Ab initio studies of electronic and dynamical properties of chosen transition metal dichalcogenides systems in hydrostatic pressure

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Recently, hexagonal transition metal dichalcogenides (TMDC) attract significant interest due to their extraordinary and tunable electronic and optical properties. [1] Their quasi two-dimensional character leads to the anisotropy of their physical properties, which has various technological applications. Moreover, the external hydrostatic pressure allows for continuous tuning of the optical transitions, rendering the TMDC the appealing materials for applications in electronic and optoelectronic devices. Hence, an experimental characterization and theoretical analysis of the properties of bulk and multilayered TMDC crystals is of fundamental importance. This work is focused on the electronic and phonon structure of chosen TMDC systems in the external hydrostatic pressure in reference to experimental results.

We study from first principles (DFT) electronic structure and lattice dynamics of bulk HfS_2 and $MoTe_2$ under hydrostatic pressure. The calculated band structures and phonon are then compared to experimental data. We are able to explain the pressure evolution of Raman modes by analysing the position of phonon modes at Γ point of Brillouin zone. [2]

The analysis of bulk $MoTe_2$ band structures allowed for identification of several optical transitions observed in photoreflectivity measurements. In particular, we confirm the presence of H point direct transitions. [3]

References

[1] H. Wang, H. Yuan, S. S. Hong, Y. Lib, Y. Cui, Chem. Soc. Rev. 44, 2664 (2015)
[2] J. Ibanez, T. Woźniak, to be submitted
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Figures

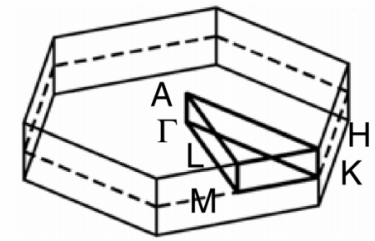

Figure 1: The Brillouin zone of the considered bulk TMDC