Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Anisotropic optical properties of few-layer transition metal dichalcogenide ReS_2 ZHENGLU LI, TING CAO, FELIPE H. DA JORNADA, MENG WU, STEVEN G. LOUIE, Physics Department, UC Berkeley and Lawrence Berkeley National Lab — We present first-principles (DFT, GW and GW-BSE) calculations of the electronic and optical properties of few-layer rhenium disulfide (ReS_2). Monolayer ReS_2 shows strong many-electron effects with a fundamental quasiparticle band gap of 2.38 eV based on G_0W_0 calculation and a large exciton binding energy of 690 meV based on solving the Bethe-Salpeter equation. Highly anisotropic linear-polarized optical absorptions are revealed for few-layer and bulk ReS_2. The band gap shows a decreasing trend with the optical polarization direction near the absorption edge gradually rotating from around 67 degree in the monolayer to 85 degree in the bulk, referencing to the Re-chain. Our calculations are consistent with recent experimental data and theoretical studies, and provide a systematic understanding of the electronic and optical properties in few-layer ReS_2. This work was supported by National Science Foundation Grant No. DMR15-1508412 and the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at Lawrence Berkeley National Laboratory's NERSC facility.

Zhenglu Li
Physics Department, UC Berkeley and Lawrence Berkeley National Lab

Date submitted: 05 Nov 2015 Electronic form version 1.4