Modelling of atomically thin nanomaterials (TIFX04-17-02)

Background
The continuing trend to miniaturization of devices in modern technology faces fundamental physical limits of applied materials. The search for novel structures with new functionalities has brought atomically thin two-dimensional (2D) nanomaterials into the focus of current research. These materials show a wide range of exceptional optical, electronic, mechanical, chemical, and thermal properties. They can also be stacked into van der Waals heterostructures (see figure) suggesting technological application in next-generation flexible and transparent nanoelectronic devices.

The most prominent representative of this new class of nanomaterials is graphene. However, there is a variety of other promising 2D materials beyond graphene, such as transition metal dichalcogenides, black phosphorus, antimonene, arsenene, etc.

Project description
The aim of the project is to calculate the electronic band structure and the optical absorption spectra of different atomically thin 2D nanostructures. The obtained insights will allow us to reveal the optical finger print of these technologically promising nanomaterials.

Type of work
Theoretical work. Analytic calculations and illustration of results with Mathematica.

Group size
The project can be performed by a group of 3-4 students.

Target group
F, Gu-Fysik

Literature tips

Handledare
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