XXXII Panhellenic Conference on Solid State Physics and Materials Science
Conference Center "Carolos Papoulias", 18-21 September 2016, Ioannina, Greece

Electronic properties engineering of transition metal dichalcogenides: strained monolayers and nanoribbons

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Abstract: We present theoretical results for the electronic and dielectric properties of single-layer (2D) semiconducting transition metal dichalcogenides MX_2 (M = Mo, W; X = S, Se, 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. 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 and are consistent with available experimental data [2]. We also present results that show how strain can be used to tune atom adsorption on TMDs, such as hydrogen on MoS_2 nanostructures [3].

[1] A.E. Maniadaki et al, Solid State Commun. 227 (2016) 33.
[2] D. Davelou et al., Solid State Commun. 192 (2014) 42.
[3] A.E. Maniadaki and G. Kopidakis, Phys. Status Solidi RRL 10 (2016) 453.

Photographs / graphics may be used if necessary to substantiate results.