

Effect of strain and electric field on charge density wave orderings in tantalum dichalcogenides: a first-principles study of TaS₂, TaSe₂ and TaSSe monolayers

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Tantalum dichalcogenides constitute a particularly interesting subgroup of transition metal dichalcogenides owing to the emergence of charge density wave (CDW) orderings related to lattice distortions in these van der Waals materials [1]. This phenomenon occurs both in bulk and monolayer systems, making them an attractive playground for fundamental physics and enhancing their potential for applications. In particular, the T polymorphs of TaS₂ and TaSe₂ are known to form a $\sqrt{13} \times \sqrt{13}$ superstructure accompanied by the formation of a CDW, which is robust even at room temperature. Furthermore, CDW ordering can be controlled by a variety of stimuli, such as temperature, electric field, doping, laser illumination, or strain.

In this paper, we discuss the influence of biaxial strain on the CDW-related properties of monolayer tantalum dichalcogenides such as TaS₂ and TaSe₂ [2], as well as a Janus-type system, TaSSe [3]. The computational study is based on a first-principles approach. We analyse structural quantities such as bond lengths, as well as the total energies of the distorted (commensurate CDW) and undistorted (normal) phases, to assess the behaviour of the lattice distortion. We then investigate the charge transfer between atoms in the supercell and the local density of states to shed light on charge-density-related features. To complete the physical picture, we analyse the electronic structure of the systems under consideration.

We find that compressive strain stabilizes the CDW ordering by increasing its energetic stability and enhancing both relative distortion and charge transfer between tantalum atoms. In contrast, tensile strain promotes the normal (undistorted) phase. The critical values of tensile strain required to induce switching between the CDW and normal phase are determined.

To gain further insight, we also investigate the influence of an external electric field applied perpendicular to the monolayers on CDW stability, finding pronounced robustness of the CDW phase against this perturbation.

The results may be relevant to understanding the effect of substrates on CDW properties in tantalum dichalcogenides. Moreover, they may aid the design of van der Waals heterostructures with spintronic functionalities involving such materials [4].

References:

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We gratefully acknowledge Polish high-performance computing infrastructure PLGrid (HPC Center: ACK Cyfronet AGH) for providing computer facilities and support within computational grant no. PLG/2025/018673.