Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Effective tight-binding model for transition metal dichalcogenides[1] YEN-HUNG HO, MIGUEL CAZALILLA, National Tsing Hua University, TAIWAN, HECTOR OCHOA, University of California, Los Angeles, USA — For transition metal dichalcogenides, various band models have been developed to describe the novel subband features. In this work, we propose a new effective minimum-band model by preforming a canonical transformation on the full-band Hamiltonian. We found that, depending on the form of transformation, both the Γ- and K-valley electrons can be well captured, including the frequency and band effective mass. And, for the full-band parameters used, starting from Wannier function basis set leads to a better result than from Slater-Koster basis set. A close inspection of the transformation projection also enables us to extract the modification on the site energy, as well as the orbital hopping between several nearest neighboring atoms. Instead of pure empirical fitting, our effective models preserve rich orbital physics inside, which is shown to be versatile in studying a variety of fundamental physical properties.

[1]Ministry of Science and Technology of Taiwan (NSC 102-2112-M-007-024-MY5)

Yen-Hung Ho
Physics, National Tsing Hua University, TAIWAN

Date submitted: 06 Nov 2015 Electronic form version 1.4