DFT study of the electrical and thermal transport properties of 2D MoS_2: Application to thermoelectricity

Dr. Christophe A. Adessi, S. Pecorario, S Thébaud and G. Bouzerar
Institut Lumière Matière, UMR 5306 Université Cluade Bernard Lyon 1 – CNRS, Université de Lyon, 69622 Villeurbanne CEDEX, FRANCE
christophe.adessi@univ-lyon1.fr

Transition metal dichalogenides like MoS_2 have received an increased interest as a new family of two dimensional (2D) materials. Unlike graphene, MoS_2 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]. However, we have pointed out in a previous work, that doping is a delicate task with MoS_2 in order to obtain good electrical properties[3]. The challenge associated with thermolectricity is to minimize thermal transport and maximize electrical transport as the thermoelectric figure of merit ZT is defined as:

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

where S is the Seebeck coefficient, σ the electrical conductivity, κ the thermal conductivity and T the temperature. During this talk, I will address the influence of a very common kind of defects in MoS_2 which are the sulfur vacancies. I will present the influence of this defects on both the electrical and the thermal transport properties of MoS_2. For this work, DFT calculations have been used, combined with the Landauer formalism allowing us to investigate more realistically the influence of the disordering of the sulfur vacancies. One of the main result is the very different behavior of the ZT depending if the material is n or p doped.

References

[1] B. Radisavlijevic, *et al.* Nature nanotechnology, 6: 147—150, 2011.
[2] L.D Hicks and M.S. Dresselhaus. Phys. Rev. B, 47: 12727, 1993.
[3] Ch. Adessi *et al. J. Phys. Chem. C, 121(23) 12577-12584, 2017.*

Figures

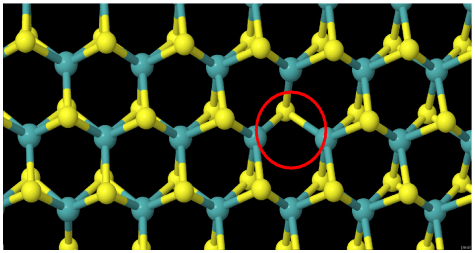

Figure 1: MoS_2 with a single sulfur vacancy.

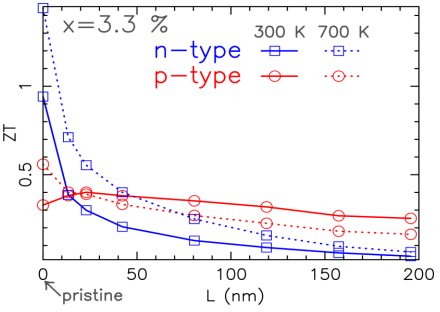

Figure 2: Figure of merit ZT for MoS_{2-x} as function of the length of the system either doped with electrons or holes for 2 temperatures.