STRUCTURAL PROPERTIES OF SOME TRANSITION METAL CLUSTERS

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Abstract: The structural properties of small $X_N$ with $6 \leq N \leq 55$ (X: Ag, Cd, Co, Cu, Ir, Ni, Pd, Pt, Rh, Ti, Zn and Zr) clusters were studied using Genetic Algorithm. Cohesion of the clusters was modeled by Gupta potential, which contains many-body atomic interactions. The global minimum energies, mean bond lengths and differences between first and second energy were calculated, and these quantities were plotted as a function of cluster size and were compared with each other. The results were evaluated with the bulk properties of metals that are melting temperatures, atomic radiiuses. Geometrical magic number clusters were obtained and were investigated. Finally, our preliminary analysis showed that one can easily optimize the classical structures with high level of accuracy considering the well established classical Gupta potential. These results can be at least for small clusters used as initial guess to deal with more efficient and precise calculations based on quantum mechanics.

Keywords: Transition Metal Cluster; Genetic Algorithm; Gupta Potential; Magic Number.