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Electronic and Magnetic properties of Transition Metal Borides. ADITI HERWADKAR, National Renewable Energy Laboratory , YUFENG ZHAO — Boron has three valance electron and a small covalent radius undergoing sp_2hybridization in many boron clusters. It is also known to form large variety of crystal structures both planer and 3D caged molecules. Our current work is to study transition metal boride clusters. This would be useful towards designing metal boride nanoclusters with tunable optical, magnetic and electron transport properties. Different stoichiometries are studied. The metal to Boron ratio varies from 0.3 to 0.75. For each of these compositions the lowest energy geometries were determined by optimizing the bond length for several initial symmetric geometries. The lowest energy structure is then chosen as the equilibrium structure. Most strikingly, all these transition-metal boride clusters are cage-like although both boron and transition metal usually favor high coordination number. We also find that some of the clusters have an extremely high magnetic moment per unit mass. This renders metal boride nanoparticles as potentially promising light-weighted magnetic materials. All the calculations are done using the spin-polarized density functional theory method implemented in the Vienna ab initio simulation package. A plane wave basis set with (400 eV cutoff) was used in combination with an all electron like projector augmented wave potential and PBE exchange correlation functional with in the generalized gradient approximation.

Aditi Herwadkar
National Renewable Energy Laboratory

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