Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Electric field and spin-orbit coupling effects on the band structure of monolayer WSe_2[1] ITTIPON FONGKAEW, School of Physics, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand, WALTER R.L. LAMBRECHT, Department of Physics, Case Western Reserve University, Cleveland, OH, USA 44106 — Transition metal dichalcogenides are known to switch from indirect to direct gap between bulk and monolayer form. Here we show that in WSe_2, an electric field perpendicular to the layer of order a few 0.1 MV/cm has strong effects on the conduction band and can convert the material back to an indirect gap. The competing minima at different points in the Brillouin zone undergo different shifts with electric field because of their different orbital character. Using first-principles GGA calculations in the presence of an electric field with and without spin-orbit coupling, we determine the critical field at which the minimum between Γ and K (where the gap occurs in bulk) becomes back the lowest conduction band minimum. For even stronger electric fields we find the CBM to shift to the Γ-point. While the electric fields considered here are much larger than the fields obtained in gated structures, they may be possible using electric double layers using an electrolyte. Such measurements have already been done on bulk WSe_2, [Nature Physics 9, 563 (2013)] but focused on the valence band and Rashba effects instead of the conduction band.

[1]This work was supported by Development and Promotion of Science and Technology Talents Project (DPST).

Ittipon Fongkaew
Suranaree University of Technology

Date submitted: 13 Nov 2014 Electronic form version 1.4