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First-principles study of magnetic properties of two-dimensional semi conductors ABX_3[1] NIKHIL SIVADAS, MATTHEW DANIELS, ROBERT SWENDSEN, Department of Physics, Carnegie Mellon University, SATOSHI OAKAMOTO, Materials Science and Technology Division, Oak Ridge National Laboratory, DI XIAO, Department of Physics, Carnegie Mellon University — We investigate the magnetic properties of monolayers of van der Waals semiconductors ABX_3 theoretically. Our density functional theory (DFT) calculations show that these materials display rich magnetic phases. We use wannier analysis to study the competition between the antiferromagnetic direct exchange and the ferromagnetic superexchange, which governs the magnetic ground state. Using the low-energy effective models derived from our DFT results, we discuss the origin of rich magnetic behavior and phase transitions at finite temperature of these materials. We conclude that monolayers ABX_3 are suitable candidates for two-dimensional magnetic semiconductors, which have immense applications in next generation spintronics.

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