Abstract Submitted
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Ab Initio Infrared Spectra and Electronic Response Calculations for the Insulating Phases of VO_2[1] CHRISTOPHER HENDRIKS, TYLER HUFFMAN, ERIC WALTER, MUMTAZ QAZILBASH, HENRY KRAKAUER, William and Mary College — Previous studies have shown[2] that, under doping or tensile strain and upon heating, the well-known vanadium dioxide (VO_2) transition from an insulating monoclinic (M1) to a metallic rutile (R) phase progresses through a triclinic symmetry (T) phase and a magnetic monoclinic phase (M2), both of which are insulating. Structurally, this progression from M1 to R through T and M2 can be characterized by the progressive breaking of the V dimers. Investigation of the effect of these structural changes on the insulating phases of VO_2 may help resolve questions surrounding the long-debated issue of the respective roles of electronic correlation and Peierls mechanisms in driving the MIT. We investigated electronic and vibrational properties of the insulating phases of VO_2 in the framework of DFT+U. We will present *ab initio* calculations of infrared spectra and optical electronic responses for the insulating phases and compare these to available experimental measurements [3456].

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[2]J. H. Park et al., Nature **500**, 431 (2013).
[3]T. J. Huffman et al., PRB **87**, 115121 (2013).
[4]A. S. Barker et al., PRL **17**, 1286 (1966).
[5]H. W. Verleur et al., PR **172**, 788 (1968).
[6]J. M. Tomczak and S. Biermann, PRB **80**, 085117 (2009).

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