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Filled and empty orbital interactions in a planar covalent organic framework on graphene

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The electronic characteristics of a planar covalent organic framework (COF) on graphene are investigated by means of dispersion-corrected density functional theory. The aromatic central molecule of the COF acts as an electron donor to graphene, while the linker of the COF acts as an electron acceptor. The concerted interaction between the filled orbitals of the central molecule and empty orbitals of the linker promotes the formation of planar COF networks on graphene. The calculation results are in very good agreement with experimental findings of an ordered hexagonal and square COF planar on graphene, which sheds light on the super molecular assembly mechanism.

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