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**Band Theory for the Electronic and Magnetic Properties of VO<sub>2</sub> Phases**<sup>1</sup> XIAO SHEN, Vanderbilt University, University of Memphis, SHENG XU, Jiangsu University of Science and Technology, KENT HALLMAN, RICHARD HAGLUND, Vanderbilt University, SOKRATES PANTELIDES, Vanderbilt University, Oak Ridge National Lab — VO<sub>2</sub> is widely studied for the insulator-metal transition between the monoclinic M1 (insulator) and rutile R (metal) phases. Recent experiments show that in addition to the M1 and R phases, VO<sub>2</sub> has a rich phase diagram including a recently identified metallic monoclinic phase, making the material particularly intriguing. The origin of the band gap in the insulating phase of VO<sub>2</sub> has been a subject of debate. It was suggested that the insulating phase cannot be described by band theory and thus strong correlations must be invoked. However, recent band calculations using density functional theory (DFT) with a hybrid functional and standard pseudopotentials correctly obtains a band gap for the M1 insulating phase. Subsequent calculations, however, found that the magnetic properties of VO<sub>2</sub> phases are not correctly described by such calculations. Here we present DFT calculations using a tuned hybrid functional and hard pseudopotentials that reproduce both the band gaps and the magnetic properties of the known VO<sub>2</sub> phases. Thus, it is appropriate to use band theory to describe VO<sub>2</sub> phases without invoking strong correlations. Furthermore, using the band theory treatment, we identify a candidate for the metallic monoclinic phase.

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