Abstract Submitted
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Theoretical search for new permanent magnets with no rare earth atoms LIQIN KE, VLADIMIR ANTROPOV, Ames Laboratory — We performed the extensive computational search for better permanent magnets containing no rare earth atoms. Our initial studies are concentrated on the intrinsic properties of magnetic materials such as magnetization, the Curie temperature and magnetic anisotropy. A computational tool based on the electronic structure methods has been developed to describe these physical properties as a function of electronic concentration. The application of this technique allowed us to provide several possible directions to perform a search for new materials. We discuss some physical limitations of required properties in iron based materials using the analysis of their electronic structure and simplified magnetic models. The issues of chemical substitutions, modification of geometry and changing the dimensionality of systems will be discussed as well. The specific results will be shown for Fe and Co based systems with the additions of N, C, W, Al and other atoms.

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