Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Monolayer II-VI semiconductors: A first-principles prediction[1]
HUI ZHENG[2], Department of NanoEngineering, University of California San Diego, NIAN-KE CHEN, College of Electronic Science and Engineering, Jilin University, China, S. B. ZHANG, Department of Physics, Applied Physics, Astronomy, Rensselaer Polytechnic Institute, USA, XIAN-BIN LI[3], State Key Laboratory on Integrated Optoelectronics, College of Electronic Science and Engineering, Jilin University, China — A systematic study of 32 honeycomb monolayer II-VI semiconductors is carried out by first-principles methods. It appears that BeO, MgO, CaO, ZnO, CdO, CaS, SrS, SrSe, BaTe, and HgTe honeycomb monolayers have a good dynamic stability which is revealed by phonon calculations. In addition, from the molecular dynamic (MD) simulation of other unstable candidates, we also find two extra monolayers dynamically stable, which are tetragonal BaS and orthorhombic HgS. The honeycomb monolayers exist in form of either a planar perfect honeycomb or a low-buckled 2D layer, all of which possess a band gap and most of them are in the ultraviolet region. Interestingly, the dynamically stable SrSe has a gap near visible light, and displays exotic electronic properties with a flat top of the valence band, and hence has a strong spin polarization upon hole doping. The honeycomb HgTe has been reported to achieve a topological nontrivial phase under appropriate in-plane tensile strain and spin-orbital coupling (SOC). Some II-VI partners with less than 5% lattice mismatch may be used to design novel 2D heterojunction devices. If synthesized, potential applications of these 2D II-VI families could include optoelectronics, spintronics, and strong correlated electronics.

[1]Distinguished Student (DS) Program of APS FIP travel funds
[2]This work is done when Hui Zheng was a master's student in Jilin University.
[3]*Corresponding author

Hui Zheng
Department of NanoEngineering, University of California San Diego

Date submitted: 09 Nov 2016 Electronic form version 1.4