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Atomic structure prediction of metal clusters using the evolutionary algorithm NABIL AL-AQTASH, University of Nebraska- Omaha, KHALDOUN TARAWNEH, Princess Sumaya University for Technology, RENAT SABIRI-ANOV, University of Nebraska- Omaha — The evolutionary algorithm coupled with density functional (DFT) method is used to identify the global energy minimum atomic structure of metal clusters. Using evolutionary crystal structure optimization algorithm, as implemented in USPEX, we studied the atomic structure, binding energies, and magnetic properties of 13-atom Cu, Co and Cr clusters. A set of metastable and global minimum atomic structures are identified. Several new lower energy configurations were identified for 13- atom Cu, Co and Cr clusters and previous known atomic structures were confirmed by our calculations. We found that the Cu_{13} cluster has a distorted hexagonal bilayer (HBL) –like structure, which is composed by two layers as in the ideal HBL structure. The distorted HBL Cu_{13} is 1.17 eV lower in total energy compared to close-packed icosahedral (ICO) configuration, which reported as the lowest-energy structure for Cu_{13} in previous studies. Our calculations show that Co_{13} has an ideal HBL structure and Cr_{13} cluster has distorted ICO structure, which are consistent with the previous studies. Moreover, our calculations show that Cr_{13} has another lower energy atomic configuration with 0.003 eV difference form ICO. Cr_{13} has ferrimagnetic (FIM) interaction which plays an important role in finding the lowest energy structure. We discuss the predictive capabilities of evolutionary algorithms for nanoclusters.

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