Unveiling Electronic Properties in Metal−Phthalocyanine-Based Conjugated Two-Dimensional Covalent Organic Frameworks

Mingchao Wang
Dr. Renhao Dong, Prof. Dr. Xinliang Feng
Center for Advancing Electronics Dresden (cfaed) and Department of Chemistry and Food Chemistry, Technische Universität Dresden, Mommsenstasse 4, 01069 Dresden, Germany.
Mingchao.wang@tu-dresden.de

Conjugated two-dimensional covalent organic frameworks (2D COFs) are emerging as a novel class of electroactive materials for (opto)electronic[1] and chemiresistive sensing[2] applications. However, understanding the intricate interplay between structure and conductivity remains elusive. We have demonstrated two novel samples consisting of Zn− and Cu−phthalocyanine-based pyrazine-linked 2D COFs (MPc-pz COF) as p-type semiconductors both with a band gap of ~1.2 eV.[3] A record device-relevant mobility up to ~5 cm^2 /(Vs) is resolved in the dc limit. Hall effect measurements (dc limit) and terahertz spectroscopy (ac limit) in combination with density functional theory (DFT) calculations confirm that varying metal center from Cu to Zn has a negligible effect in the conductivity (~10^{-6} S/cm), charge carrier density (~10^{12} cm^{-3}), charge carrier scattering rate (~10^{13} s^{-1}), and effective mass (~2.3m_0) of majority carriers (holes). Notably, charge carrier transport is found to be anisotropic, with hole mobilities being practically null in-plane and finite out-of-plane for these 2D COFs. This work highlights the potential of high-mobility conjugated 2D COFs as semiconductors for (opto)electronics and provides a rational approach to ascertain structure−property relationships.

References

[1] M. Dogru, M. Handloser, F. Auras, T. Kunz, D. Medina, A. Hartschuh, P. Knochel, T. Bein, Angew. Chem. Int. Ed., 52 (2015) 2920−2924.
[2] Z. Meng, R. M. Stolz, K. A. Mirica, J. Am. Chem. Soc., 141 (2019) 11929−11937.
[3] M. Wang, M. Ballabio, M. Wang, H.-H. Lin, B. P. Biswal, X. Han, S. Paasch, E. Brunner, P. Liu, M. Chen, M. Bonn, T. Heine, S. Zhou, E. Canovas, R. Dong, X. Feng, J. Am. Chem. Soc., 141(2019) 16810−16816.

Figures

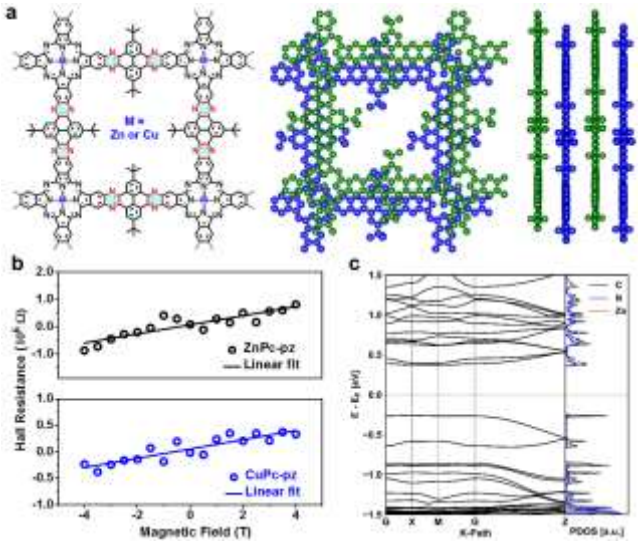

Figure 1: (a) Structural schematics of serrated AA-stacked multilayers of MPc-pz COF. (b) Hall effect measurements of ZnPc-pz and CuPc-pz COF at 300 K. (c) Electronic band structure of ZnPc-pz COF.