Quasi-freestanding graphene on Ni(111) by Cs intercalation

It is of technological interest to achieve quasi-freestanding graphene on a substrate. A possible approach is the intercalation of alkali metal atoms. We investigate Cs intercalation between graphene and Ni(111) using density functional theory, incorporating van der Waals corrections. It is known that direct contact between graphene and Ni(111) perturbs the Dirac states. We find that Cs intercalation restores the linear dispersion characteristic of Dirac fermions, which is in agreement with experiments, but the Dirac cone is shifted to lower energy, i.e., the graphene sheet is n-doped. Cs intercalation therefore effectively decouples the graphene sheet from the substrate except for a charge transfer. On the other hand, the spin polarization of Ni(111) does not extend through the intercalated atoms to the graphene sheet, for which we find virtually spin-degenerate electronic states.