Electronic and conductive properties of the $Cu[Ni(pdt)_2]$ metal-organic framework: a periodic-DFT investigation

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Conductive and chemiresistive metal–organic frameworks (MOFs) are an emerging class of materials that can be employed as chemical sensors. [1,2] Moreover, because of their porosity and crystallinity they show remarkable gas-adsorption properties. A wise combination of such features can lead to a smart design of conductive materials that operate at near-ambient conditions.

The electronic nature of $Cu[Ni(pdt)_2]$ (pdt^{2-} = 2,3-pyrazinedithiolate) MOF is investigated by means of density functional theory (DFT) calculations, and related to the experimental characterization of its conductivity, which in the pristine material is 200-fold greater than in the solvated material.

Possible reasons and mechanisms for conductivity of the pristine MOF are explored, through the study of band structure, density of states and polaron formation.

A polaron-conduction mechanism can only be hypothesized: an explicit charge carrier species has not been identified.

References

1) Kobayashi, Y. et al., *Chem. Mater.* **2010**, *22*, 4120–4122.
2) Aubrey, M. L., et al., *Nature Materials* **2018***, 17,* 625–632.