Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Ab initio modeling of STM elastic and inelastic tunneling spectra of tetramantane on Au(111) surface. EMMANOUIL KIOUPAKIS[1], R. YAMACHIKA, Y. WANG, X.H. LU, Department of Physics, University of California at Berkeley, M.F. CROMMIE, STEVEN G. LOUIE, Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — The recent discovery of the higher diamondoids in crude oil has stimulated interest in their study and several potential technological applications of these molecules have already been proposed. In studying the electronic properties of molecular or nanoscale structures on surfaces, the scanning tunneling microscope is usually the probe of choice. Currently, scanning tunneling microscopy experiments of isolated tetramantane molecules on a (111) gold surface are being carried out. We have performed ab initio pseudopotential density functional theory calculations of the electronic properties of tetramantane and provide a comparison of the elastic and inelastic tunneling spectra between our simulation and the ongoing experiment. This work was supported by the NSF Grant Nos. DMR04-39768 and EEC-0425914 and U.S. DOE Contract No. DE-AC03-76SF00098.

[1]Fellow of the Onassis Foundation

Emmanouil Kioupakis
Department of Physics, University of California at Berkeley

Date submitted: 04 Dec 2005 Electronic form version 1.4