Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Energy band structure of bulk and monolayer vanadium pentoxide (V_2O_5) beyond the quasiparticle self-consistent GW approximation: lattice polarization effects[1] CHURNA BHANDARI, WALTER R.L. LAMBRECHT, Department of Physics, Case Western Reserve University, MARK VAN SCHILFGAARDE, King's College, London — The quasiparticle self-consistent GW method (QSGW) is known to systematically overestimate the band gaps in semiconductors by about 20% due to the underestimate of screening by the random phase approximation (RPA). We show that for V_2O_5, a layered oxide material, the overestimate is significantly larger. The smallest direct gap in QSGW is found to be 4.83 eV compared to 2.35 eV experimentally. The evidence for the experimental gap and optical properties are reviewed. We suggest that a major contribution to the self-energy reduction results from the lattice polarization contribution to the dielectric screening. This results from the large LO/TO splittings in this material. We make a simple estimate of the reduction of $W(q{=}0, \omega{=}0)$, and obtain a factor $\sim$0.38, which if assumed to apply for all W and reduces the gap to 2.60 eV. The remainder of the gap overestimate is tentatively ascribed to shortcomings of the RPA. We also consider the band structure of this material in monolayer form. We find that the GW correction depends strongly on the layer separation (L) as 1/L. The lattice polarization itself depends on distance between the layers because of the dependence of the phonons on the long-range Coulomb interactions and hence reduced screening in a 2D system.

[1]Supported by DOE, AFSOR, Simons Foundation.

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Date submitted: 10 Nov 2014 Electronic form version 1.4