Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Ab Initio calculations of phonons in metallic rutile and insulating monoclinic M1 and M2 VO_2[1] CHRIS HENDRIKS, ERIC WALTER, HENRY KRAKAUER, College of William and Mary — Vanadium dioxide (VO_2) undergoes a first-order metal-insulator transition (MIT) at 340 K from a metallic, high-temperature rutile phase (R) to an insulating, low-temperature monoclinic phase (M1). Under tensile strain, two other insulating phases, a second monoclinic phase (M2) and a low symmetry triclinic phase (T), are also known to exist. Recently, Park *et al.*[2] observed a solid-state triple point of these phases in strained VO_2 nanobeams. More recently, phonon frequencies for strain-stabilized M2 have been observed.[3] Understanding the vibrational properties of these phases may help resolve questions surrounding the long-debated issue of the respective roles of electronic correlation and Peierls mechanisms in driving the MIT. We will present *ab initio* DFT and DFT+U calculations of phonon frequencies for the M2 phase and compare these to measured results and to previous calculations and measurements for the R and M1 phases.[4]

[1]Supported by ONR
[2]J. H. Park, Nature **500**, 431 (2013).
[3]M. M. Qazilbash, private communication
[4]T. J. Huffman et al., PRB **87**,115121 (2013).

Eric Walter
College of William and Mary

Date submitted: 15 Nov 2013 Electronic form version 1.4