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Strain induced change in electronic and thermoelectric properties in few layers of MoS_2 TRIBHUWAN PANDEY, SWASTIBRATA BHATTACHARYYA[1], ABHISHEK K. SINGH, Materials Research Centre, Indian Institute of Science, Bangalore — The sensitivity of the electronic and thermoelectric properties of MoS_2 on application of strain can open up a variety of applications in the emerging area of straintronics. Using first principles calculations, we investigate the effect of normal compressive (NC), bi-axial compressive (BC), and bi-axial tensile (BT) strain on the electronic properties of few layered MoS_2. Regardless of the manner of strain, a reversible semiconductor-to-metal transition is observed in this material. We further show that under NC strain, the inter-layer interactions between Mo-d_{z^2} and S-p_z causes the S-M transition, whereas under BC and BT strain it is caused by the strong hybridization of the intra-layer Mo-$d_{x^2-y^2}$ and S-p_x orbitals and Mo-d_{z^2} and S-p_z orbitals, respectively. We also study number of layer (nL)and stain dependent transport properties using Boltzmann transport theory. Our study reveals that the 3L and 2L-MoS_2 emerge as the most efficient thermoelectric materials under NC and BT strain, respectively. The concept proposed from our study can also be extended to other semiconducting TMDs owing to similar crystal structure and electronic properties.

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