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Theory of spin-orbit coupling in fluorinated graphene[1] MARTIN GMITRA, TOBIAS FRANK, SUSANNE IRMER, DENIS KOCHAN, JAROSLAV FABIAN, University of Regensburg — We performed first-principles calculations of the spin-orbit coupling in graphene with fluorine adatom. The chemisorption of fluorine modifies the structural symmetry of graphene by breaking the pseudospin symmetry and inducing local corrugation towards sp^3 hybridization. We show that there are two dominant contributions to the spin-orbit field – Rashba term and a term due to pseudospin inversion asymmetry (PIA). In addition to the sp^3 induced spin-orbit coupling enhancement the spin-orbit split of the fluorine p orbitals is substantially transferred to graphene. Using group theoretical arguments we propose a realistic minimal Hamiltonian that reproduce the relevant spin-orbit effects calculated from first-principles. Our realistic effective Hamiltonian should be useful for spin transport and spin relaxation investigations.

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