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π-Magnetism of Surface Supported Molecular Structures

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π-Conjugated radical architectures offer a chemically programmable platform for low-dimensional magnetism, where weak spin-orbit coupling and delocalized frontier spins can support diverse collective spin phenomena. In this talk, we will first show a nitrogen-doped polycyclic aromatic hydrocarbon in which the π-magnetism is induced by molecule-substrate charge transfer and can be further tuned by atomic manipulation, enabling precise control of its charge and spin states. Beyond individual molecules, antiferromagnetic (AFM) nanographene chains have recently established atomically precise π-electron prototype for low-dimensional quantum magnetism. In the second part of the talk, we will discuss the spin models of ferromagnetically (FM) coupled and AFM-FM mixed nanographene chains in length less than six units. Their excitation energies and real-space spectral-weight profiles are quantitatively described by Heisenberg Hamiltonians constructed using exchange constants independently determined from dimer excitation. Moreover, we introduce fluorenes in phenyl-based chains. We will demonstrate that distinct linkage topologies result in nearly an order-of-magnitude variation in intermolecular hopping strength, which in turn reshapes spin-exchange coupling and lattice response, giving rise to AFM, FM, and Jahn-Teller competitive regimes in infinite one-dimensional chains.

References:

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