P3: Multiscale Modelling of Chemical Vapor Deposition

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Introduction

- Chemical vapor deposition (CVD) is widely used to deposit 2D and 3D materials.
- CVD enables to synthesize large-area high quality carbon based materials, but they are not perfect, which affect material properties.
- Better understanding and control of graphene and carbon nanotubes growth, influence of the feedstock decomposition and the nucleation mechanism are needed.

The grand challenge of the CVD modelling is the development of an approach to calculate accurate potential energies and gradients on-the-fly to study the growth of graphene on metal particles and surfaces.

Objectives

- Development of a new multiscale on-the-fly Monte Carlo workflow based on quantum chemical calculations and classical MD simulations.
- Atomic structure understanding of processes guiding the CVD growth mechanism of graphene and carbon nanotubes using recursive simulation approach.
- Combination of theoretical methods using high degree of automatization and workflow engineering tools.
- To provide the doctoral researchers experience in expertise in multi-scale modelling beyond application of standard software packages.

Qualification program – example

- Curriculum for a PhD 2 with a background in (quantum) chemistry, working within P3

Synergies with the other sub-projects

- P4 – Machine learning, DFTB parametrization
- P6 – Workflow approaches

References