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Pd-based dichalcogenides: the 1T and the novel $1O_T$ regular and Janus structures: from electronic to thermal properties

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Abstract

The discovery of two dimensional (2D) graphene has opened the doors to investigate a myriad of new 2D materials that have better characteristics. Out of these are the transition metal dichalcogenides (TMDs). In this talk, I will shine light on the electronic, optical and thermal properties of the 1T [1] Pd-based dichalcogenides, namely PdS_2, $PdSe_2$, PdSSe, PdSTe, and PdSeTe systems, that do not have a fair share of research like the Mo or W-based TMDs. Our results show that the thermal electronic conductivity (κ_e), the electronic conductivity (σ_e), the Seebeck effect (*S*), and the figure of merit (ZT) along the x and *y* directions register the largest values in the case of electron doping for the $PdSe_2$ and PdSeTe 2D crystals [1]. Additionally, ZT of the Janus structures are larger than their corresponding pristine PdX_2 (X = S, Se) structures [1]. Once synthesized, such information is crucial for the implementation of the PdXY (Y = Se, Te) structures in industrial applications.

I will also discuss the electronic and optical properties for the novel $1O_T$ [2] metastable (with monoclinic symmetry) structures that we have modelled in our group. Our calculations reveal that, without the inclusion of spin-orbit coupling, all structures considered have a semi-metallic behavior with a non-zero (DOS) at the Fermi level. Furthermore, they demonstrate a wider range of absorption spectra than 1T systems, and can emit or absorb within the infrared (IR) regime. They are dynamically stable and their thermal lattice conductivities should be lower than their 1T analogs, making them suitable candidates for thermoelectric devices. The Born-Oppenheimer Molecular Dynamics (MD) simulations [3] show that the $1O_T$ PdS2 and PdSe2 structures are thermally stable at temperatures above 300 K, while the Janus PdSSe system remains stable up to temperatures close to 600 K and is completely destroyed at 900K [2].

References

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Figures

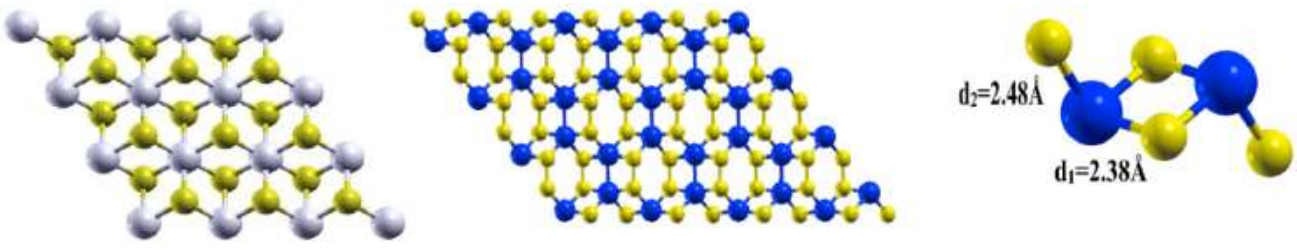

Figure 1: top view of 1T (left) and $1O_T$ (middle) supercells of the PdX_2 materials. Blue and grey spheres are Pd atoms; yellow spheres represent S or Se. (Right) unit cell of the $1O_T$ structure, showing optimized bond lengths.