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Effect of 3d-metal doping on magnetic properties of Fe₃Se₄ RENAT SABIRIANOV, NABIL AL-AQTASH, Univ of Nebraska - Omaha, DEBASIS SENGUPTA, CFDRC — Fe₃Se₄ exhibits large magnetocrystalline anisotropy (MAE) and coercivity up 40kOe. The large anisotropy of Fe₃Se₄ should be accompanied by large magnetization for permanent magnet applications. The magnetization of Fe₃Se₄ suffers from antiferromagnetic (AFM) superexchange coupling of Fe across the Se planes. We present density functional theory study of the magnetic properties of Fe₃Se₄ doped with TM (Co, Cr, Ni and Mn), TM ions doped in Fe sites, Fe_{3-x}(TM)_xSe₄ (x = 0.5), to examine a potential increase of the magnetization and Curie temperature of Fe₃Se₄. We performed screening of the exchange interactions and magnetization modifications upon the substitution of Fe by 3d-transition metals at various Fe sites in the Fe₃Se₄. We find that the doping of Fe₃Se₄ with 3d-elements does not remove AFM coupling across layers. The increase in the strength of exchange interactions on doping with Cr should increase the Curie temperature of the system. We compare the results of doped alloy with the ones for Cr₃Te₄. This compound is analogous to Fe₃Se₄ because Te has same electron configuration as Se, but Cr has only four d-electrons. We find that Cr₃Te₄ has ferromagnetic coupling and magnetization larger than one possible in Fe₃Se₄. Magnetization per unit cell is 18.24 μ_B . MAE of this material is large (MAE = 1.67 MJ/m³)

Renat Sabirianov
Univ of Nebraska - Omaha

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