Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Structural, electronic, and magnetic properties of the Mn3N2(001) surfaces J. GUERRERO-SANCHEZ, KANGKANG WANG, NOBORU TAKEUCHI, ARTHUR R. SMITH, Department of Physics and Astronomy, Nanoscale and Quantum Phenomena Institute, Ohio University, Athens, Ohio 45701, United States — Structural, electronic, and magnetic properties of theMn3N2(001) surfaces have been investigated experimentally in recent years. The molecular beam epitaxy technique has been used for the sample preparation. Scanning tunneling microscopy measurements show two different surface terminations: a Mn3N2(001)-(1x1)structure with MnN-layer termination and a Mn3N2-c(4x2) structure with the formation of Mn tetramers [1]. Spin-polarized STM studies have revealed a spin anisotropy in antiferromagnetic Mn3N2(001) nanopyramids. To explain these results it has been proposed an induced anisotropy as a result of the atomic strain generated by the absence of N atoms that drives the structure to a non-collinear magnetic configuration or by the formation of molecule-like Mn tetramers on the surface [2]. In this work we perform first principles total energy calculations to investigate the Mn3N2(001)-(1x1) and Mn3N2(001)-(2x2) surfaces. We have determined the structural, electronic and magnetic properties of bulk Mn3N2 and compare results with those reported previously. The most favorable configuration for both surfaces has been obtained by calculating the surface formation energy. We have also studied the electronic and magnetic properties of the most stable surface structures. References [1] Rong Yang.; et al. Appl. Phys. Lett. 88, 173101 (2006). [2] Kangkang Wang and Arthur R. Smith, Nano Lett. 12, 5443 (2012).

Arthur R. Smith
Department of Physics and Astronomy, Nanoscale and Quantum Phenomena Institute, Ohio University, Athens, Ohio 45701, United States

Date submitted: 15 Nov 2013 Electronic form version 1.4