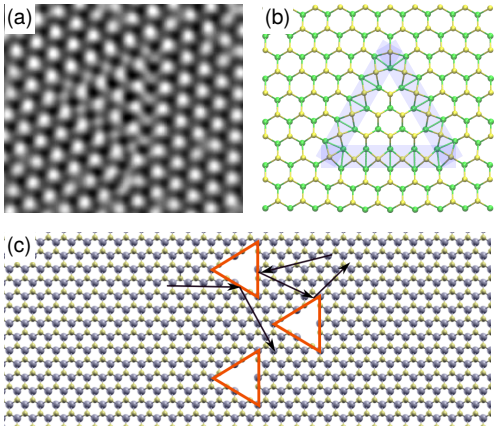
Thermal conductivity of defective MoS_2 by molecular dynamics

Introduction.



MoS_2 is a layered material, meaning that it can be exfoliated into atomically thin layers like graphene. Unlike metallic graphene, however, MoS_2 is a semiconductor and thus it has recently attracted significant attention in the materials research community for its possible uses in ultra-thin, flexible optoelectronic applications. These applications prospects can be hampered by the heat generated within the active region, unless it can be efficiently transported out. On the other hand, controlling the balance between thermal and electrical conductivities can be useful for thermoelectric applications.

The thermal transport of the material depends sensitively on the types and concentrations of defects they possess. Recently, it has been found that MoS_2 also hosts a particular type of defects called "inversion domains" (see figure). Their formation can be controlled during the material growth or after it by irradiation, annealing, or atom deposition. They are extended, triangular-shaped defects and the lattice inside the domain is rotated 180° with respect to the host within which it is embedded.

Project description.

The goal in this project is to investigate the effect of inversion domains on thermal transport of MoS_2 via molecular dynamics simulations. First, however, suitable atomistic models need to be constructed. To this end, the student writes a program which automatically generates embedded inversion domain structures with desired concentrations and sizes (or size distribution).

The MD simulations are then carried out using GPUMD code. This is fast and efficient software that has been developed at Aalto University and is run on GPU nodes on our local cluster.

The first aspect of the results will simply be the sensitivity of thermal conductivity on the defects. Next, the student can analyze the path of the heat current through the sample, i.e., does it go around or through the inversion domains. Finally, since the atomic structures of inversion domains inherently possess a three-fold symmetry, it will be interesting to find out if such a symmetry can also be retained in the thermal conductivity. This could provide an experimentally viable way to realize a thermal rectifier/diode.

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Accurate Basis Functions for Hybrid Density Functional Theory

Introduction

Majority of electronic structure theory today relies on the solution of the famous Kohn-Sham equations in the density functional theory (DFT) framework. Computational solution of the Kohn-Sham equations requires a discretization that is usually done using a set of basis functions. The quality of the basis has a considerable effect on the accuracy of the solution as well as on the speed of the calculation.

Depending on the desired level of theory in DFT several approximations to the exchange and correlation energy of the electrons can be made. The simplest ones assume that only local density or its gradient have an effect on the energy whereas more complex approximations accounting for the exchange energy exactly lead to so called hybrid functionals. [1]

While universal and transferable basis sets are desirable it turns out in practise that for hybrid functionals optimizing the basis further pays off due to smaller basis leading to decreased calculation time without sacrificing too much accuracy.

Project description

In this project the student will start from optimized basis function sets for local and semi-local density functionals and tune them further for use with the hybrid functionals. The work is implemented to an existing electronic structure theory code, FHI-aims. [2]

Requirements

Apart from basic understanding of quantum mechanics some experience in solid state physics is required as the tuning of the basis needs to consider also periodic systems. Bachelor level courses in engineering physics provide sufficient background. Since basis tuning requires many small calculations to find the optimum some familiarity of the Linux / Unix operating system and its scripting capabilities is required. Basic knowledge of numerical methods for partial differential equations is an additional merit.

Gains

In this project the student will

- familiarize herself/himself with the use of a modern electronic structure code including its algorithmic and numerical foundations
- gain insight into the use of an electronic structure code for obtaining physical properties of molecules and matter
- contribute to a project that has hundreds of users worldwide

Contact

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[1] J. Heyd, G.E. Scuseria, M. Ernzerhof, *Hybrid functionals based on a screened Coulomb potential,* The Journal of Chemical Physics **118**, 8207 (2003); https://doi.org/10.1063/1.1564060
[2] https://aimsclub.fhi-berlin.mpg.de/