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Theoretical study of tunneling spectra of tetramantane on Au(111) surface EMMANOUIL KIOUPAKIS[1], Y. WANG, R. YAMACHIKA, X. LU, M. F. CROMMIE, STEVEN G. LOUIE, Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — Diamondoids are a class of carbon-based molecules in which the carbon atoms are structured in a diamond-like fashion with all dangling bonds saturated with hydrogen atoms. Recently, scanning tunneling microscopy experiments were carried out to study the tunneling spectra of tetramantane on Au (111) surface. The elastic tunneling images have a LUMO-like character in a broad energy range around the Fermi level, while the inelastic signal shows spatial localization. We use ab-initio density functional theory calculations to study the molecule-surface system and discuss the observed elastic and inelastic tunneling spectra. This work was supported by National Science Foundation Grant No. DMR04-39768, by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231, and by an NSF Graduate Research Fellowship. Computational resources have been provided by NERSC and NPACI.

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