Electronic Properties of Metal-Phthalocyanine-Based 2D Conjugated Covalent Organic Frameworks

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Two-dimensional (2D) conjugated covalent organic frameworks (*c*-COFs) are emerging as a unique class of semiconducting 2D conjugated polymers for (opto)electronics and energy storage.[1,2] However, understanding the intricate interplay between structure and conductivity remains elusive. We have demonstrated two metal−phthalocyanine-based pyrazine-linked 2D *c*-COFs (MPc-pz, M = Cu or Zn) as *p*-type semiconductors with a band gap of ∼1.2 eV and charge mobility up to ∼5 $cm^2/(Vs)$.[3] Hall effect measurements and terahertz spectroscopy in combination with density functional theory calculations confirm that varying metal center from Cu to Zn has a negligible effect on the charge transport behaviors. After reversible *p*-type doping with I_2, the doping-defined 2D *c*-COF displays enhanced conductivity by 3 orders of magnitude, due to the elevated carrier concentration.[4] Remarkably, charge mobility also increased upon doping, which can be traced to increased scattering time for free charge carriers, indicating that scattering mechanisms limiting the mobility are mitigated by doping.

References

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Figures

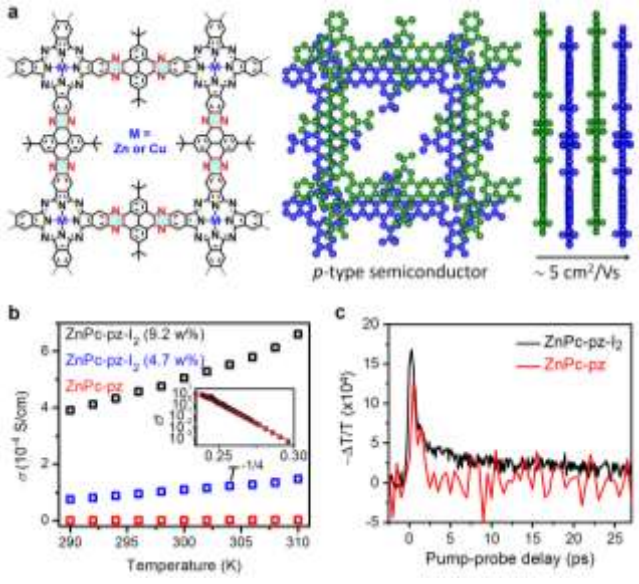

Figure 1: (a) Structural schematics of MPc-pz COF. (b) Variable-temperature conductivity of pristine and doped MPc-pz. (c) Terahertz spectroscopy.