DFT study of the thermal transport properties of MoS_2: Application to thermoelectricity

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Transition metal dichalogenides (TMDC) have received an increased interest as a new family of two-dimensional (2D) material. Unlike graphene, TMDC exhibit a large band gap and have already been used promisingly as field effect transistor [1]. Moreover, 2D materials are expected to lead to higher thermoelectric figure of merit compared to bulk materials due to poor thermal conductivity [2].

We previously demonstrate that potassium doping seems a promising path to improve the Seebeck coefficient S and the electrical conductance σ [3]. However, the efficiency of thermoelectric modules depends both on the electronic and the thermal transport properties as the figure of merit ZT is defined as:

$$ZT = \frac{\sigma S^2 T}{\kappa}$$

During this talk, I will address the thermal transport properties of MoS_2 and its thermal conductance κ. The calculations have been performed using the SIESTA DFT package based on atomic orbitals. A comparison with a plane wave calculation is given on Fig.1.

I will mainly focus on the influence of sulfur vacancies [4] on κ and also the influence of adsorbed potassium. Using Green's function technic and the Landauer formalism, we will also present the influence of realistic disordering on κ.

References

[1] B. Radisavljevic, *et al.* "Single-layer MoS_2 transistors". Nature nanotechnology, 6:147--150, 2011.

[2] L.D. Hicks and M.S Dresselhaus. "Effect of quantum-well structures on the Thermoelectric figure of merit". Physical Review B, 47:12727, 1993.

[3] Ch. Adessi, S. Thébaud, R. Bouzerar and G. Bouzerar. "First Principle Investigation on Thermoelectric Properties of Transition Metal Dichalcogenides: Beyond Rigid Band Model". Journal of Physical Chemistry, 121(23) 12577–12584, 2017.

[4] Ch. Adessi *et al.* "Influence of sulfur vacancies on the thermal conductance of MoS_2. A DFT study". Submitted.

Figures

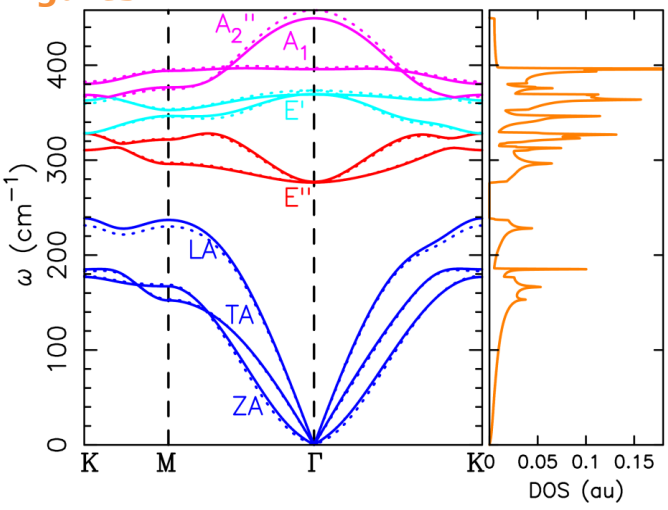

Figure 1. Phonon dispersion and density of states for MoS_2. The solid lines correspond to the SIESTA (atomic orbitals) calculation, the dotted lines to the VASP (plane waves) calculation.