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First principles calculations of insulator-to-metal transition in photoexcited monoclinic VO2 LEDE XIAN, University of the Basque Country, MATTEO GATTI, Ecole Polytechnique, PIERLUIGI CUDAZZO, University of the Basque Country, DANIEL WEGKAMP, MARC HERZOG, Fritz Haber Institute of the Max Planck Society, CHRISTINA MCGAHAN, ROBERT MARVEL, RICHARD HAGLUND, Vanderbilt University, MARTIN WOLF, JULIA STAHLER, Fritz Haber Institute of the Max Planck Society, ANGEL RUBIO, University of the Basque Country — The insulator-to-metal phase transition of VO2 has been discovered for a long time, but its origin remains elusive. In recent experiments, ultrafast band gap collapse of monoclinic VO2 upon photo excitation was observed through time resolved photoelectron spectroscopy (TRPES). In order to study this issue, we have performed first principles calculations based on many-body perturbation theory. We show that the band gap in monoclinic phase is extremely sensitive to small changes in the occupation of the localized d bands of V atoms. In particular, the photo-induced hole doping in VO2 can strongly alter the dynamical screening, which then leads to a collapse of the band gap. Our results support the experimental findings and point to the electronic origin of the insulator-to-metal phase transition of monoclinic VO2 in the TRPES experiments.

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