

High magnetocrystalline anisotropy in oxides with near cubic local environments

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We investigate magnetic coercivity in double perovskite related oxides, based on first principles calculations of the magnetic properties and magnetocrystalline anisotropy. The Re-based materials studied have large magnetic moments on Re (nearly $1 \mu_B$ in $\text{Sr}_2\text{CrReO}_6$) and relatively large magnetocrystalline anisotropy energies. This is unexpected considering the octahedral coordination. Based on this, we studied an intergrowth of double perovskite $\text{Sr}_2\text{CrReO}_6$ -like and SrTiO_3 -like blocks. We obtain a very high predicted coercive field in excess of 90 T. This shows that it is possible to have large coercive fields arising from magnetocrystalline anisotropy associated with transition elements in nearly cubic local environments.