Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

First-principle Investigation of the Stability and Vibrational Spectrum of MoSx Nanostructures Grown on Cu(111)[1] TALAT S. RAHMAN, MARAL AMINPOUR, DUY LE, MARISOL ALCÁNTARA ORTIGOZA, University of Central Florida, Department of Physics, Orlando FL 32816-2385, USA — Recent experiments have successfully synthetized MoS_X nanostructures in a controlled manner by evaporating Mo adatoms on the copper sulfide monolayer that forms on Cu(111) upon sulfur preloading [1,2]. STM observations and total-energy calculations based on density functional theory, including van-der-Waals interactions, have proposed several structures for MoS_X/Cu(111). In this study, we investigate the plausibility of those structures and provide elements for further experimental substantiation or refutation. In particular, we perform density-functional-theory calculations (including ab intio van-der-Waals interactions) of vibrational spectrum of the proposed structures to (1) attest their dynamical stability; (2) compare their thermodynamic stability as obtained from the total free energy; and (3) provide the vibrational frequencies that uniquely fingerprint the proposed structures.

[1] Kim et al., Langmuir 27, 11650 (2011)
[2] Dezheng D Sun, Angew Chem. Int. Ed. **51**, 10284-8 (2012)

[1]This work was supported in part by DOE grant DE-FG02-07ER15842

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Date submitted: 28 Nov 2012 Electronic form version 1.4