Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Interstitial hydrogen in vanadium dioxide[1] W. B. FOWLER, M. STAVOLA, WEIKAI YIN, YING QIN, Lehigh University, L. A. BOATNER, Oak Ridge National Laboratory — It has long been recognized that VO_2 has a monoclinic-to-rutile phase transition as the temperature increases through 340K, accompanied by a remarkable increase in conductivity from insulator to metal[1,2]. Recently it has been found that interstitial hydrogen can modify both the structural and the electronic phase transition[3]. The way hydrogen does this has only recently begun to be studied[4]. We are using infrared spectroscopy to study the properties of H_i, and are also using the CRYSTAL06 code[5] with hybridized DFT Hamiltonian to determine equilibrium positions and vibrational frequencies. IR spectroscopy finds several OH vibrational lines in hydrogenated VO_2 samples. Within the monoclinic structure of VO_2 there are four inequivalent sites for H_i which may lead to distinct spectroscopic signatures. [1] F. J. Morin, Phys. Rev. Lett. **3**, 34 (1959). [2] A. Zylbersztejn and N. F. Mott, Phys. Rev. B **11**, 4383 (1975). [3] J. Wei *et al.*, Nature Nanotechnology **7**, 357 (2012). [4] K. H. Warnick *et al.*, Appl. Phys. Lett. **104**, 101913 (2014). [5] R. Dovesi *et al.*, *Crystal06 User's Manual* (University of Torino, Torino, 2006).

[1]Supported by NSF grant DMR-1160756.

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Date submitted: 14 Nov 2014 Electronic form version 1.4