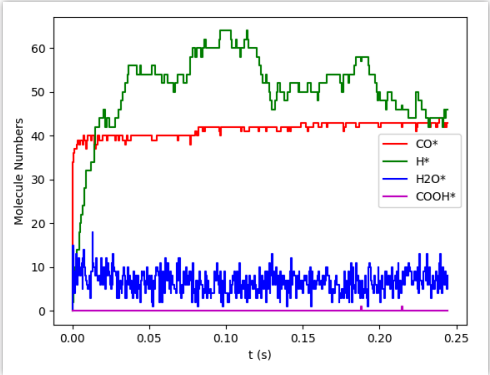
Oil, gas & catalysis

with the Amsterdam Modeling Suite

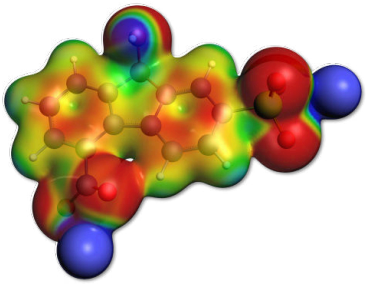
Understand mechanisms and processes, at the atomic scale

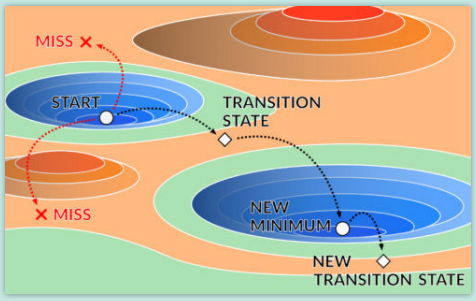
With the continuous development of oil and gas exploitation, the focus of research in the oil industry has shifted from macro to micro. Molecular simulation technology is gaining widespread attention because of its cost-saving benefits, reduced experimental timelines, and the ability to simulate extreme conditions that are nearly impossible to replicate in physical experiments.



What can you compute with AMS?

- Kinetics and catalytic activity
- Thermodynamic properties of mixtures (activity, vapor pressures, boiling points, solubilities, partition coefficients, LLE, VLE)
- Adsorption energies and isotherms
- Phase diagrams
- Resilience of materials, tribology



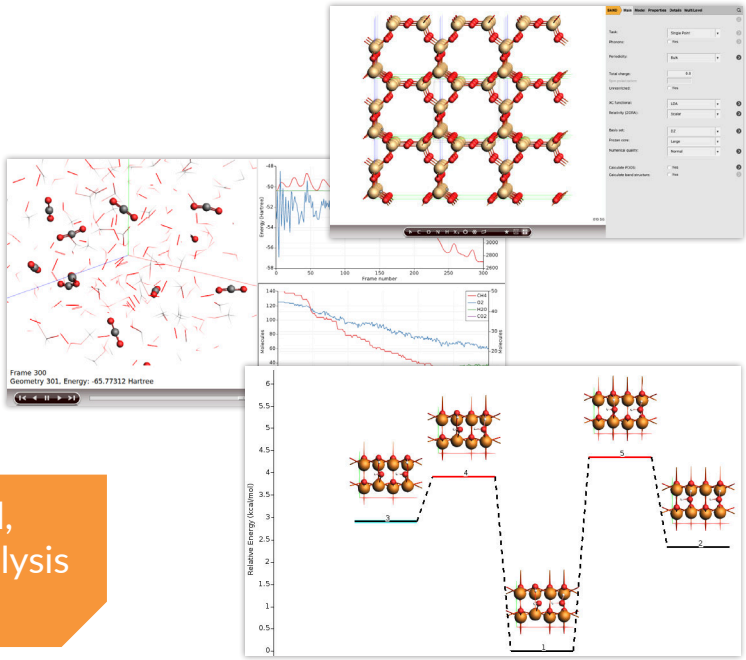


Key methods for oil, gas & catalysis modeling

- √ Periodic DFT with BAND and Quantum Espresso (QE)
- √ ReaxFF, Machine Learning Potentials, UFF4MOF
- √ COSMO-RS for thermodynamic properties (solvents and mixtures)
- √ Grand-canonical and kinetic Monte Carlo
- √ Accelerated molecular dynamics

Tools and analysis for oil, gas & catalysis modeling

- Molecular, crystal and framework builders
- Interactive molecular dynamics analysis
- Automatically extract reaction paths, rates, and reaction networks
- Automatic PES and reaction exploration



SCM
Software for Chemistry & Materials

Explore oil, gas & catalysis with AMS

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SCM
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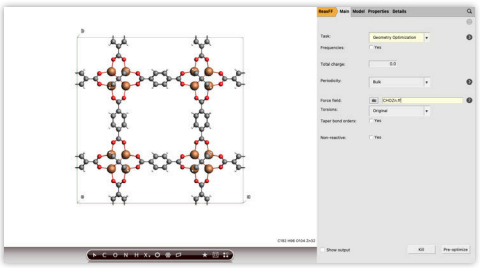
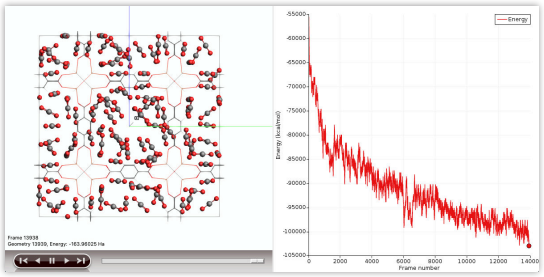
Compute adsorption isotherms

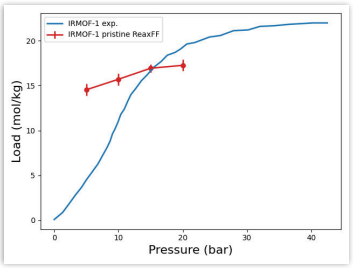
Adsorption isotherms represent the property of a host materials to intake a given quantity of a guest molecule at a given temperature and varying pressures. The shape of an isotherm holds information regarding the nature of the adsorption process. Atomistic simulations can help connect the macroscopic adsorption properties to the microscopic origin of the adsorption process (physisorption, chemisorption, catalytic reaction).



Methods and results

Adsorption isotherms can be computed directly from molecular dynamics with Grand-canonical Monte Carlo (GCMC). We computed the storage capacity for CO_2 in IRMOF-1 at room temperature with ReaxFF. Define the host material and the guest molecule with the graphical user interface and setup the GCMC simulation (pressure, temperature, etc.). Analyze the atomic structure interactively as CO_2 is loaded into the framework and compute the entire adsorption isotherm by reproducing the simulation at various pressures.





"What I really like about the Amsterdam Modeling Suite is that the programs were clearly written by chemists for dealing with real chemical problems. A great suite of programs!"

– Roald Hoffmann, Nobel Laureate

About SCM

Scientists at SCM are passionate about making computational chemistry work for you. Our mission is to develop powerful, easy-to-use software for your research and development needs. We love to discuss your research and learn how we can serve you better in the future.

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