Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Quasiparticle self-consistent GW calculations of monolayer, bilayer and bulk MoS_2 TAWINAN CHEIWCHANCHAMNANGIJ, WALTER LAMBRECHT, JIE SHAN, Department of Physics, Case Western Reserve University, 10900 Euclid Avenue, Cleveland, Ohio 44106 — Photoluminescence and absorption spectra of monolayer MoS_2 indicate a direct gap behavior while bulk MoS_2 is known to have an indirect gap. The details of these spectra and the band structure are not yet fully understood. Here, the quasiparticle self-consistent GW method is used to study the electronic structure of monolayer, bilayer, and bulk MoS_2. Band structures, effective masses, and dielectric functions are extracted from our calculations. In contrast to another recent GW calculation, we find the monolayer to have a direct gap of 2.84 eV at K, which is large compared to the photoluminescence energies. The exciton binding energy for this transition is estimated within an effective mass approximation using our calculated effective masses and dielectric constants and amounts to about 0.90 eV, leading to good agreement with the experimental data for the lowest direct transition. We find a second conduction band local minimum along Γ-K about 0.44 eV higher but do not find it to give rise to a bound state exciton. When spin-orbit coupling is included, we find a spin-splitting of the levels along Γ-K in the monolayer related to the absence of an inversion center. In the bilayer, we find an indirect gap from Γ-K and a splitting of the valence band at K, mainly due to the interlayer interaction but also increased by spin-orbit coupling. The splitting between the lowest two absorption features A and B is consistent with the slightly larger splitting calculated in the bilayer than the monolayer.

Tawinan Cheiwchanchamnangij
Department of Physics, Case Western Reserve University,
10900 Euclid Avenue, Cleveland, Ohio 44106

Date submitted: 27 Nov 2011 Electronic form version 1.4