

Abstract Submitted
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Bottom-up design of optoelectronic properties: on-surface synthesis of iron-terpyridine macromolecular complex AGUSTIN SCHIFFRIN, CORNELIUS KRULL, MARINA CASTELLI, NIKHIL MEDHEKAR, YUE-FENG YIN, Monash Univ, MARTINA CAPSONI, GELAREH FARAHI, TANYA ROUSSY, KATHERINE COCHRANE, SARAH BURKE, University of British Columbia, CHEN-GUANG WANG, WEI JI, Renmin University of China — Supramolecular chemistry allows for the design of atomically precise materials with tailored (opto)electronic properties. In particular, metal-organic complexes resulting from the coordination of π -conjugated molecules with metals exhibit electronic properties which can translate in efficient light absorption and photo-induced charge separation. Here, we report the on-surface synthesis of 1D nanostructures based on an iron-terpyridine interaction borrowed from functional complexes used for photovoltaics and catalysis. Thermally activated on-surface conformational changes and molecular and adatom diffusion leads to formation of macromolecular chains via terpyridine-iron coordination. Our low-temperature scanning tunnelling microscopy and spectroscopy, photoelectron spectroscopy and density functional theory studies reveal an unusual poly-iron linkage between ligands accompanied by a metal-to-ligand electron transfer. This results in highest occupied (lowest unoccupied) orbitals dominated by metal (ligand, respectively) states, potentially allowing for efficient visible light absorption and photo-induced electron-hole separation. This novel coordination configuration has not been observed from solution synthesis methods, and is mediated by the constraint the surface provides in this “bottom-up” approach.

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