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Anisotropy of Zr-Co and Hf-Co nanoclusters using the evolutionary algorithm NABIL AL-AQTASH, Hashemite University, RENAT SABIRIANOV, University of Nebraska at Omaha — Nanostructures of Hf-Co and Zr-Co rare earth free magnetic material that exhibit a high room-temperature energy product. In our study, the evolutionary algorithm coupled with density functional (DFT) method is used to identify the global energy minimum atomic structure 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 ZrxCoy and HfxCoy (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 Zr2Co11, Zr1Co5, Zr1Co7, Hf2Co11, Hf1Co5 and Hf1Co7clusters by our calculations. We discussed the magnetic interaction between the atoms of the clusters which is critical in finding the lowest energy structure. Our calculation show that Zr-Co and Hf-Co have ferromagnetic coupling and large magnetization. We will also discuss the magnetocrystalline anisotropy (MAE) variation in these clusters.

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