Unveiling the Semiconducting Properties in Four Different Metal Triphenylenehexathiol-based Metal-Organic Frameworks

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Abstract: Optical Pump-THz Probe analysis of charge transport reveals semiconducting behavior in THT-based 2D MOFs, showing increased photoconductivity after excitation and dispersive spectra well-described by the Drude-Smith model.

Metal-organic frameworks (MOFs) constitute a class of hybrid coordination polymers consisting of metal ions connected by organic ligands. The intrinsic porosity of these structures, that gives an extraordinary surface area per unit volume, has resulted in a natural appeal to use MOF in gas sieving and storage. Thanks to the recent discovery of the unique combination of the high porosity and electrical conductivity in materials that were seen essentially as insulators, we have begun to explore yet other broad areas of potential applications of MOFs as active elements in optoelectronics and chemiresistive sensing, but also in electrocatalysis and energy storage [1].

In particular, 2D layered MOFs and especially graphene analogues MOFs have been reported to have high conductivity [2,3]. Among those example, we shall mention MOFs based on triphenylene linkers. In this work we interrogate a broad family of triphenylenehexathiol (THT) MOF, prepared with four different transition metal cations (Fe, Co, Ni and Cu), to analyze their electro-optical properties in the attempt to establish a more clear relation between the metal centers and the charge transport.

Optical Pump-THz Probe (OPTP) represents a powerful technique to study the complex-valued photoconductivity of these materials in a fully non-contact fashion (Fig. 1a). All of the samples present a semiconducting response, predicted by DFT analysis and hereby demonstrated by the increase of conductivity upon light excitation (Fig. 1b). Photoconductivity spectra obtained from OPTP, revealed also a characteristic dispersion that can be adjusted with the Drude-Smith model (Fig. 1c).

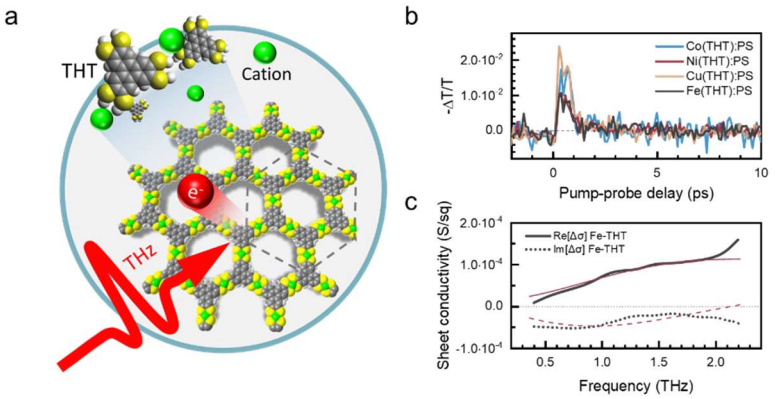

Fig.1 | a) Graphical representation of metal triphenylenehexathiol (M-THT) MOFs irradiated by THz light. b) Differential transmission in (M-THT) MOFs measured via OPTP. c) Frequency resolved photoconductivity in Fe_2THT_3 MOF (black) and fit according to the Drude-Smith model (burgundy).

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References

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