Multiphysics simulations of atomically-thin sensors

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Background

Two-dimensional layered materials (2DLM), such as graphene and transition metal dichalcogenides, consist of stacks a single or few-atom-thick layers. 2DLM are ideal for sensing especially in their monolayer form, as they offer the highest possible surface to volume ratio. For example, graphene has been successfully used in several sensing applications, ranging from single gas molecule detection, DNA sequencing, electrophysiology and even for identification of SARS-CoV-2 spike protein. Moreover, the surface of 2DLM can be engineered to interact with specific targets, such as specific DNA sequences via suitable functionalization.

Aims and objectives

This project aims to model and simulate sensors based on 2DLM using COMSOL Multiphysics®, e.g. chemically-sensitive field effect transistors (ChemFETs) where 2DLM are used as sensing channel. The Multiphysics environment provided by the simulator will enable studying the combined effect of different physical phenomena, such as electron transport and surface electrochemistry.

Planned outcomes

The intended outcomes of the project are:

- Understanding basics of finite-element simulations
- Performing multiphysics simulations using COMSOL Multiphysics®
- Define new materials in the simulation environment
- Couple different physical phenomena in a multiphysics simulation
- Perform parametric studies and optimization
- Estimate sensor performance