Heavy adatoms and Anderson localization in graphene

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We analyze electronic localization in a graphene layer doped with adatoms sitting in the center of the honeycomb hexagon, as happens with the heaviest adatoms. In this configuration, the hybridization between the adatom orbitals and its neighboring carbon atoms mediate hopping processes that connect all six vertices of the honeycomb hexagon around the impurity(see Illustration 1.a). The amplitudes of the hopping depend on the symmetry of the orbital that hybridizes with graphene, leading to an orbital-dependent "plaquete disorder". To capture the physics of localization, we propose an effective graphene-only Hamiltonian that preserves the associated orbital symmetries and conduct a scaling analysis of the local density of states(LDOS) for large system sizes. We show that some adatoms will form a zero-energy resonant state(See illustration 1.b) in the plaquette of the impurity that leads to Anderson Localization in the vicinity of the Dirac point and to a metal-insulator transition at a well defined energy. We show that when the discrete rotational symmetry of graphene is broken, charge puddles with non characteristic sizes appears at energies near the Dirac point, which also happens for a strong scalar disorder(On the plaquete) (See Illustration 2.a and 2.b) in agreement with the Anderson Localization scenario. But when the symmetry is preserved, destructive interference between the different hybridization paths in the plaquette of the adatom suppresses Anderson Localization and leads to a non-homogeneous metallic state with large charge puddles, that localizes only at the Dirac point(See Illustration 2.c and 2.d).

Therefore, the quest for finding Anderson Localization in graphene hence relies on empirically identifying species of adatoms that sit at the center of the honeycomb plaquettes and do have a resonance at the Dirac point.

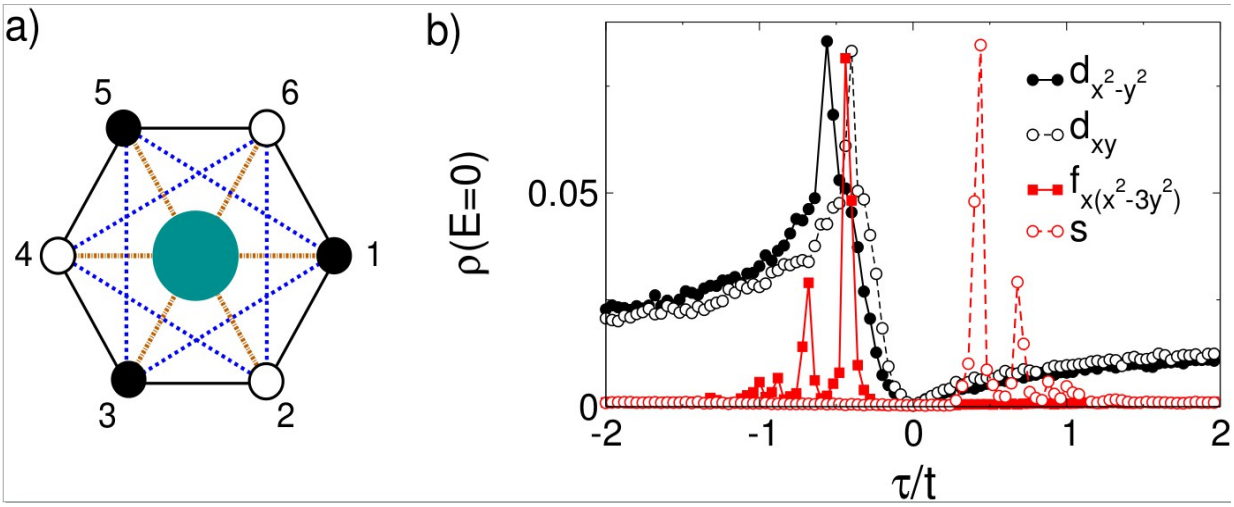

Illustration 1: a)Impurity plaquette for an adatom(center) stting at an H-site, with six carbon atoms: white circle(sublattice A); black circles(sublaticce B). Hopping processes mediated by the adatom:Solid lines(Nearest Neighbors), dashed (Next Nearest Neighbors), dot-dashed(Next Next Nearest Neighbors). b) DOS at the Dirac point vs effective hopping parameter for different orbital symmetries for a concentrarion of 0.5% adatoms per carbon and 10^7 atoms.

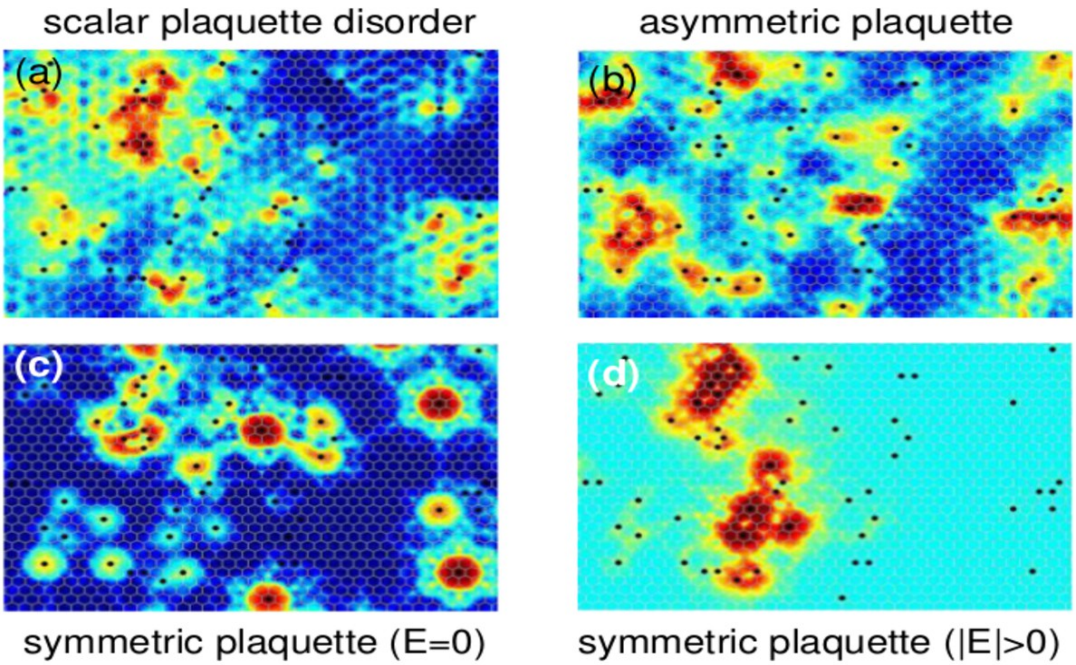

Illustration 2: Normalized LDOS at the Dirac point for a) Scalar plaquete disorder and b) asymmetric plaquette disorder for d orbitals. c) Symmetric plaquette disorder(s-wave orbital), at the Dirac point and d) Away from it (E=0.1t)