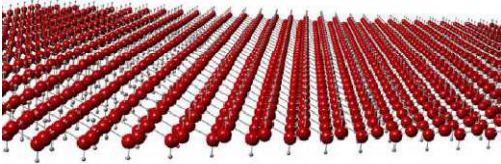


## Modelling of transport properties of advanced van der Waals heterostacks

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Two-dimensional (2D) layered materials [1] such as the graphene or transition metal dichalcogenides (TMDs) have emerged as promising materials for electronic, optoelectronic, and valleytronic applications. It is the nature of two-dimensional

materials that the physical properties are highly anisotropic in the plane of the two-dimensional crystal and in the out-of plane direction. The reason for this anisotropy is the strong covalent or ionic bonds within the plane and weak van der Waals coupling between different layers. The real advantage of two-dimensional materials is their capability for the integration in heterostructures and heterostacks with anisotropic charge and heat transport properties for thermoelectric application and for devices with controlled heat management.

**Master thesis project: To be able to predict the electron and phonon transport in the 2D heterostacks (HS)** a support will be provided by numerical simulations. The simulations require to be multiscale and multiphysics at the same time. In fact, the transport through the HS needs to couple quantum mechanical models with semiclassical hopping processes and both electrical and thermal transport. The numerical model will be implemented using the TiberCAD software [2] which already includes most of the models (both classical and quantum) for the multiscale approach. The aim of the thesis work is to implement and calibrate, within the TiberCAD architecture, a model able to capture transport characteristics of the HS. Primary target is the electron transport, secondary target the heat transport and their coupling in the thermoelectric effect. The aim of the thesis is strongly device oriented.

[1] S. Z. Butler et al., ACS Nano Review, **2013**, 7 (4), pp 2898–2926.

[2] [www.tibercad.org](http://www.tibercad.org)