Abstract Submitted
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Structural and vibrational properties of VO2 from DFT and DFT+U calculations[1] ERIC J. WALTER, HENRY KRAKAUER, TYLER J. HUFFMAN, PENG XU, M. M. QAZILBASH, College of William and Mary — Vanadium dioxide (VO_2) undergoes a metal-insulator transition (MIT) at 340 K from a metallic, high-temperature rutile phase to a insulating, low-temperature monoclinic phase. In thin films, the extremely fast switching times ($\simeq$ 100 femtoseconds) of the MIT have led to many suggested device applications. Understanding the MIT driving mechanism and the long-debated importance of electronic correlation is important to these developments. We have computed the relaxed geometry and phonon frequencies using DFT and DFT+U for both phases of VO_2. The dependence of vibrational mode frequencies and oscillator strengths on the Hubbard U parameter and their sensitivity to the Born effective charges in the insulating monoclinic phase will be reported. The calculated frequencies for $U = 5$ eV are in good agreement with recent experimental infrared micro-spectroscopy measurements on single crystal platelets of VO_2 [2]. Our results indicate that strong electron-electron correlation must be included to describe the vibrational properties.

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[2]T. J. Huffman et al., PRB, submitted.

Eric J. Walter
College of William and Mary

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