

Layer-Oriented 2D Conjugated Metal-Organic Framework Films Enabling Directional Charge Transport

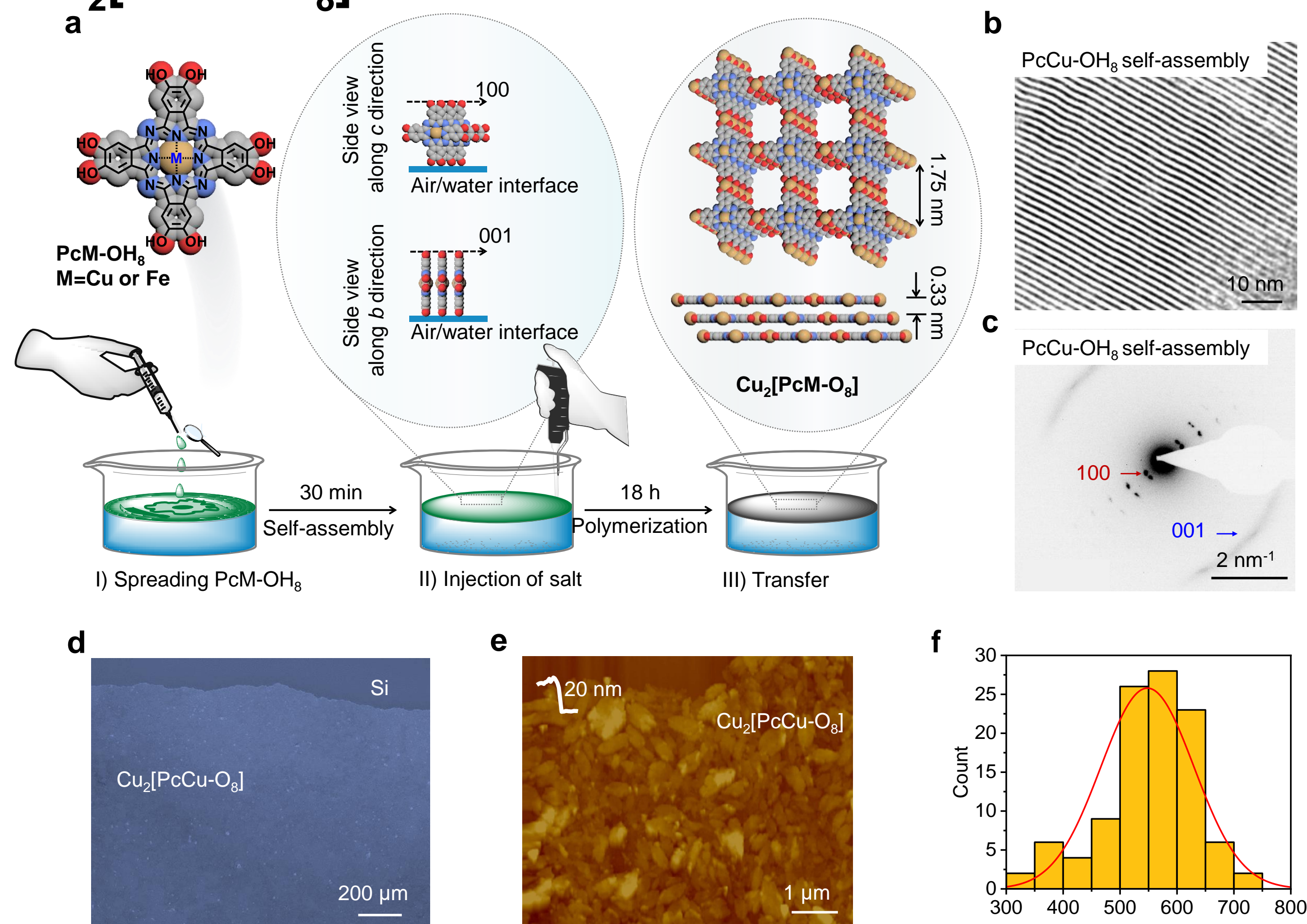
Zhiyong Wang, Renhao Dong, Xinliang Feng

Center for Advancing Electronics Dresden (cfaed) and Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, 01062 Dresden

Abstract

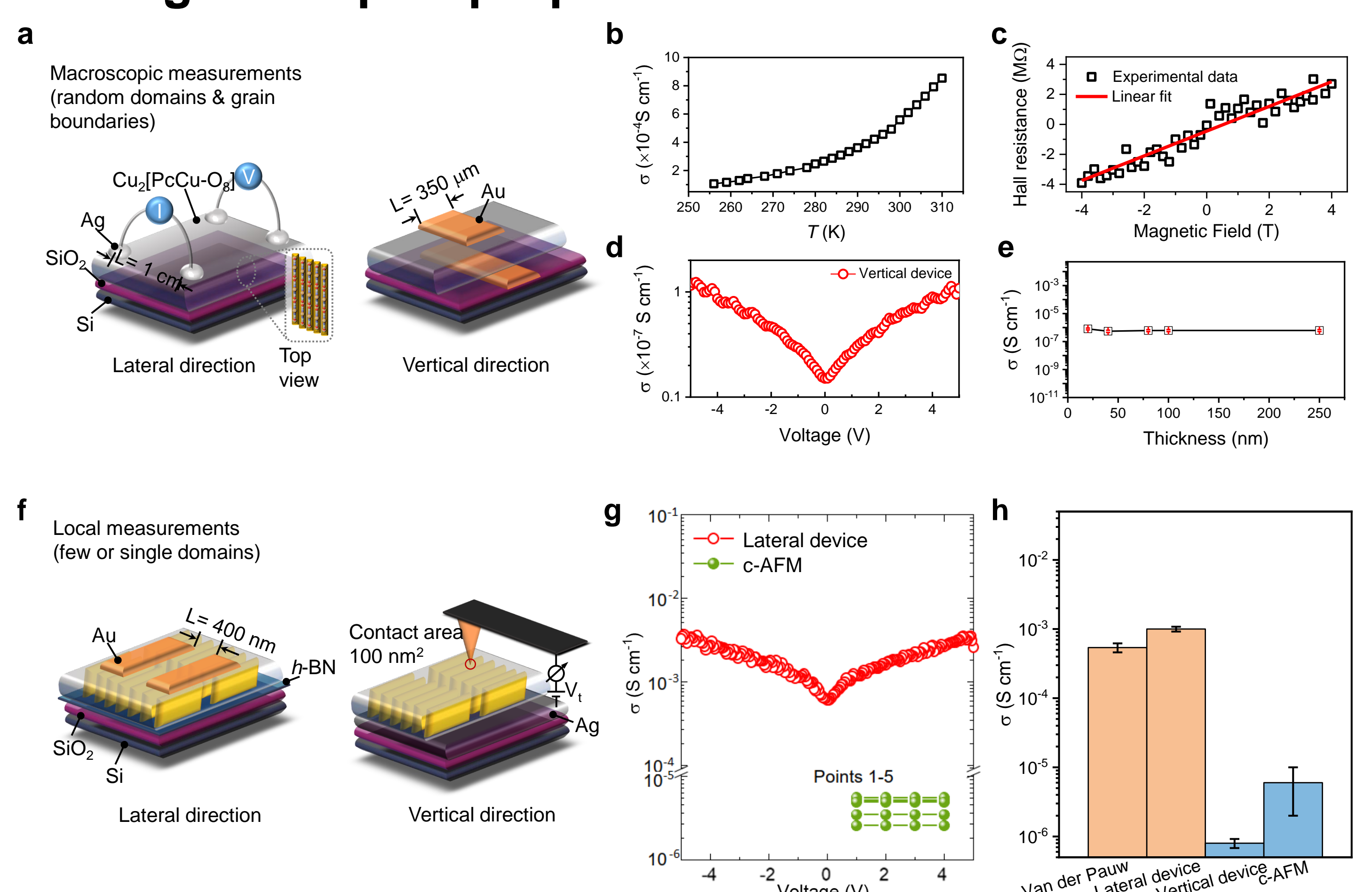
Edge-on layer-oriented *p*-type semiconducting 2D conjugated MOF (2D c-MOF) films comprising phthalocyanine ligands have been obtained at the air/water interface. The correlation between ligands and their alignment at the air/water interface was established. Macroscopic and local (sub- μm) charge transport measurements, combined with theoretical calculation have disclosed that the intrinsic conductivity is dominated by the charge transfer along the interlayer pathway.

Synthesis and morphological characterization of the $\text{Cu}_2[\text{PcCu-O}_8]$ film



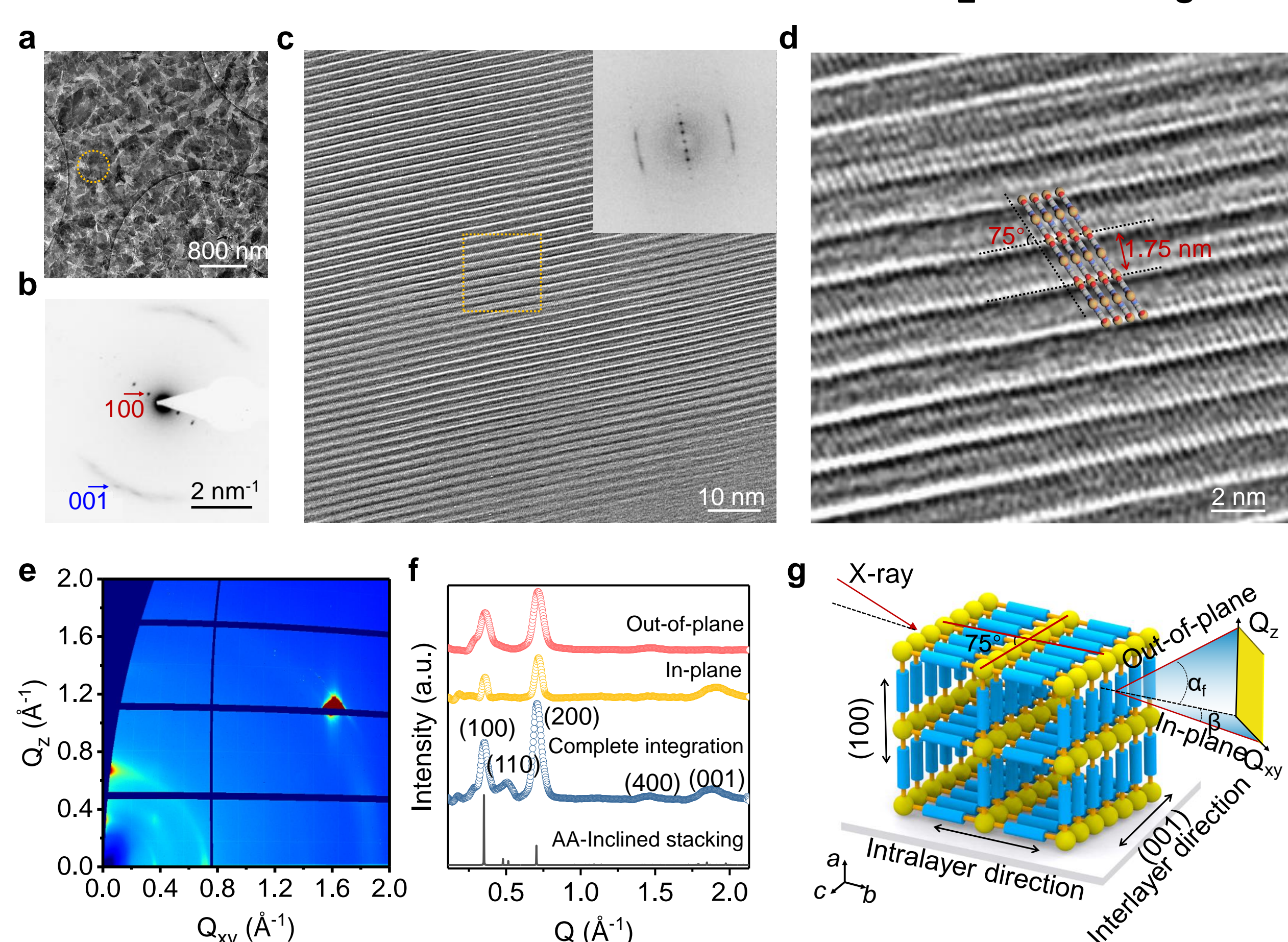
- π - π interaction and hydrophobicity guide the molecular arrangement and the edge-on structure formation of $\text{Cu}_2[\text{PcCu-O}_8]$.
- Thickness 20 nm, domain size, ~ 600 nm.

Charge transport properties



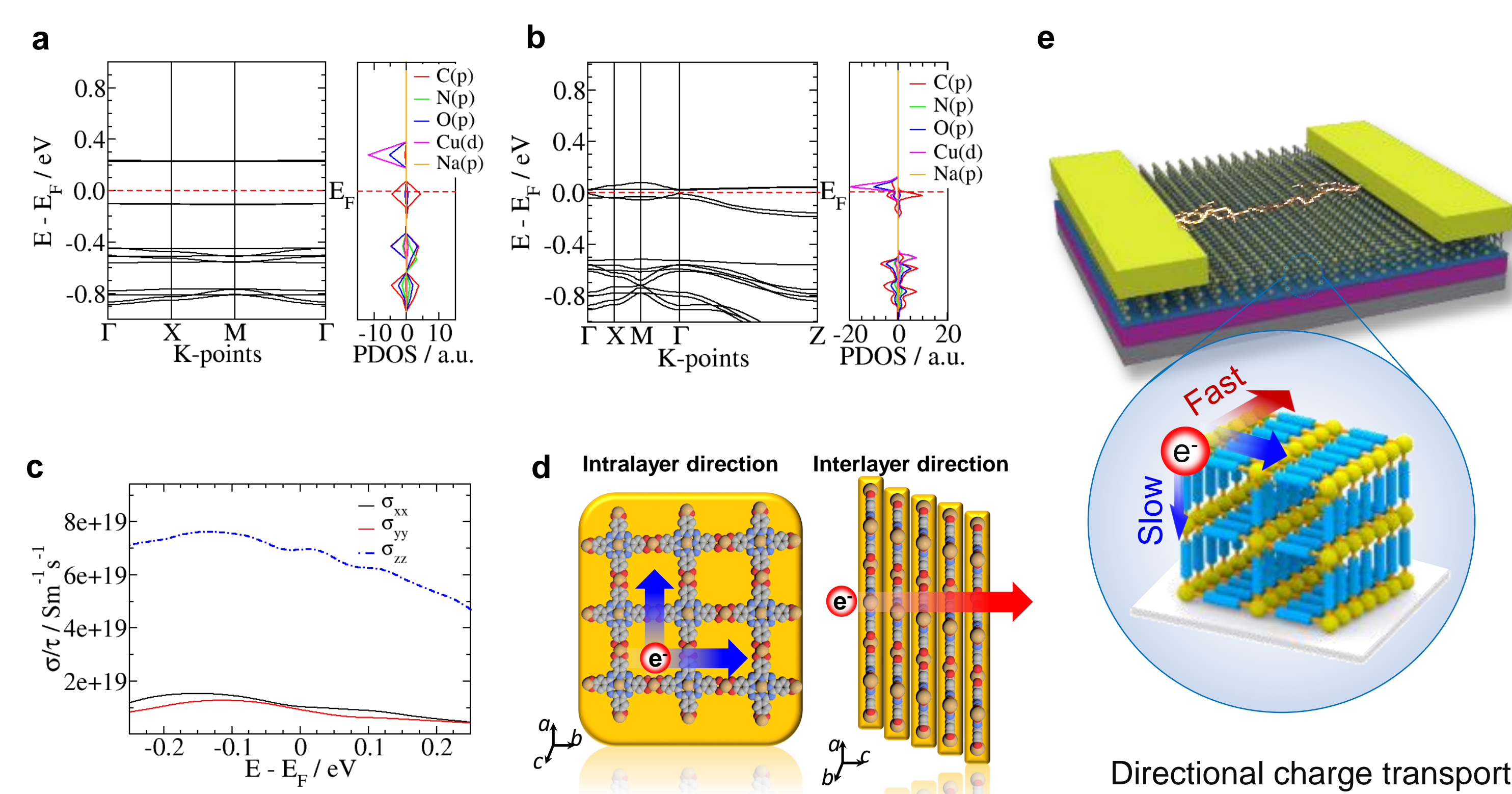
- Lateral direction: room-temperature mobility: $\sim 4.4 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$; Conductivity: $10^{-4} \sim 10^{-3} \text{ S cm}^{-1}$.
- Vertical direction: Conductivity: $10^{-6} \sim 10^{-5} \text{ S cm}^{-1}$.
- Such anisotropic behavior can be attributed to the preferential charge transport along the layer-stacking direction.

Crystal structural characterization of $\text{Cu}_2[\text{PcCu-O}_8]$



- AC-HRTEM image presents highly ordered linear arrangement with a lattice distance of 1.80 nm and a interlayer distance of 0.33 nm.
- GIWAXS measurement demonstrates a preference of $\text{Cu}_2[\text{PcCu-O}_8]$ for the edge-on orientation.

Mechanism of directional charge transport property



- Conjugation direction: **no dispersion in both conduction and valence bands** near the Fermi level; band gap 0.35 eV.
- π - π stacking direction: Small band gap 0.03 eV; **higher dispersion of the valence bands**

CONTACT PERSON

Z. Wang
wang.zhiyong@tu-dresden.de

REFERENCES

Z. Wang et al., *J. Am. Chem. Soc.* **2021**, doi.org/10.1021/jacs.1c05051.