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Effect of Uniaxial Strain on Band Structure of Multi-layer WS_2*[1]

CONRAD TROHA[2], DUY LE, TALAT RAHMAN, Univ of Central Florida — The ability to tailor band structure of a multi-layer transition metal dichalcogenide is of interest because it opens up utilizations of the material for various applications. Strain is considered a robust way to alter the electronic structure of a material. We performed calculations, using density functional theory, of band structure of multi-layer WS_2 under the effects of uniaxial strain. We show that the position of the bottom of conduction band (BCB) at $\sum$ moves to higher, and at K to lower, energy levels under the effects of uniaxial tensile strain, making multi-layer WS_2 closer to a direct band gap material. Our results suggest that uniaxial tensile strain can be used to alter band structure of multi-layer WS_2 to achieve higher yield photo luminescence.

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