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Electronic properties of bilayer mixtures of WS2 and MoS2 with different stackings[1] HUMBERTO TERRONES, ANA LAURA ELIAS, NESTOR PEREA-LOPEZ, The Pennsylvania State University, HUMBERTO R. GUTIERREZ, University of Louisville, AYSE BERKDEMIR, ANDRES CASTRO-BELTRAN, RUITAO LV, The Pennsylvania State University, FLORENTINO LOPEZ-URIAS, The Pennsylvania State University, IPICYT, TAKUYA HAYASHI, YOONG AHM KIM, MORINOBU ENDO, Shinshu University, MAURICIO TERRONES, The Pennsylvania State University — Besides graphene and hexagonal boron nitride, transition metal chalcogenides (TMC) such as MoS2, WS2, NbS2 and WSe2 also exhibit a layered structure in which the layers weakly interact via Van der Waals forces, and for this reason these materials exhibit excellent lubrication properties. For TMC, the layers are formed by the transition metal atom sandwiched by the sulfur atoms. MoS2 and WS2 in bulk are indirect band gap semiconducting materials. However, an isolated sheet of MoS2 or WS2 becomes a direct gap semiconductor. This particular behavior makes them very attractive in terms of optical properties such as spin polarization, in which the lack of center of inversion of one layer plays a crucial role. Therefore, it is important to study the properties of different configurations of WS2 and MoS2 mixtures bi-layer TMC systems with different stackings. First principles calculations are carried out to study how the indirect and the direct gaps behave, thus shedding light in a new type of bi-layered material.

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