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A study for magnetic properties enhencement of strontium hexaferrite by first principles calculations VIVEK DIKSHIT, CHANDANI NANDADASA, Department of Physics and Astronomy, Mississippi State University, Mississippi State, MS 39762, USA, SEONG-GON KIM, Department of Physics and Astronomy, Mississippi State University, Mississippi State, MS 39762, USA and Center for Computational Sciences, Mississippi — Owing to high magnetic anisotropy and saturation magnetization Strontium Hexaferrite is one of the most commonly used materials for hard magnets. In order to further improve the magnetic properties of the material we investigated the substitution different elements at Fe atom sites. Our calculation (using quantum mechanical DFT package, VASP) shows that both the properties: magnetization as well as magnetic anisotropy energy can be improved by a proper substitution.

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