Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Giant valley drifts in uniaxially strained monolayer MoS_2[1]

QINGYUN ZHANG, YINGCHUN CHENG, LI-YONG GAN, UDO SCHWINGENSCHLOGL, Physical Sciences and Engineering, King Abdullah University of Science and Technology, COMPUTATIONAL PHYSICS AND MATERIALS SCIENCE TEAM — Using first-principles calculations, we study the electronic structure of monolayer MoS_2 under uniaxial strain. We show that the energy valleys drift far off the corners of the Brillouin zone (K points), about 12 times the amount observed in graphene. Therefore, it is essential to take this effect into consideration for a correct identification of the band gap. The system remains a direct band gap semiconductor up to 4% uniaxial strain, while the size of the band gap decreases from 1.73 to 1.54 eV. We also demonstrate that the splitting of the valence bands due to inversion symmetry breaking and spin-orbit coupling is not sensitive to strain.

[1]Computational resources have been provided by KAUST IT. This work is supported by a KAUST CRG grant.

Qingyun Zhang
Physical Sciences and Engineering,
King Abdullah University of Science and Technology

Date submitted: 12 Nov 2014 Electronic form version 1.4