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Supporting Information

Architecting *Pyrediyne Nanowalls* with Improved Inter-Molecular interactions, Electronic Features and Transport characteristics

Palani Prabakaran, Sitakanta Satapathy, Edamana Prasad* and Sethuraman Sankararaman*

Department of Chemistry, Indian Institute of Technology Madras, Chennai 600036, India

Phone: (+91) 44 2257 4232; Fax: (+91) 44-2257-4202

*E-mail:pre@iitm.ac.in

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Figure S1. a) SEM image used for elemental mapping, elemental mapping images of b) Copper (Cu) and c) Carbon (C)



Figure S2. **a)** Image used for SEM- energy dispersive x-ray spectrometry (EDS) and **b)** EDS of pyrediyne nanowalls (substrate: Silicon wafer).



Figure S3. a) Image used for SEM-energy dispersive x-ray spectrometry (EDS) and **b)** EDS of pyrediyne powder (substrate: Indium tin oxide glass).



Figure S4. Thermogravimetric analysis (TGA) depicting the thermal stability of the pyrediyne powder synthesized in bulk



Figure S5. FT-IR spectra of the pyrediyne nanowall (black) and the as synthesized pyrediyne powder in bulk (red) after washing with nitric acid



Figure S6. XPS focusing on the Cu 2p region for copper powder.



Figure S7. Pyrediyne with **a**) lesser conjugation and its corresponding density of states (DOS) diagram and **b**) extended conjugation and its corresponding density of states (DOS) diagram. (Level of theory: Grimme's dispersion corrected B3LYP-D/6-31G(d).