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A DFT-based method of calculating optical properties of transition metal oxide materials JOHN E. COULTER, Florida State University, ADAM GALI, Institute for Solid State Physics and Optics - Hungarian Academy of Sciences, MANOUSAKIS EFSTRATIOS, Florida State University — As part of an ongoing investigation of optical properties of transition metal oxide materials, we have examined the optical properties of Vanadium Dioxide using an *ab-initio* method. Starting from hybrid DFT, we apply the GW approximation and solve the Bethe-Salpeter Equation (BSE) on the wavefunctions obtained from the DFT starting point. We find that the hybrid functional is not fully satisfactory for description of the optical spectrum of VO2, and that corrections are required. The hybrid functional results may be a good starting place for many-body perturbation theory. We apply the GW approximation and then solve the BSE from that starting point. We show that including single particle-hole quasiparticles is not sufficient for the optical spectrum, and that two-particle-two-hole effects must be included via the BSE to give agreement between the integrated strength of the optical spectrum at low energies and the experimental spectrum. We also find that a large number of high energy states must be included for a convergent description of the low energy optical spectrum.

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