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Strong magneto-crystalline anisotropy in transition metal intercalated dichalcogenides VAIDEESH LOGANATHAN, ANDRIY NEVIDOMSKYY, Rice University, JIAN-XIN ZHU, Los Alamos National Laboratory — A figure of merit for hard ferromagnets is proportional to the magneto-crystalline anisotropy energy (MAE), which measures the energy cost of deviations from easy-axis magnetization. Materials containing elements with strong spin-orbit coupling and large ordered moment have been found to be strongly anisotropic. Due to the scarce availability of rare earths, hard magnets without rare earths are desirable, and intercalated metal dichalcogenides, $A_{0.25}MS_2$ (A=Fe,Mn; M=Ta,Nb), are one such candidate. We have performed first-principles LDA+U calculations on these materials. The MAE was calculated using two approaches, from the total energy difference between easy and hard magnetic directions using the non-collinear method; and using the torque method. Along with a saturated moment of $4\mu B$, we find MAE of about 10meV. This corresponds to an anisotropy field of about 60 T, comparable to those of rare-earth magnets. Substitution of Ta with Nb yields minor change in MAE, suggesting that the spin-orbit coupling effect contributes less to the anisotropy than the crystal structure. We find that the MAE in Fe intercalated compounds strongly depends on the value of the Hubbard U. We also study the effect on MAE of lattice strain, which can be used to tune the anisotropy.

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