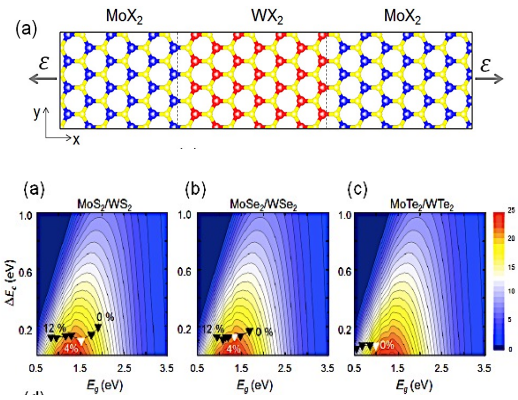
Stretching Semiconductors to Tune Optoelectronic Properties

Achievement: First-principles calculations reveal how mechanical strain be used to enhance the optoelectronic properties of two-dimensional transition metal dichalcogenide (TMD) lateral heterostructures.

Significance and Impact: The work unambiguously shows that strain can simultaneously control the the bandgap, thus opening a route for tuning of optoelectronic properties in TMD lateral heterostructures.

Research Details:

- Using first-principles density functional theory and quasiparticle GW calculations, the study reports the influence of strain on the optoelectronic properties (power conversion efficiency (PCE)) of TMD-based lateral heterostructures.
- Lateral MoX_2/WX_2 (X=S, Se, Te) heterostructures develop type II band alignment with greatly tunable PCE by strain.



Top: (a) The lateral heterostructure, MoX_2/WX_2 (X=S, Se, Te), under a uniaxial strain ε.

Bottom: Computed power conversion efficiency contours as a function of the bandgap (Eg) of WX2 and conduction band offset (ΔEc) of WX2, where the computed Eg and ΔEc at each strain are overlaid on

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PI and affiliation: ???

Team: J. Lee, J. Huang, B. G. Sumpter, and M. Yoon

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Overview:

In this work we report the influence of strain on the optoelectronic properties (power conversion efficiency) of TMD-based lateral heterostructures such as MoX2/WX2 (X=S, Se,Te), by first-principles density functional theory and quasiparticle GW calculations. The results unambiguously show that strain can simultaneously control the energetic distribution of bandgap, thus open a route for tuning of optoelectronic properties in TMD lateral heterostructures. Specifically we find that lateral MoX2/WX2 (X=S, Se, Te) heterostructures develop type II band alignment that facilitates efficient electron–hole separation for light detection/harvesting. In addition, the type II character is robust and can be preserved up to 12% of uniaxial strain. From the strain-dependent bandgap and the band offset, we find that uniaxial tensile strain can significantly increase the power conversion efficiency of lateral heterostructures. For example, 4% uniaxial tensile strain increases the power efficiency of both lateral MoSe2/WSe2 and MoS2/WS2 heterostructures by 15% up to 35%. We thus expect that these strained TMD lateral heterostructures can be utilized as novel architectures for efficient optoelectronic device development by selective control of the bandgap in energetic distribution.