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Ab initio **study of optical excitations in VO_2** JOHN COULTER, Florida State Univ, ADAM GALI, Wigner Research Center, Hungarian Academy of Sciences, EFSTRATIOS MANOUSAKIS, Florida State Univ, NHMFL — Motivated by recent experimental efforts to fabricate p-n junctions from transition metal oxides (TMOs) and a recent theoretical study claiming TMOs to be good absorbers and promising materials for efficient carrier multiplication, we study the optical properties of a prototypical TMO, the insulator M_1 phase of vanadium dioxide (VO_2), by *ab initio* methods. We applied the Bethe-Salpeter equations (BSE) to calculate the optical properties, starting from self-consistent GW quasi-particle energy levels and states. In contrast to expectations, the exciton binding energy obtained by BSE is in good agreement with the experiment. We find that the electron-electron interaction is very strong which makes this material promising for efficient carrier multiplication that might lead to an enhanced efficiency in photo-voltaics applications. To illustrate this more quantitatively, we calculated the impact ionization rate within the independent quasiparticle approximation, and find that the rate is significantly higher than silicon in the region of highest solar intensity, due to the strong multiple carrier excitations.

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