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Unique playground for complex magnetism: Fe monolayers on hexagonal transition-metal surfaces STEFAN HEINZE, BJOERN HARDRAT, PAOLO FERRIANI, Institute of Applied Physics, University of Hamburg, Germany, ALI AL-ZUBI, GUSTAV BIHLMAYER, STEFAN BLUEGEL, Institut fuer Festkoerperforschung, Forschungszentrum Juelich, Germany — Recently, the complexity of magnetic order even in single monolayer (ML) thick magnetic films on non-magnetic substrates has been dramatically demonstrated by the discovery of a spin-spiral state for a Mn ML on W(110) [1] and a nanoscale magnetic structure for an Fe ML on Ir(111) [2]. Here, we use density functional theory calculations based on the full-potential linearized augmented plane wave method to systematically study the magnetic order of an Fe ML on hexagonal hcp (0001) and fcc (111) surfaces of 4d- and 5d-transition metals. We show that due to substrate d-band filling the exchange coupling changes gradually from antiferromagnetic (AFM) on Tc, Ru, Re, and Os to ferromagnetic (FM) on Rh, Ir, Pd, and Pt. On Ru and Re the AFM coupling leads to a non-collinear Néel ground state due to topological frustration of exchange interaction. On Ru, Rh and Ir, the nearest-neighbor exchange coupling is small and exchange beyond nearest-neighbors, higher order spin interactions, and anisotropic exchange interaction compete making these systems a playground for intriguing magnetic order. [1] M. Bode et al., Nature 447, 190 (2007). [2] K. von Bergmann et al., PRL 96, 167203 (2006).

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