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Electronic and structural properties of $M_3(HITP)_2$ (M = Ni, Cu and Co) metal-organic frameworks ORLANDO SILVEIRA, HELIO CHACHAM, SIMONE ALEXANDRE, Federal University of Minas Gerais — Theoretical and experimental works have demonstrated that electrical and structural properties of metal-organic frameworks (MOF) can be significantly changed by the identity of the metal center, leading to a potential strategy for tuning the selectivity of the material toward different types of technological applications. In this work, we use first principle calculations to investigate the electronic properties of 2D MOF $M_3(HITP)_2$ (M is Ni, Cu and Co and HITP = 2,3,6,7,10,11 hexaiminotriphenylene). Our results show that for M=Ni and Co, the structures are perfect planar and there is a full charge delocalization in the 2D plane of stacking due to the predominance of $\pi - \pi$ bonding. The band structure for M = Ni shows that this material is a semiconductor with an indirect band gap of 132 meV, whilst for M = Co the band structure shows that this material is a ferromagnetic semiconductor with a direct band gap of 386 meV for spin down and a indirect band gap of 246 meV for spin up. For M=Cu, the material is a metal and adopts a distorted structure due to a different hybridization of the metal atom in comparison with its counterparts. We also propose a tight binding model that can represent the electronic structure near the Fermi level of this family of MOF.

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