"Cobalt adatoms on graphene: Role of the realistic Coulomb interaction matrix in a QMC simulation"

Impurities on surfaces experience a geometric symmetry breaking not only induced by the on-site crystal-field splitting and the orbital-dependent hybridization, but also in their Coulomb interaction properties due to different optimality of screening in different directions. Here we present a many-body study of the Anderson impurity model for the Co/graphene system taking into account all anisotropies of the Coulomb matrix which we obtained by the constrained random phase approximation. The most pronounced differences are naturally displayed by the many-body self-energy projected onto the single-particle states.