Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Vibrational properties of an adamantane monolayer on a gold surface[1] YUKI SAKAI, Tokyo Institute of Technology and University of California, Berkeley, GIANG D. NGUYEN, University of California, Berkeley, RODRIGO B. CAPAZ, Universidade Federal do Rio de Janeiro and University of California, Berkeley, SINISA COH, IVAN V. PECHENEZHSKIY, University of California, Berkeley and Lawrence Berkeley National Laboratory, XIAOPING HONG, University of California, Berkeley, MICHAEL F. CROMMIE, FENG WANG, University of California, Berkeley and Lawrence Berkeley National Laboratory, SUSUMU SAITO, Tokyo Institute of Technology, STEVEN G. LOUIE, MARVIN L. COHEN, University of California, Berkeley and Lawrence Berkeley National Laboratory — We study the vibrational properties of an adamantane monolayer on a Au(111) surface. The IR spectrum of a self-assembled monolayer of adamantane on Au(111) is measured by a newly developed infrared scanning tunneling microscopy (IRSTM) technique. We analyze the IR spectrum of this system by a density functional theory and find that the IR spectrum is severely modified by both adamantane-gold and adamantane-adamantane interactions. One of three gas-phase C-H bond stretching modes is significantly red-shifted due to the molecule-substrate interactions. The intermolecular interactions cause a suppression of the IR intensity of another gas-phase IR peak. The techniques used in this work can be applied for an independent estimate of molecule-substrate and intermolecular interactions in related diamondoid/metal-substrate systems.

[1]This work was supported by NSF grant No. DMR10-1006184 and U.S. DOE under Contract No. DE-AC02-05CH11231.

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Date submitted: 30 Oct 2013 Electronic form version 1.4