Abstract Submitted
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Theory of copper induced spin-orbit coupling in graphene: substrate, clusters, and adatoms[1] TOBIAS FRANK, Univ Regensburg, SUSANNE IRMER, DENIS KOCHAN, MARTIN GMITRA, JAROSLAV FABIAN, University of Regensburg — We present a DFT study of graphene functionalized by copper adatoms and clusters, as well as of graphene on the (111) Cu surface, focussing on spin-orbit coupling effects. In the single copper adatom limit we study two energetically favored adsorption positions: the top and bridge positions and their corresponding diffusion barrier. Based on symmetry arguments we propose an effective tight-binding model Hamiltonian to describe low energy electronic states and determine realistic orbital and spin-orbit coupling parameters. We consider also copper clusters adsorbed on graphene and graphene on the Cu (111) surface, for which we as well fit to a model Hamiltonian to extract Rashba and intrinsic spin-orbit coupling strengths.

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