Workshop for academia & industry
Chemistry, Materials & Processes with the Amsterdam Modeling Suite

SCM
Software for Chemistry & Materials

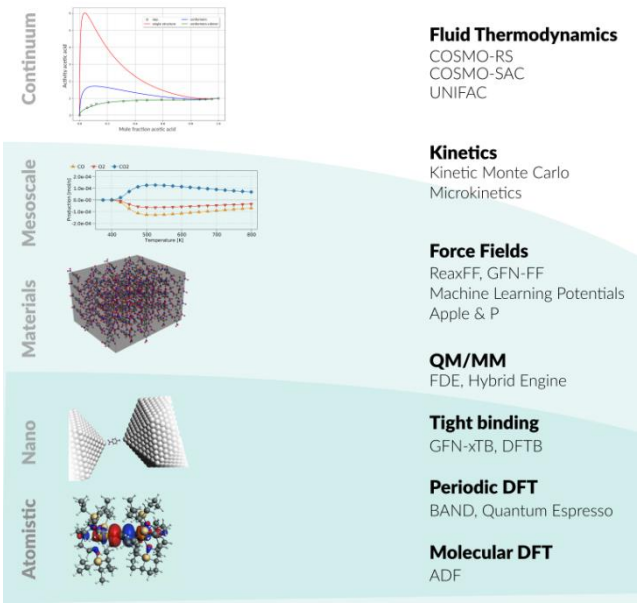
Hosted by GPC, Qatar University, Muftah El-Naas
Tutors: Fedor Goumans, Mohamad SAAB
Thu 19 September 2024, 8.00-12.30

جامعة قطر
QATAR UNIVERSITY

Researchers in industry and academia have been using the Amsterdam Modeling Suite (AMS) for over half a century to understand and predict chemistry, materials & processes.

We will discuss relevant use cases from the oil & gas industry, using atomistic and multiscale simulations as well as machine learning methods.

Then we will get started with hands-on examples to run simulations ourselves with the Amsterdam Modeling Suite, including spectroscopic properties, catalysis, thermodynamic properties and using machine learning.



We would love to hear about your interests, so we can try to include relevant examples in the workshop

Participants should register and install AMS and additional packages beforehand on their laptop. The Amsterdam Modeling Suite can be used for 1 more month after the workshop.

Program
08.00-08.30: Amsterdam Modeling Suite: intro to the different modules, case studies
08,30-10.15: Hands-on: geometry optimization, spectra, transition states (ADF, DFTB)
10.15-10.45: Coffee & tea break
10.45-11.30: Bulk & surfaces (DFTB, BAND, QE, combustion & reaction analysis (ReaxFF)
11.30-12.15: Thermodynamic properties and machine learning predictions with COSMO-RS
12.15-12.30: Wrap up, Q&A