Abstract Submitted
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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_xCo_y and Hf_xCo_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_2Co_{11}, Zr_1Co_5, Zr_1Co_7, Hf_2Co_{11}, Hf_1Co_5 and Hf_1Co_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.

Ahmad Alsaad
Department of Physics, Jordan university of sci.
Technology, Irbid, Jordan

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