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Induced Magnetization and Band Gap in Graphene-Like Materials: Towards Spintronics XUAN LUO, National Graphene Research and Development Center, JESSE CAI, Thomas Jefferson High School for Science and Technology, NGRD-TJHSST TEAM — We use first principles calculations incorporated within the ABINIT package to\pardanalyze the potential of two dimensional graphene-like materials in spintronics. Spintronics haspotential to vastly improve upon and decrease the size of existing silicon based technology.use four transition metals, Mn, Fe, Co, and Ni, to dope six graphene-like materials: graphene, boron nitride, silicene, molybdenum disulfide, molybdenum diselenide and black phosphorene. With the addition of a transition metal dopant, boron nitride, silicene, molybdenum disulfide, molybdenum diselenide and black phosphorene all displayed magnetization and a band gap in at least one configuration. Doped graphene, however,showed magnetization but no band gap. By using a hybrid graphene/boron nitride surface, or by placing graphene on top of boron nitride, magnetization and a band gap was observed. By altering the surface and the metal dopant, we have the ability to tune the band gap and magnetization. In conclusion, we find that all six graphene-like materials show promise in developing spintronics.

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