Giant valley drifts in uniaxially strained monolayer MoS$_2$\textsuperscript{1}

QINGYUN ZHANG, YINGCHUN CHENG, LI-YONG GAN, UDO SCHWINGEN-SCHLOGL, 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.

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