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The nearly free electron like superatom states in fullerenes and nanotubes[1] JIN ZHAO, MIN FENG, HRVOJE PETEK, Department of Physics & Astronomy, University of Pittsburgh — Motivated by the discovery of the superatom states of C_{60} molecules,[1] by DFT calculations we investigate their origin and the factors that influence their energy and wave function hybridization into nearly-free electron bands in molecular solids. We show that the superatom states are derived from the universal image potential states of molecular sheets by rolling and wrapping them into 0D fullerenes. Unlike the well-known π orbitals, superatom orbitals hybridize more extensively among the neighboring molecules to form bands with nearly free-electron dispersion. The prospect of exploiting the strong intermolecular coupling to achieve metal-like conduction in applications may be attained by lowering the energy of superatom states from 3.5 eV, for single chemisorbed C_{60} molecules, to proximity of the Fermi level; therefore, we study how the superatom state energies depend on factors such as the aggregation into 1D - 3D solids, their cage size, and exo and endohedral doping by metal atoms. We also study the superatom states of 1D nanotubes.

[1] Min Feng, Jin Zhao, Hrvoje Petek *Science*, **320**,359, 2008.

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