

Strain-induced modification of electronic properties in transition metal dichalcogenide monolayers and nanostructures

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We present theoretical results for the electronic and dielectric properties of single-layer (2D) semiconducting transition metal dichalcogenides MX_2 ($\text{M} = \text{Mo}, \text{W}$; $\text{X} = \text{S}, \text{Se}, \text{Te}$) under isotropic, uniaxial (along the zigzag and armchair directions), and shear strain. Our Density Functional Theory (DFT) calculations show that electronic band gaps decrease while dielectric constants increase for heavier X. The direct gaps of equilibrium structures often become indirect under certain types of strain, depending on the material. The effects of strain and of broken symmetry on the band structure are discussed. Gaps reach maximum values at small compressive strains or in equilibrium, and decrease with larger strains. In-plane dielectric constants generally increase with strain, reaching a minimum value at small compressive strains. The out-of-plane constants exhibit a similar behavior under shear strain but under isotropic and uniaxial strain they increase with compression and decrease with tension, thus exhibiting a monotonic behavior. These DFT results are theoretically explained using only structural parameters and equilibrium dielectric constants [1]. We also discuss nanoribbon (quasi-1D) structures in comparison to the single-layer (2D) and bulk (3D) materials. Besides metallic edge states, our DFT results reveal several interesting electronic and dielectric properties which are interpreted with simple models [2]. Our findings are consistent with available experimental data. Results that show how strain can be used to tune atom adsorption, such as hydrogen, on TMD nanostructures are also presented. In graphene supported nanostructures, H adsorption changes significantly w.r.t. to the free-standing ones when the substrate induces strain [3].

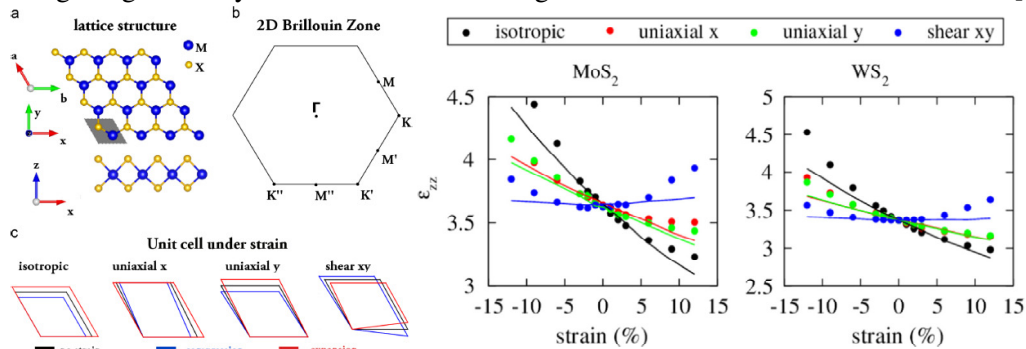


Figure 1: Left, MX_2 monolayer lattice (a) and BZ (b) and strain types imposed (c). Right, out-of-plane dielectric constants vs strain, theory (lines) and DFT results (points) [1].

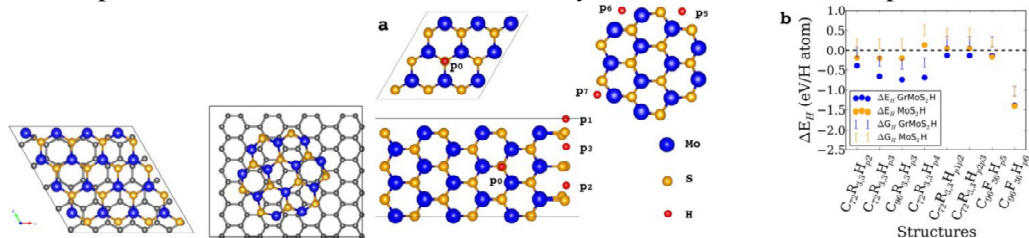


Figure 2: From left to right, MoS_2 /graphene heterostructures, H atoms adsorbed on MoS_2 , H adsorption energies for several nanostructures, with and without graphene substrate [3].

References

- [1] A.E. Maniadaki, G. Kopidakis, I.N. Remediakis, *Solid State Commun.* **227** 33 (2016).
- [2] D. Davelou, G. Kopidakis, G. Kioseoglou, I.N. Remediakis, *Solid State Commun.* **192** 42 (2014).
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