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OPTICAL SPECTROSCOPY OF THE M_2 AND T PHASES OF VANADIUM DIOXIDE T.J. HUFFMAN, M.M. QAZILBASH, C. HENDRIKS, E.J. WALTER, H. KRAKAUER, College of William and Mary, JOONSEOK YOON, HONGLYOUL JU, Yonsei University, R. SMITH, G.L. CARR, Brookhaven National Laboratory — The salient feature of the familiar structural transition that accompanies the metal-insulator transition in bulk VO_2 is a pairing of all of the vanadium ions in the M_1 insulating phase. This pairing has long been thought critical to the emergence of insulating behavior. However, there exist two less familiar insulating states, M_2 and T. These phases notably exhibit distinctly different V-V pairing. In the M_2 phase, only half of the vanadium ions exhibit pairing while the other half carry local spin 1/2 magnetic moments and are equally spaced in quasi-one dimensional chains. The T phase has two types of inequivalent vanadium chains, each consisting of V-V pairs but with different spacing between V ions in the pairs. The M_1 phase has been studied extensively with optical spectroscopy. By studying the two less familiar insulating phases, M_2 and T, one can investigate how changes in V-V pairing affect the properties of the VO_2 insulating state. We performed infrared and optical spectroscopy on the M_2 and T phases in the same sample. Despite a clear change in the lattice structure, the inter-band transitions are insensitive to changes in the V-V pairing. This result conclusively establishes that intra-atomic Coulomb repulsion between electrons provides the dominant contribution to the energy gap in all insulating phases of VO_2 . Our work highlights the necessity of considering the M_2 and T phases of VO_2 in future experimental and theoretical research.

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