

Abstract Submitted
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Superatom states in an endohedral fullerene¹ TIAN HUANG, MIN FENG, JIN ZHAO, HRVOJE PETEK, Dept. of Physics and Astronomy, University of Pittsburgh, SHANGFENG YANG, LOTHAR DUNSCH, Group of Electrochemistry and Conducting Polymers, Leibniz-Institute for Solid State and Materials Research (IFW), Dresden — Motivated by the recent discovery of superatom states in C₆₀[1], we studied the electronic structures of an endohedral fullerene, Sc₃N@C₈₀, adsorbed on copper surface by LT-STM experiment and DFT calculation. Both experimental and calculated results show that superatom states also exist in Sc₃N@C₈₀. Different from the C₆₀, the encapsulated cluster (Sc₃N-) in Sc₃N@C₈₀ distorts the nearly-spherical potential of the carbon cage, making the atom-like orbitals look asymmetric in the STM images. The adsorbed molecules exhibit various shapes of superatom orbitals due to the different orientation of the Sc₃N@C₈₀ on the surface. When two molecules form a dimer, however, the strong intermolecular hybridization overcomes the perturbation induced by the inside clusters, making all the dimers to have similar H₂like molecular orbitals with clear bonding and anti-bonding characteristics. [1] Min Feng, Jin Zhao, Hrvoje Petek Science, 320,359, 2008.

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