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Isotropic Wave Function Delocalization in C_{60} Molecular Assemblies MIN FENG, JIN ZHAO, HRVOJE PETEK, University of Pittsburgh — Electronic wave function delocalization in a molecular material is highly surprising. Here, we describe a new paradigm of strong intermolecular hybridization of a hollow core-bound molecular state in C_{60} assemblies. In 1D C_{60} wire and 2D C_{60} island, LT-STM revealed extensive, isotropic wave function delocalization at energy above 3.5eV, in contrast with the poor intermolecular wave function overlap of the π-molecular orbitals. DFT indicates that a new kind of molecular orbital, which is derived from the central potential of the hollow cage shape of C_{60}, is responsible for this NFE like wave function delocalization. This central potential derived from the screening interaction and gives rise to s, p, d, etc., symmetry atom-like orbitals, which we dub the superatom molecular orbitals (SAMOs). Studies show how these atomlike orbitals hybridize into H_2 molecule-like σ and π symmetry bonding/antibonding orbitals of C_{60} dimmers, and for larger aggregates, with alkali atom-like NFE dispersions. As a common consequence of a hollow topology, we expect that similar SAMO states will exist in other molecules derived by wrapping and rolling molecular sheets into hollow cages and nanotubes.

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