Shell Structure of Electronic States of Noble-Metal Microclusters and Magnetic Anomaly of Transition-Metal Microclusters

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Electronic states of Cu_N and Ni_N clusters are calculated for N=4,6,8,13,14 and 19 by the DV-Xα-LCAO method.

In Cu clusters, the valence 3d electrons are localized within atoms and isolated from the valence 4s electrons extending over the whole cluster. The main feature of the 4s electronic states well corresponds to that of one-electron in the spherical potential well *i.e.* the shell model. The fact that noble clusters of some specific sizes (magic number) are abundant is explained by closing the highest group of nearly degenerate occupied levels.

In Ni clusters, the 3d electrons are also localized within atoms and the 4s electrons extend over the whole cluster. The main feature of the 4s electronic states is the shell structure. By the spin-polarized-DV-Xα-LCAO calculation, it is found that the number of 3d holes becomes discontinuous as a function of the cluster size and that this results in the step-wise change in the net magnetic moments of clusters. This magnetic anomaly is due to two facts that 3d electronic states are dense around the highest occupied level and that the 4s electronic states have the shell structure.

Electronic structure of Co clusters is similar to that of Ni clusters. Then, the anomaly of magnetism is expected in a series of the ferromagnetic-transition-metal clusters.