Abstract Submitted
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The Magnetism in 3d and 4f Intercalated Graphene-Surface Systems[1] NICOLAE ATODIRESEI, VASILE CACIUC, STEFAN BLÜGEL, Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — Graphene adsorbed on Ir(111) [1] is a widely used two-dimensional template which can be functionalized via metal intercalation [2, 3] or molecular adsorption [4]. Our first principles density functional theory (DFT) calculations employing a non-local correlation vdW-DF functional unveiled that the bonding mechanism of graphene on Ir(111) is physisorption with a local chemical modulation. Furthermore, our theoretical investigations of a 3d Co and Fe monolayer intercalated between graphene and Ir(111) demonstrated that the strong hybridization at the interface drastically modifies the magnetic properties of both graphene and substrate. With the prospect of using graphene in spintronics, we will show how the spin-splitting of the graphene π system can be tailored through a fine interplay between the weak hybridization, electrostatic and vdW interactions by intercalating 4f Eu between graphene and Ni(111). *E-mail address: n.atodiresei@fz-juelich.de ;* [1] C. Busse et al. Phys. Rev. Lett. **107** 036101 (2011); [2] R. Decker et al. Phys. Rev. B **87**, 041403(R) (2013); [3] J. Brede et al. Nature Nanotech. **9**, 1018 (2014); [4] F. Huttmann et al. Phys. Rev. Lett. **115** 236101 (2015)

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Nicolae Atodiresei
Peter Grünberg Inst., (PGI-1) and Inst., for Adv., Simulation (IAS-1)

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