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Theoretical and Experimental Investigation of Fe and Ni-TCNQ on Graphene

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Abstract : Due to the outstanding properties of the 2D metal-organic frameworks (MOF), intensive computational and experimental studies have been done. However, the lack of fundamental studies of MOFs on the graphene backbone is observed. This work studies Fe and Ni as metal and tetracyanoquinodimethane (TCNQ) with a high electron affinity as an organic linker functionalized on graphene. Here we present DFT calculations results to unveil the electronic and magnetic properties of iron and nickel-TCNQ physisorbed on graphene. Adsorption and Fermi energies, structural, and magnetic properties will be reported. Our experimental observations prove Fe- and NiTCNQ@Gr/Ir(111) are thermally highly stable up to 500 and 250°C, respectively, making them promising materials for single-atom catalysts or high-density storage media.

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