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 $\pi$-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 $\sigma$ and $\pi$ 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.