Prediction of novel magnetic materials[1] SAEED RAHMANIAN KOSHKAKI, Skolkovo Institute of Science and Technology, Moscow Institute of Physics and Technology, Department of Physics-University of Texas at Dallas, ARTEM OGANOV, Skolkovo Institute of Science and Technology, Moscow Institute of Physics and Technology, Department of Geosciences Stony Brook University, SAEED RAHMANIAN KOSHKAKI, Moscow Institute of Physics and Technology, QIAN GUANG-RUI, Department of Geosciences and Center for Materials by Design,Stony Brook University, OGANOV LAB TEAM — Discovery of new magnetic materials is a big challenge to modern material science. In this presentation, we attempt to report our results in the discovery of new hard magnetic materials candidate, with no rare earth elements in their chemical formula. Besides this, we also investigated the effect of electron correlation on the thermodynamic stability of materials by means of DFT calculation. To predict hard magnet, We utilized the state of art algorithm, USPEX, and then we used the micro-magnet model to compute hard magnetic properties of predicted materials. Searches were performed at zero pressure using GGA and GGA+U (to account for correlation effects). Successfully, we predicted new hard magnet candidates, with a perfect agreement between predicted crystal structure and experimental data, but the magnetic properties yet to be confirmed experimentally.

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