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Spin-orbit induced splitting in presence of non-uniform strain in 2D materials

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Introduction and Motivation:

Strain fields are present in 2D materials due to synthetic procedures or as a way to modulate their properties. Moreover, the occurring strain fields can be uniform or inhomogeneous. Herein, we model the wrinkles of transition metal dichalcogenides (TMDC) as an example of 2D structures with inhomogeneous strain fields.

We would like to answer the following questions:

- ✓How are properties and strain field related?
- ✓How can this be modeled efficiently?
- ✓What level of theory is suitable?
- ✓How can it be used in future applications?

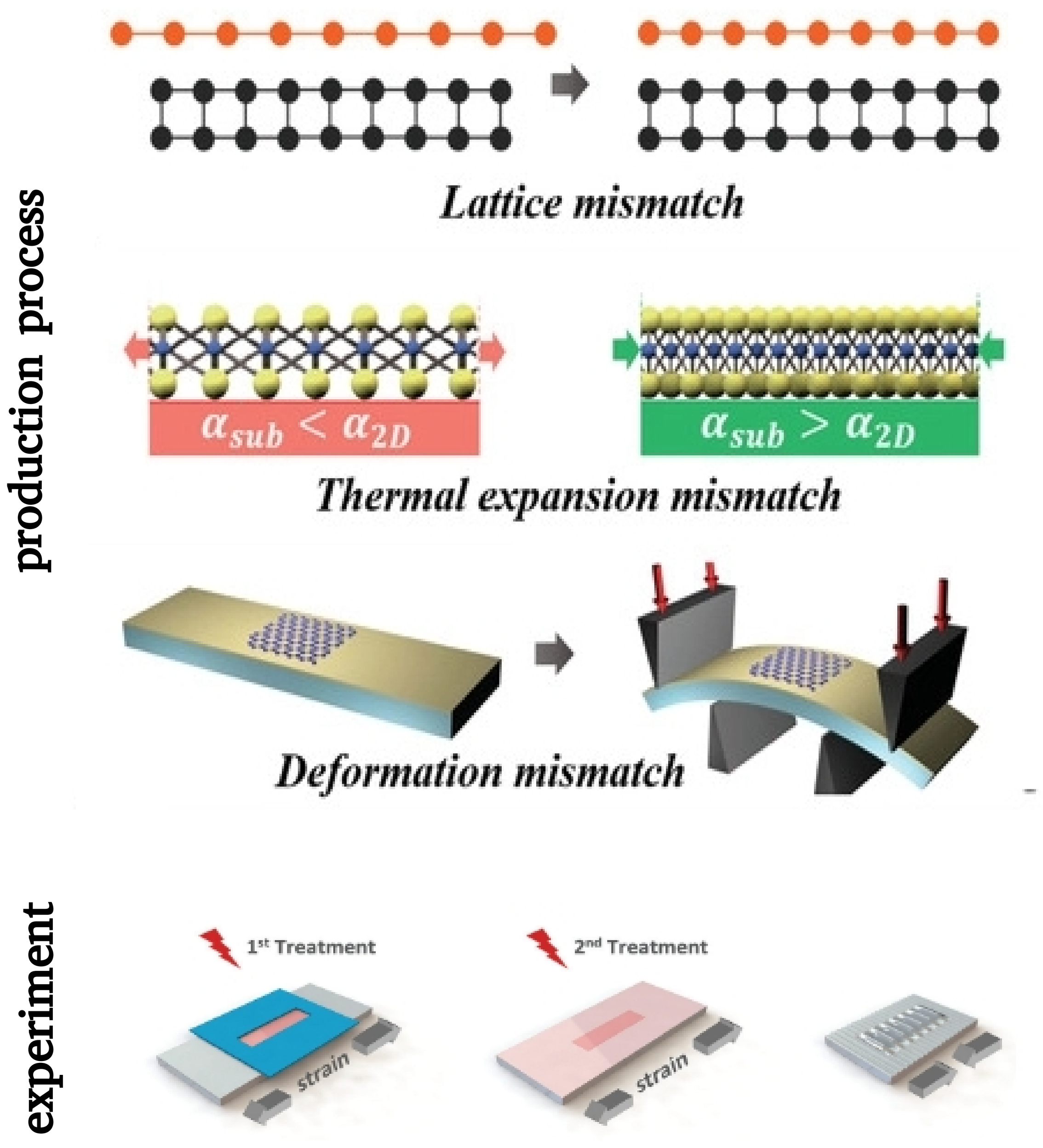

Figure 1. Introduction of the strain field in 2D materials. **Top:** a secondary effect **Bottom:** a direct effect [1,2].

Methods:

Density **F**unctional **T**heory (DFT) with **PBE** functional, **T**katchenko-**S**cheffler (TS) dispersion and spin-orbit coupling

- ✓Helical boundary condition is avoided
- ✓WSe_2 and MoS_2 as model systems
- ✓Nanotube and wrinkle geometries

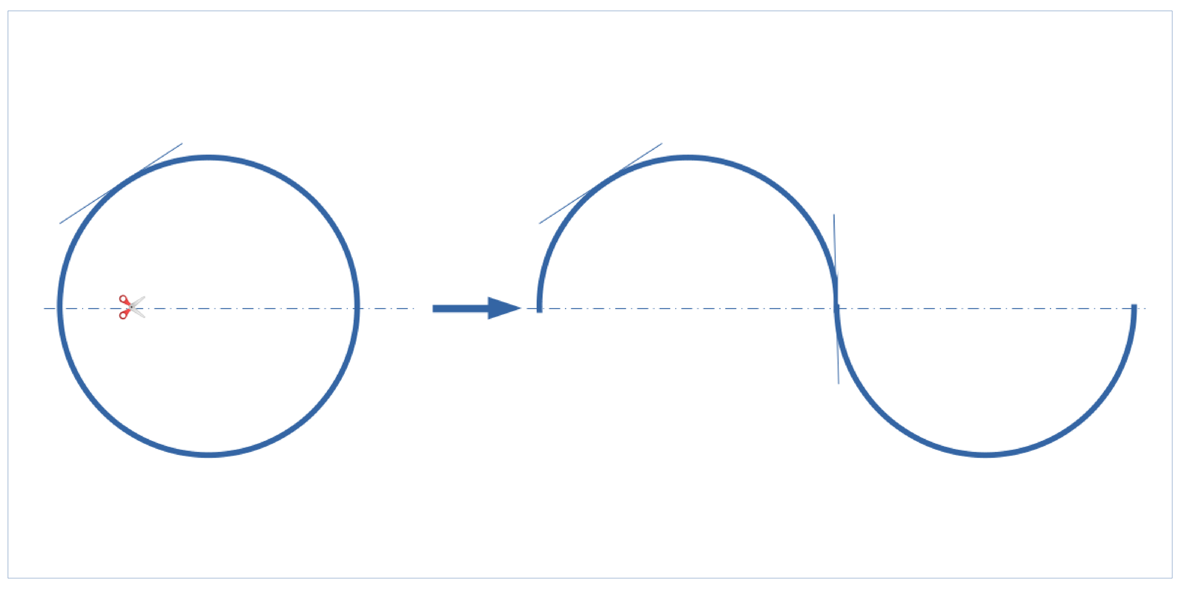

Figure 2. Creation of the initial wrinkle structures from nanotubes.

Non-uniform strain in transition metal dichalcogenides induces **Rashba-like splitting** in their band gap which allows their usage for future spintronic applications.

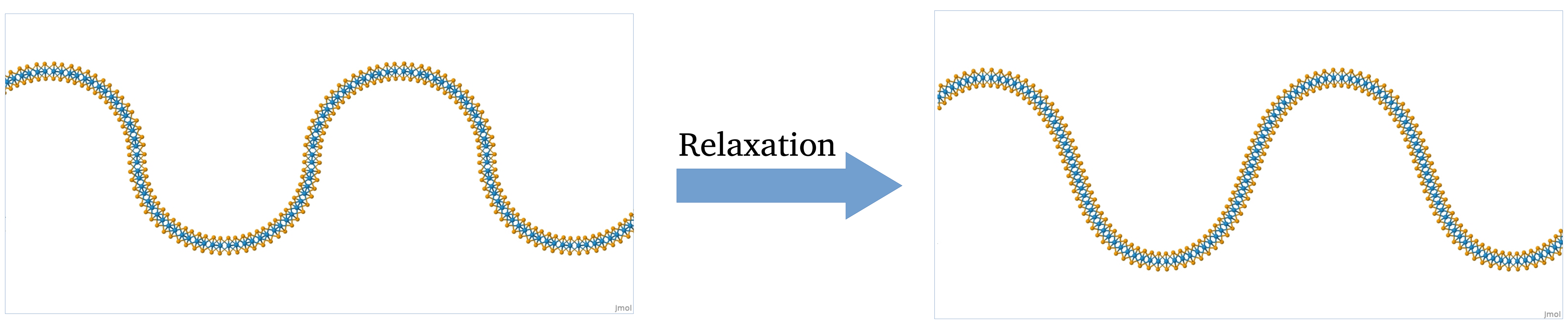

Figure 3. Evolution of wrinkle structures of 2D WSe_2 during the geometry relaxation. **Left:** initial **Right:** relaxed structure.

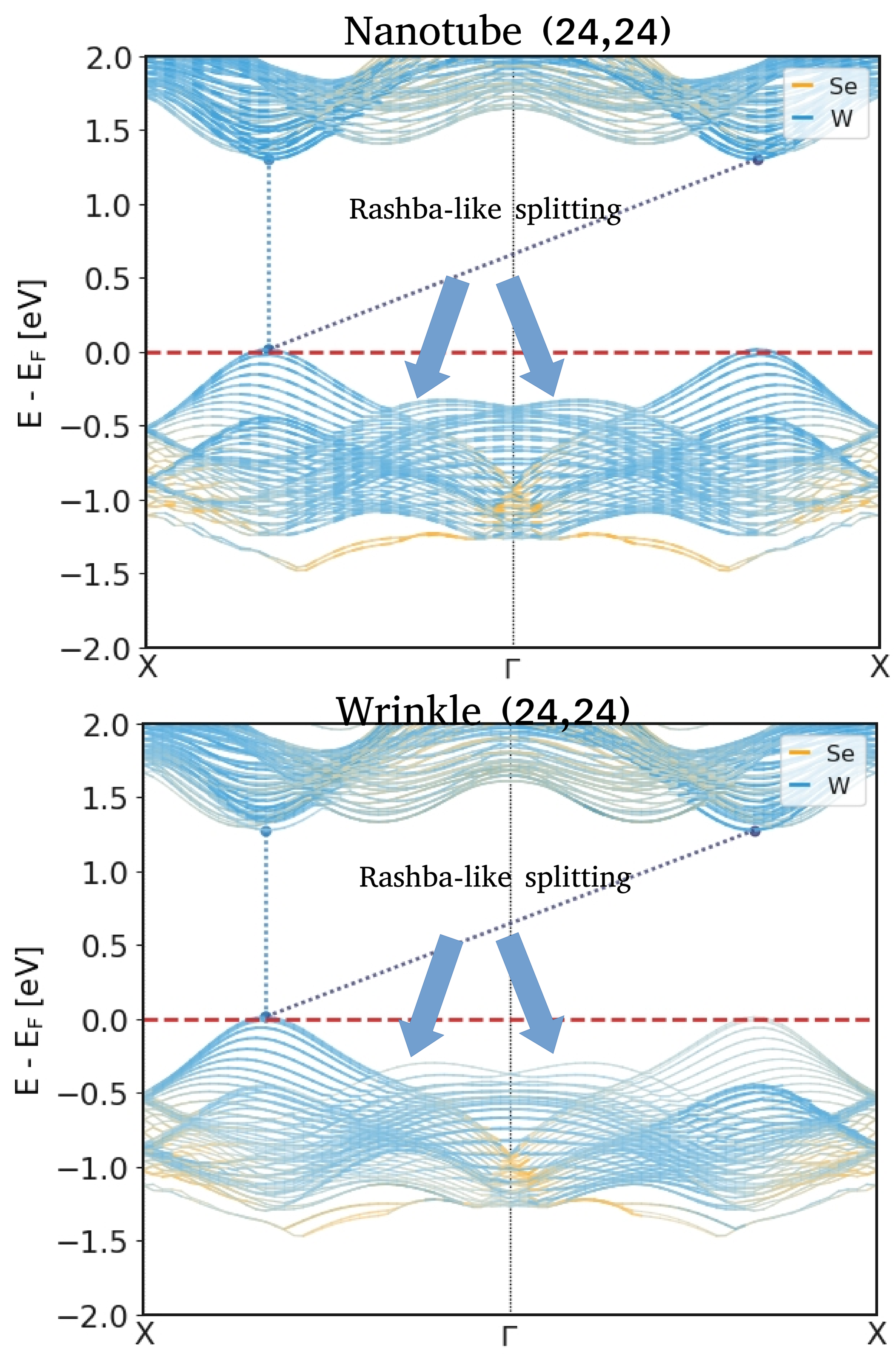

Figure 4. Comparison of the band gap of **Top:** nanotube and **Bottom:** wrinkle of the WSe_2. The formation of a splitting in momentum direction is visible (Rashba Splitting).

Results:

- ✓The relaxed shape of the wrinkles differs from the nanotubes.
- ✓There is a clear variation of the strain field in the wrinkles.
- ✓Splitting along momentum space.
- ✓Band gap differences in nanotubes and wrinkles are due to different strain fields.

Conclusion:

- ✓Large supercells (representative of all curvature) are needed to model effects present in the wrinkle.
- ✓Spin-orbit coupling influences the band gaps.
- ✓Band gaps of TMDC wrinkles and nanotubes are similar.
- ✓States and splitting are different; strongest change around the Γ point.

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