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# Rational Design of Low-Dimension Organic Frameworks

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On-surface synthesis and design of magnetic carbon-based low dimensional nanostructures are of vital importance for advancing molecular spintronics and nanoscience. First, I will present that a type of novel antiferromagnetic (AFM) nanostructures can be realized in 2D hydrogen-bonded organic frameworks (HOFs) via nesting honeycomb and Kagome lattices. In these “nesting-AFMs”, each sublattice is ferromagnetic with opposite spin polarization, constructed separately using donor and acceptor molecules. Density functional theory calculations confirm that five designed nesting HOFs are nesting-AFMs. Importantly, the ferromagnetic ordering of each sublattice originates from charge transfer between hydrogen-bond-connected donor and acceptor. These AFM frameworks can be synthesized by on-surface deposition of different molecules on certain transition metal dichalcogenides. Second, I will introduce the controlling magnetic coupling in diradical nonbenzenoid nanographenes via on-surface synthesis. Using first-principles calculations, we elucidated the reaction thermodynamics/kinetics of precursor DMPI-I on Au(111): selective cyclization and Ullmann coupling are governed by distinct energy barriers, guiding the synthesis of several molecule-based nanostructures. Ground-state and spin density calculations revealed magnetic states of different nanostructures, in good agreement with experimental observations. For dimers, spin density sign at connection sites dictates the magnetic ground state.

References:

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