

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

All-electron GW calculation of vanadium dioxide REI SAKUMA, TAKASHI MIYAKE, FERDI ARYASETIAWAN, JST-CREST, AIST — We present the results of the GW calculation of metallic and insulating vanadium dioxide using a full-potential LMTO basis set. Our calculations show that it is crucial to take into account both the frequency dependence and the off-diagonal elements of the self-energy. We find that the usual 1-shot GW scheme, where the frequency expansion of the self-energy is truncated in the first-order, yields a large error ($> 0.1\text{eV}$) in quasiparticle energies due to the unsmoothness of the self-energy. In both phases, the dynamical correlation effect within RPA leads to a plasmon satellite above the Fermi level, but not below. This difference can be attributed to matrix element effects. Our 1-shot GW calculation does not reproduce insulating VO_2 due to the mixing of conduction and valence bands in the LDA calculation, and we reconstruct G and W by updating the quasiparticle wavefunctions and energies to obtain the band gap. The result indicates the importance of self-consistency in GW calculations. Our results are more in line with the Peierls picture of gap opening due to the lattice distortion, rather than the Mott-Hubbard picture of strong correlations.

Rei Sakuma
JST-CREST, AIST

Date submitted: 26 Nov 2007

Electronic form version 1.4