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Strain engineered optoelectronic properties of transition metal dichalcogenides lateral heterostructures[1] JAEKWANG LEE, MINA YOON, Oak Ridge National Lab — Most three-dimensional bulk-scale materials rarely survive beyond 1% strain, while recently spotlighted two-dimensional (2-D) materials can sustain a high elastic strain (up to 10%) to optimize optical quantities such as band gaps and absorption spectra governing optoelectronic device performance. Despite the enormous interest in strained 2-D materials, most researches are focused on single materials or vertical heterostructures where precise control of stacking orientation is challenging. Here, using first-principles density-functional calculations, we explore how uniaxial tensile strains modify overall electronic and optical properties of transition metal dichalcogenides lateral heterostructures, such as MoX_2/WX_2 (X=S, Se). Based on the detailed optoelectronic information, we predict the optimal strain condition for maximal power efficiency. Furthermore, we find that uniaxial tensile strain readily develops a continuously varying direct-bandgap across the lateral heterojunctions, which results in the broad range absorption of solar spectrum useful for future optoelectronic devices.

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