On-Surface Synthesis of Heisenberg Spin-1/2 Antiferromagnetic Molecular Chains

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Magnetic exchange interactions between localized spins in π-electron magnetism of carbon-based nanostructures have attracted tremendous interest due to their great potential for nano spintronics. Unique many-body quantum characteristics, such as gaped excitations, strong spin entanglement, and fractionalized excitations, have been demonstrated, but the spin-1/2 Heisenberg model with a single antiferromagnetic coupling J value remained unexplored. Here, we realized the entangled antiferromagnetic quantum spin-1/2 Heisenberg model with diazahexabenzocoronene oligomers (up to 7 units) on Au(111).[1] Extensive low-temperature scanning tunneling microscopy/spectroscopy measurements and density functional theory and many-body calculations show that even-numbered spin chains host a collective state with gapped excitations, while odd-numbered chains feature a Kondo excitation. We found that a given antiferromagnetic coupling J value between first neighbors in the entangled quantum states is responsible for the quantum phenomena, strongly relating to their parities of the chain. The tunable molecular building blocks act as an ideal platform for the experimental realization of topological spin lattices.

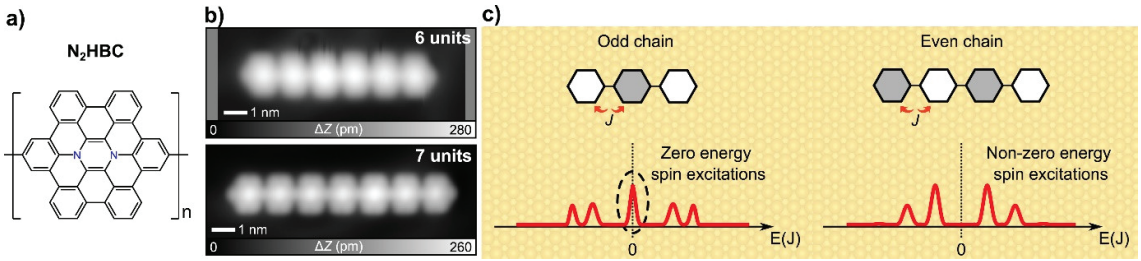

Figure 1. (a) N_2HBC chain structures. (b) STM images of 6- and 7-unit N_2HBC chains. (c) Heisenberg S = 1/2 antiferromagnetic chains with even and odd units and corresponding magnetic couplings.

Reference

[1] K. Sun, N. Cao, O. J. Silveira, A. O. Fumega, F. Hanindita, S. Ito, J. L. Lado, P. Liljeroth, A. S. Foster, S. Kawai. Sci. Adv. **11**, eads1641 (2023).