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Electronic and optical properties of $LaVO3$ and $LaVO3/SrTiO3$ interface using Ab Initio techniques SUVADIP DAS, EFSTRATIOS MANOUSAKIS, Florida State Unversity — We have investigated the electronic structure and optical anisotropy of the strongly correlated system $LaVO_3$ using DFT+U and Many body perturbation theory (MBPT) techniques implemented by the Vienna Ab Initio Simulation Package (VASP) code. LDA+U predicts $LaVO_3$ to be an antiferromagnetic insulator with C-type spin and G-type orbital ordering in the monoclinic phase. We will discuss the nature of the transitions leading to the in-plane and out of plane anisotropy in the optical conductivity of $LaVO_3$ using GGA+U. The GW self-energy correction have been incorporated by solving the quasiparticle energies self consistently and the two particle-hole excitonic effects have been included by further solving the Bethe Salpeter equations (BSE). The electronic structure and nature of the low energy optical peaks and their dependence on temperature in the $LaVO_3/SrTiO_3$ interface will be presented. The prospect of using $LaVO3/SrTiO3$ as a photovoltaic cell with enhanced photo current by the generation of multiple elctron-hole pairs will also be discussed.

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