High Spin States of Small Transition Metal Clusters: A Computational Study with Density Functional Theory

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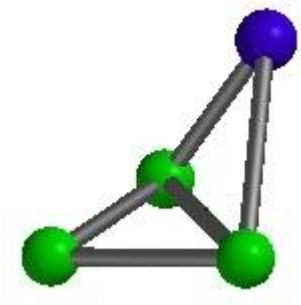
Small transition metal clusters have recently been found to exhibit unusually high spin states. This research focuses on discovering the root cause of these high spin states. Absolute energies, orbital energies, spin densities, and NBO analysis have been used to examine the relation between low spin states, which follow the aufbau principle, and high spin states, which are favorable due to energy exchange. The geometries of MCo3 (M = Co, Ni, Fe, Cu) have been optimized for various spin states with the PW91PW91 density functional method and Stuttgart RSC1997 ECP basis set. It is hoped that an increased knowledge of the cause of these high spin states will lead to a greater understanding of the bonds in these potentially catalytic molecules.



Metal cluster: Green = Cobalt, Dark Blue = Co, Fe, Ni, Cu.