# DFT Investigation of Charge Density Waves in 2D Transition Metal Dichalcogenides

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## Abstract

Transition metal dichalcogenides (TMD) often exhibit charge-density wave (CDW) phases. This is notably the case for $TaS_2$ and $TaSe_2$ with their Star of David $\sqrt{13} \times \sqrt{13}$ CDW pattern [3, 4], or for $VSe_2$ and $VTe_2$ with their $\sqrt{3} \times \sqrt{7}$ or $4 \times 4$ CDW patterns [1, 2]. These structures have been studied in collaboration with 2 groups of experimentalists. The group of experimentalists from the Nanjing University reported a dependance of the charge transfer between $TaX_2$ and monolayer graphene (MLG) on the CDW state and the polytype of $TaX_2$. Independently, the group of experimentalists at the MPQ showed using STM that, in particular, the CDW state of $VSe_2$ changes from $\sqrt{3} \times \sqrt{7}$ in its monolayer form when deposited on MLG to a $4 \times 4$ CDW when deposited on $VTe_2$ which also exhibits a $4 \times 4$ CDW. *Ab-initio* calculations have then been conducted to investigate those observations by means of Density Functional Theory (DFT) and Density Functional Perturbation Theory (DFPT) using the Quantum ESPRESSO suite of codes , within the PBE approximation, AiiDA as automation tool and the SSSP pseudopotential family The charge transfer between $TaX_2$ and MLG has been determined in the pristine and CDW states of $TaX_2$, to be then benchmarked with respect to the different combinations of polytypes and number of layers of the TMD. Results show an influence of the CDW state of the TMD on the charge transfer. Conversely, calculations also show that the CDW state of the monolayer $VSe_2$ is influenced by its charge (or doping). Ultimately, we have the result that the difference of the charge transfer between MLG and $VTe_2$ with $VSe_2$ is at the origin of the switch between its different CDW states.

## References

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