Abstract Submitted
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The optical gap in VO_2 insulating phases is dominated by Coulomb repulsion[1] CHRISTOPHER HENDRIKS, ERIC WALTER, HENRY KRAKAUER, TYLER HUFFMAN, MUMTAZ QAZILBASH, College of William and Mary — Under doping, tensile strain or heating, vanadium dioxide (VO_2) transforms from an insulating monoclinic (M1) to a metallic rutile (R) phase, progressing through intermediate insulating triclinic (T) and magnetic (M2) phases. Broadband optical spectroscopy data have been obtained [2] on the T and M2 phases in the *same* sample. While only half the V atoms are dimerized in M2 compared to M1 and T, the measured optical gap is essentially unaltered by the first-order structural phase transition between them. Moreover, the optical interband features in the T and M2 phases are remarkably similar to those previously observed in the well-studied M1 phase. This shows that the electronic structure is insensitive to the lattice structure. Our ab-initio HSE optical conductivity calculations on the insulating phases of VO_2 are in excellent agreement with the experimental measurements. We will discuss the choice of α, the fraction of exact exchange. As the energy gap is insensitive to the different lattice structures of the three insulating phases, we rule out Peierls effects as the dominant contributor to the opening of the gap. Rather, the energy gap arises from intra-atomic Coulomb correlations.

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[2]T. J. Huffman *et al.* arXiv:1608.08227.

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