Chemically Tunable Transport Phenomena of Functionalized Graphene

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We present an ab initio multiscale study and quantum transport simulations using the Kubo formalism [1] of chemically modified graphene based materials, whose properties are tuned by changing the density and nature of grafted molecular units. Depending on the nature of the introduced molecular bonding different conduction mechanism are obtained, including transition from weak to strong Anderson localization [2,3], as well as spin-dependent phenomena [4] and magnetoresistive fingerprints [5].

References

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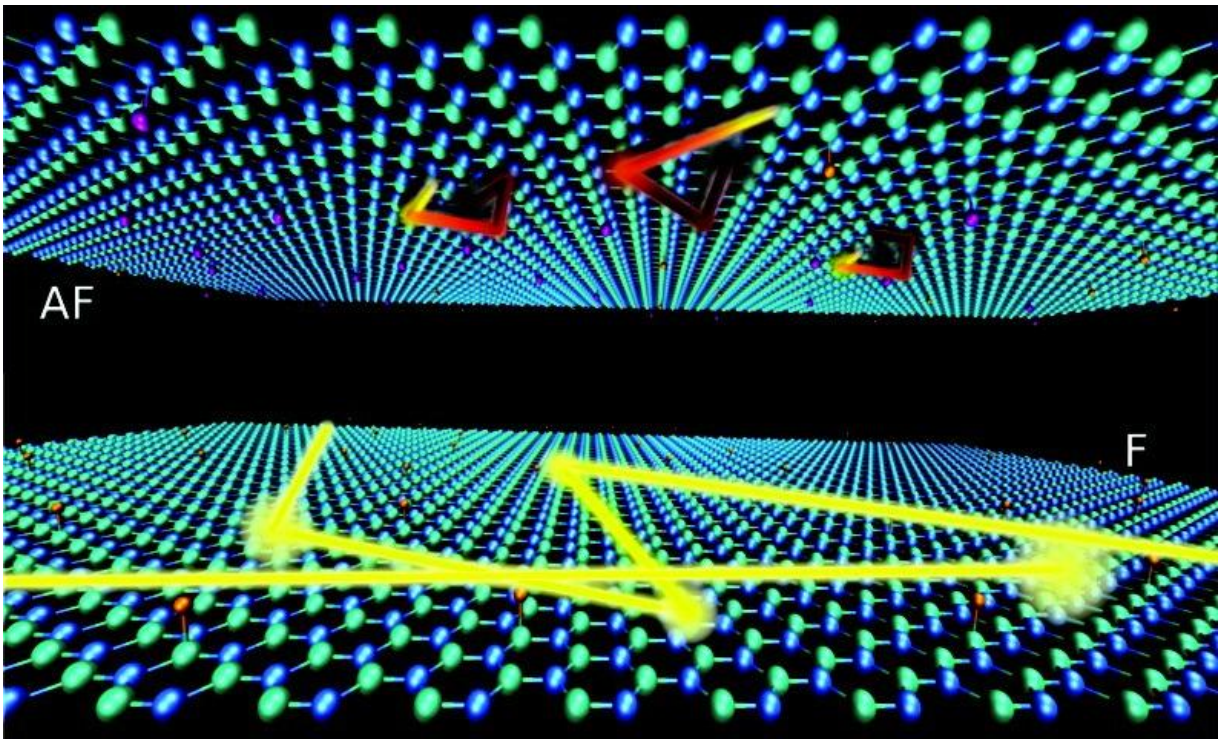
Figures



Different localization behavior depending on the type of intrinsic magnetic ordering of hydrogen atoms on graphene. All atoms distributed on the same lattice (ferromagnetic ordering) do not localize charge carriers. Atoms randomly distributed over both sub-lattices (antiferromagnetic ordering) induce quantum localization effects.