Atomic structure prediction of Zr-Co and Hf-Co nanoclusters using the evolutionary algorithm. AHMAD ALSAAD, Department of Physics, Jordan university of sci. Technology, Irbid 22110, Jordan, NABIL AL-AQTASH, Department of Physics, The Hashemite University, Zarqa 13133, Jordan, RENAT SABIRIANOV, Department of Physics, University of Nebraska at Omaha, 6001 Dodge St., Omaha, NE, USA — Nanostructures of Hf-Co and Zr-Co rare earth free magnetic materials exhibit a high room-temperature energy product. In our study, the evolutionary algorithm coupled with density functional theory (DFT) is used to identify the global energy minimum atomic structures of Zr-Co and Hf-Co clusters. Using evolutionary crystal structure optimization algorithm, as implemented in USPEX, we studied the atomic structure, binding energies, magnetic properties, and anisotropy of Zr\(_x\)Co\(_y\) and Hf\(_x\)Co\(_y\)(x=1,2 and y=5,7,11) clusters. A set of metastable and global minimum atomic structures are identified. Several new lower energy configurations were identified for Zr\(_2\)Co\(_{11}\), Zr\(_1\)Co\(_5\), Zr\(_1\)Co\(_7\), Hf\(_2\)Co\(_{11}\), Hf\(_1\)Co\(_5\) and Hf\(_1\)Co\(_7\) clusters by our calculations. We discussed the magnetic interaction between the atoms of the clusters which is critical in finding the lowest energy structure. Our calculations show that Zr-Co and Hf-Co clusters have ferromagnetic coupling and large magnetization. Magnetocrystalline anisotropy energies (MAE) of these clusters were also found to be large.

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