Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Ab Initio phonon calculations in metallic and insulating phases of VO_2[1] CHRISTOPHER HENDRIKS, ERIC WALTER, HENRY KRAKAUER, William and Mary College — Vanadium dioxide (VO_2) undergoes a first-order metal-insulator transition (MIT) from the high-temperature rutile phase (R) to an insulating, low-temperature monoclinic phase (M1). Several competing insulating phases exist, with phase boundaries in a narrow temperature and strain range close to the MIT[2,3]. Recently, novel IR and Raman measurements of micro- and nano-structured VO_2 samples have become increasingly available; this allows the phases to be studied while avoiding many difficulties with bulk samples, such as twinning and cracking on cycling through the MIT. Theoretical calculations of vibrational properties can assist in the interpretation of such experiments[4]. We will present *ab initio* DFT+U calculations of phonon frequencies for the various phases and compare these to reported measurements for the R, M1[5], M2 and T phases[6].

[1]Supported by ONR
[2]J. H. Park, Nature **500**, 431 (2013).
[3]J. M. Atkin et al, PRB **85**, 020101 (2012).
[4]T. J. Huffman et al., PRB **87**, 115121 (2013).
[5]P. Schilbe et al., Mat. Sci. and Eng. A **370**, 449-452 (2004).
[6]C. Marini et al., PRB **77**, 235111 (2008).

Christopher Hendriks
William and Mary College

Date submitted: 14 Nov 2014 Electronic form version 1.4