Hands-on workshop
Chemistry, Materials & Processes with the Amsterdam Modeling Suite

SCM
Software for Chemistry & Materials

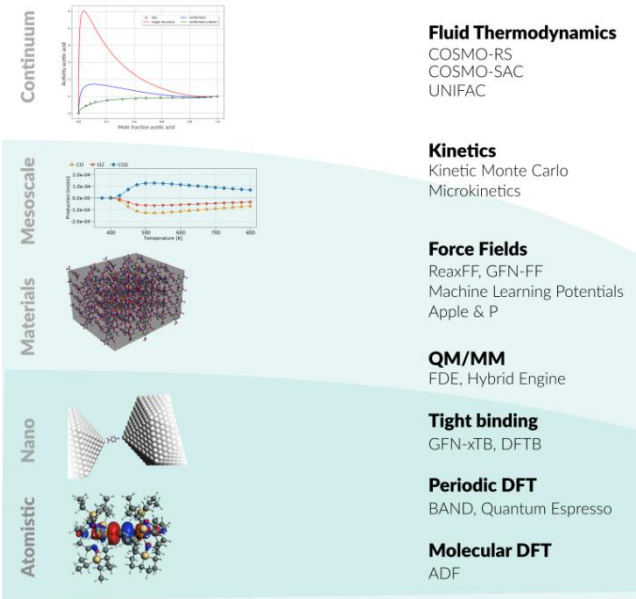
Hosted by KAUST, Luigi Cavallo
Tutors: Fedor Goumans, Mohamad SAAB
Tue 17 September 2024, 9.00-17.00

KAUST

Learn hands-on how easy it is to use the powerful Amsterdam Modeling Suite for understanding and predicting chemical and materials properties.

In the morning, we will start with the basics: building molecules & surfaces, visualizing spectra, orbitals, and band structures, and thermodynamics with COSMO-RS.
In the afternoon we will examine several ways to find transition states and reaction pathways, including ReaxFF.

We can be flexible and adjust the program according to interest!



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, and researchers may be able to access the KAUST site license locally and on the HPC Shaheen.

Program
09.00-09.30: Registration, checking installation
09.30-10.00: Amsterdam Modeling Suite: intro to the different modules
10.00-10.30: Short GUI demo
10.30-10.45: Coffee & tea break
10.45-11.15: Your first geometry optimization & spectra with ADF & DFTB (IR, UV/VIS, NMR)
11.15-11.45: Bulk and surfaces with DFTB & BAND
11.45-12.00: COSMO-RS: solubility, vapor-liquid equilibrium
12.00-13.30: Lunch
13.30-14.30: Transition States: NEB, PES Scans, restart from lower-level
14.30-15.30: Automatic reaction search: PES exploration, Reaction discovery
15.30-16.00: Coffee & tea break
16.00-16.45: Combustion simulations with ReaxFF
16.45-17.00: Wrap up, Q&A