements with valence d-states having more than half-occupation, at the end of each series. The magnetic exchange interactions play an important role for particular systems such as Fe, Cr, and Mn. Most of the properties can be explained by the occupation of the bonding and anti-bonding states

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