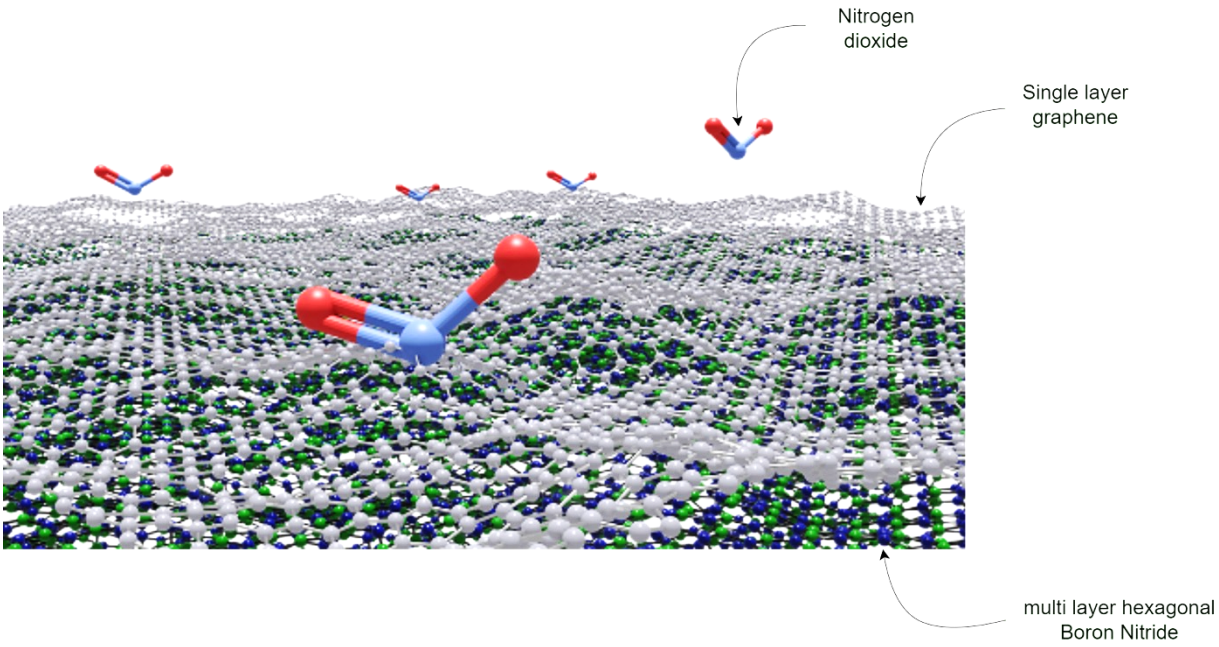
Bachelor Thesis, Semester Project, Master Thesis

Molecular binding kinetics modelling of NO_2 on graphene/hBN heterostructure



Keywords

DFT modelling, heterostructure, binding kinetics, quantum transport

About the Project

Graphene/hBN heterostructures offer optimal transistor performance metrics due to the excellent encapsulation properties of hBN. Graphene transferred onto a multi-layer hBN film with its top face exposed to molecules, as shown above, allows to explore its potential in gas sensor applications. To study the influence of certain reactive molecules, this project aims to study the molecular binding kinetics of nitrogen dioxide on graphene/hBN heterostructure and its influence on the (quantum) transport properties of this system.

Your profile

- Student of ITET, PHYS, MAVT, or MATL
- Strong interest in semiconductor device physics and simulation
- Basic programming skills in Python and/or MATLAB
- Previous experience with DFT calculations is welcome, but not mandatory

Contact

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