Electronic-Properties Engineering of TMDs: Strained Monolayers and Nanoribbons

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We present theoretical results for the structural, electronic and optical properties of nanoribbons (quasi-1D) and single-layer (2D) transition metal dichalcogenides MX_2 (M = Mo, W; X = S, Se, Te) under various types of strain. Our results are obtained through Density Functional Theory (DFT) calculations.

We find that the direct gap of single-layer MX_2 changes to an indirect gap for biaxial strain and uniaxial strain in the x- and y- direction, whereas for shear strain the structure remains a direct gap material. For both, tensile and compressive strain the gap decreases, with the reduction rate being smaller for tensile strain.

We also investigate the behaviour of the optical properties that are obtained using linear response theory. The results show qualitatively similar behaviour between the MX_2 materials and strain types. We show that the static dielectric constant decreases when the structure is under tensile strain and increases under compressive strain. Our DFT results are interpreted with simple models and are shown to be consistent with available experimental data.

For the quasi-1D structure, as far as the static dielectric constant is concerned, the behaviour under strain remains similar to the 2D structure. Additionally the dielectric constant increases with increasing ribbon width, reaching values which approach the dielectric constant found for the single-layer [1]. We interpret our results with a simple model by separately considering the contributions of the metallic edges and the semiconducting interior of the ribbons.

References

[1] Davelou et al, Solid State Commun., 192 (2014) 42.

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