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First-principles study of the electronic structure of single-layer MnX/TM(001) (X=B, N, TM=Ag, Cu) surfaces SHOGO NAKAMURA, YOSHIHIRO GOHDA, Department of Materials Science and Engineering, Tokyo Institute of Technology — We propose new candidates of ferromagnetic monolayer, manganese boride (MnB), on the TM(001) substrate by first–principles calculations. Ferromagnetic thin films have attracted great attention not only as key materials for developing spintronic devices but also scientific interest in the magnetic mechanism. Our calculated results show that MnB/TM(001) and MnN/TM(001) become ferromagnetic and antiferromagnetic, respectively. We have also revealed the differences of the electronic structures of MnX/TM(001), suggesting the key role of the Mn $3d_{x^2-y^2}$ contribution to the hybridization around the Fermi energy for obtaining ferromagnetism. The exchange interaction constants are also evaluated from first–principles calculations. Moreover, we show the spin band splitting of MnN/Cu(001) in only a peculiar direction, whose electron–spin degeneracy is lifted as a consequence of the strain effects induced by a lattice mismatch.

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