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MoS_2-WSe_2 Hetero Bilayer: Possibility of Mechanical Strain Induced Band Gap Engineering MUNISH SHARMA, ASHOK KUMAR, P.K. AHLUWALIA, Department of Physics, Himachal Pradesh University, Shimla-171005 (India) — The tunability of band gap in two-dimensional (2D) hetero-bilayers of MoS_2-WSe_2 with applied mechanical strains (in-plane and out-of-plane) in two different types of stackings (AA and AB) have been investigated in the framework of density functional theory (DFT). The in-plane biaxial tensile strain is found to reduce electronic band gap monotonically and rendered considered bilayer into metal at 6% of applied strain. The transition pressure required for complete semiconductor-to-metal transition is found to be of 7.89 GPa while tensile strength of the reported hetero-bilayer has been calculated 10 GPa at 25% strain. In case of vertical compression strain, 16 GPa pressure has been calculated for complete semiconductor-to-metal transition. The band-gap deformation potentials and effective masses (electron and hole) have been found to posses strong dependence on the type of applied strain. Such band gap engineering in controlled manner (internal control by composition and external control by applied strain) makes the considered hetero-bilayer as a strong candidate for the application in variety of nano scale devices.

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