Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Atomic structure prediction of Zr-Co and Hf-Co nanoclusters using the evolutionary algorithm NABIL AL-AQTASH, The 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 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 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.

Renat Sabirianov
University of Nebraska at Omaha

Date submitted: 01 Dec 2015 Electronic form version 1.4