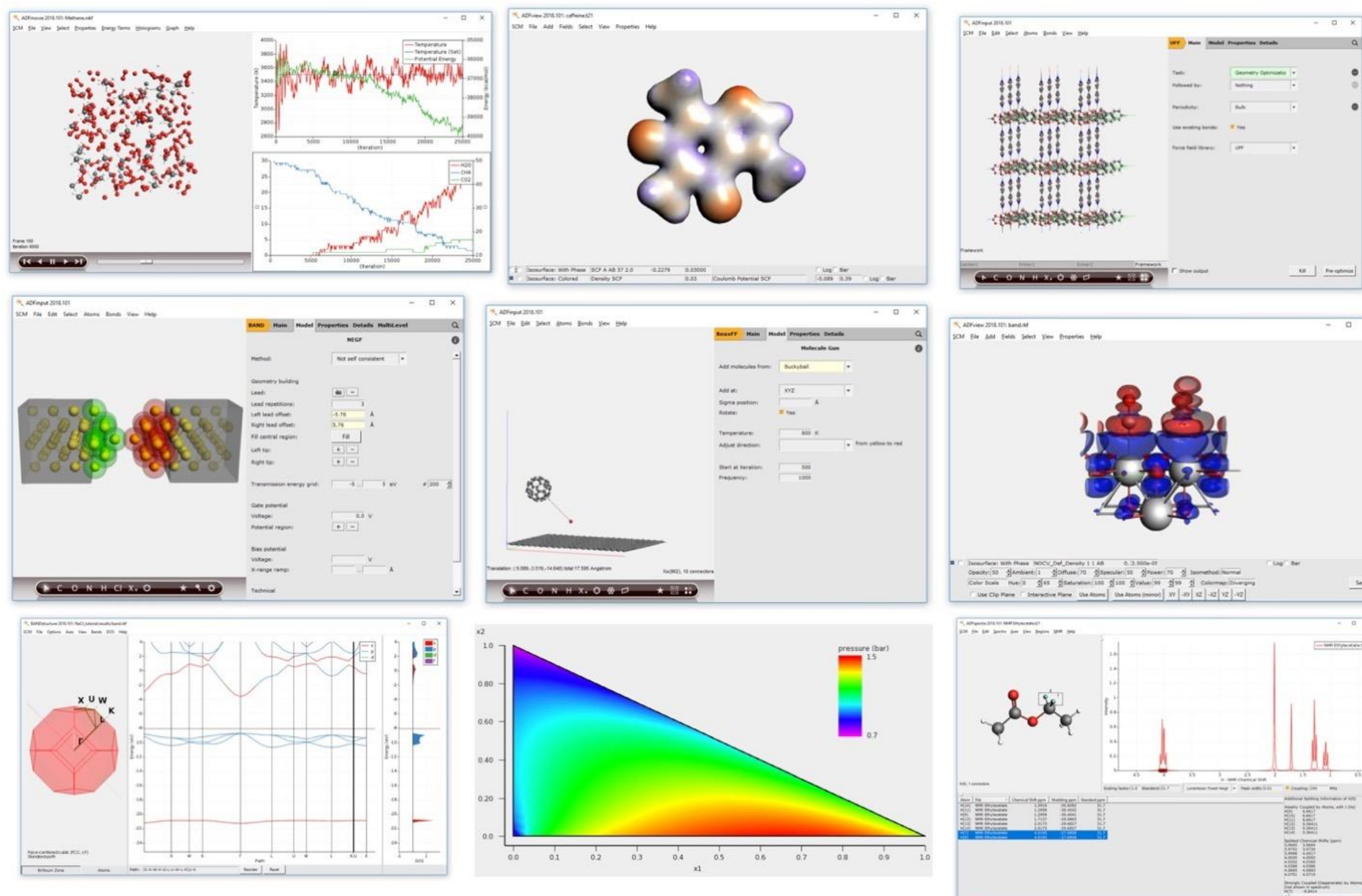


Online workshop: Using the Amsterdam Modeling Suite on HPC



SURF AMS hands-on workshop: 10 February 2021

Fedor Goumans, goumans@scm.com, Thomas Soini

SCM support: support@scm.com

SURF: Carlos, Ana

SCM experts: Remco, Marcel & Matthias

Program

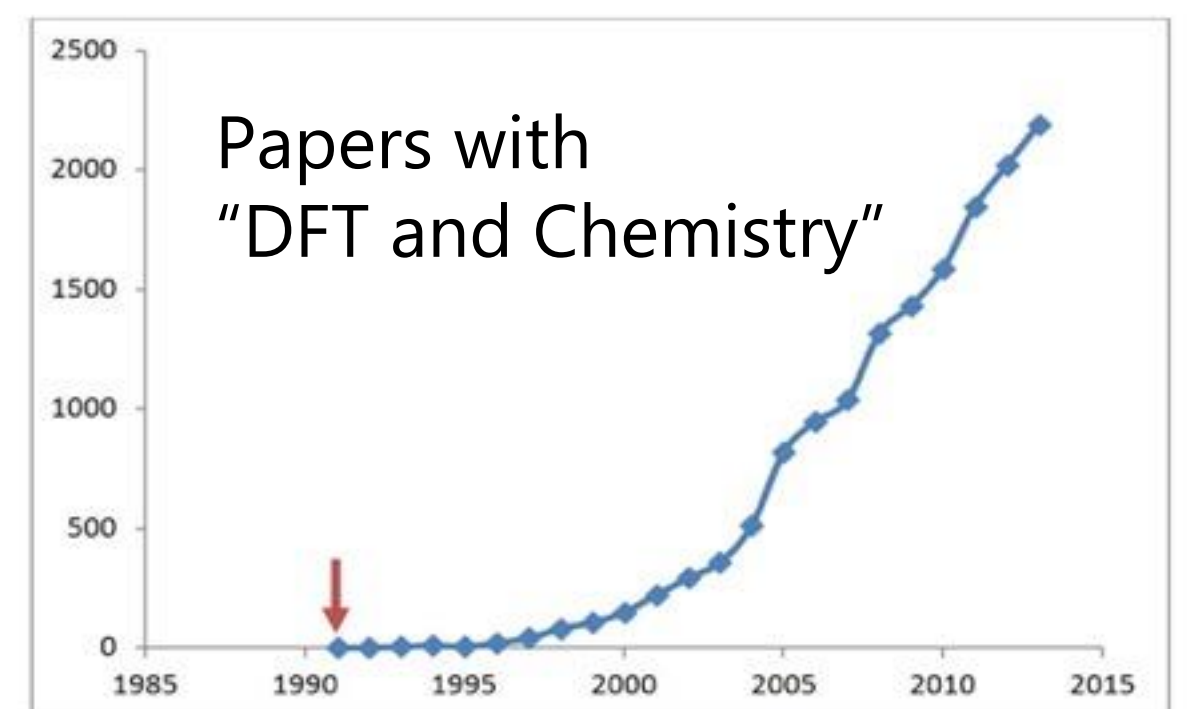
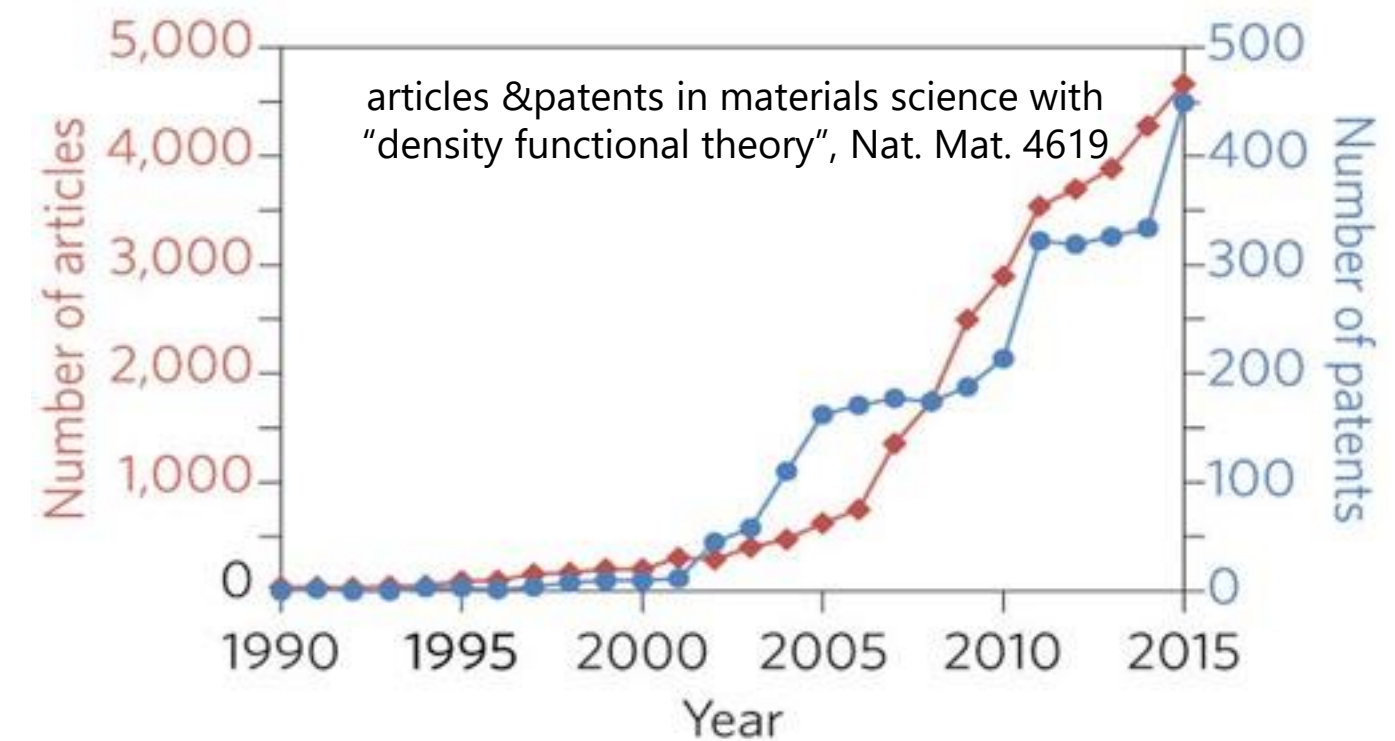
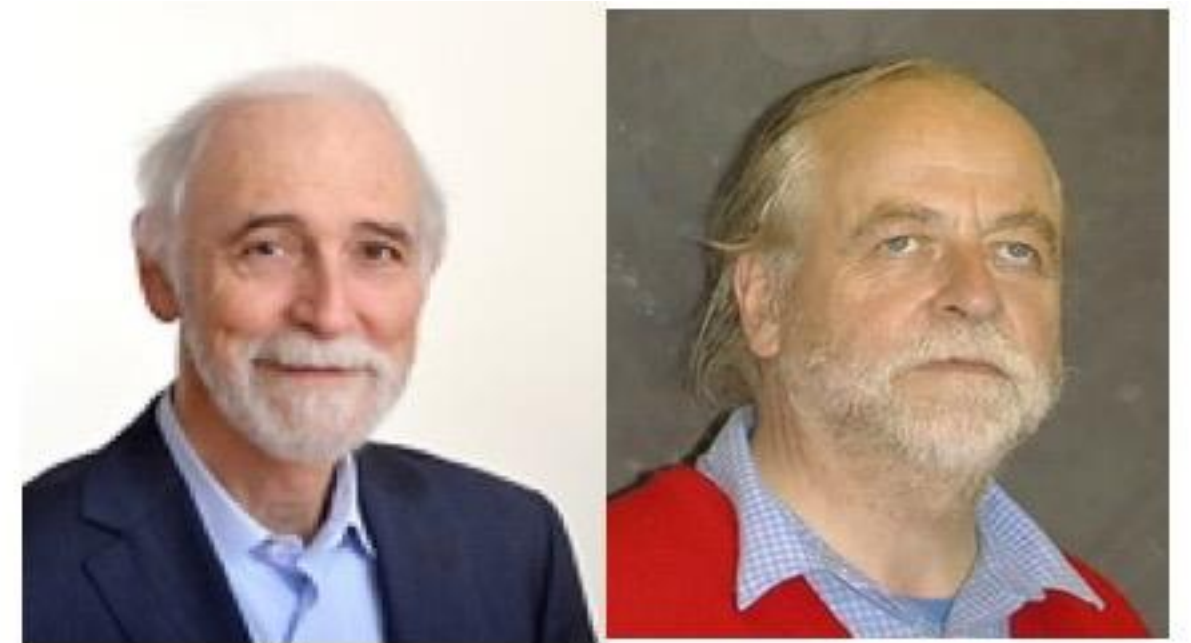
- 9.00-9.30: intro SCM & Amsterdam Modeling Suite
- 9.30-11.30: GUI, simple molecular calculations (Thomas)
scm.com/SURF (slides)
scm.com/SURFstruct (structures, py scripts)
- 11.30-12.00: HPC intro, connection to SURF
- 12.00-13.00: break
- 13.00-13.30: HPC & Chemistry
- 13.30-14.00: Remco Havenith (TDDFT)
- 14:00-16.30: Marcel Swart (Multi-layer: QM/MM, QM/QM)
- 16.30-18.00: Matthias Bickelhaupt: (TS, bonding & reactivity)

SURF: unl. license Amsterdam Modeling Suite (academic use)

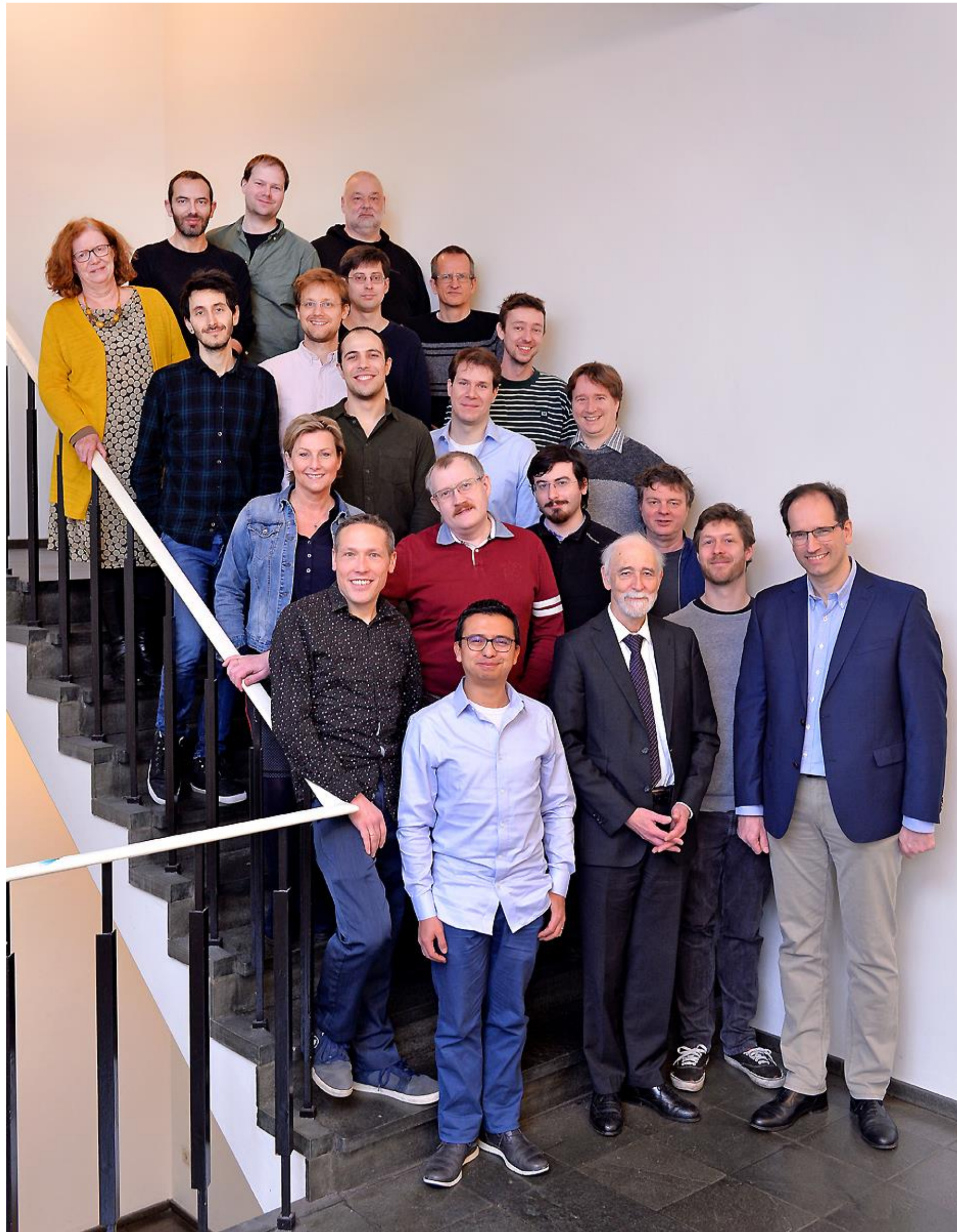
Universities also local (site) licenses: smaller calculations, GUI

Background: SCM, ADF & AMS

- ADF = first DFT code for chemistry (1970s)
Baerends@VU (>'73), Ziegler@Calgary⁽⁺⁾ (>'75)
 - 80s: support industrial users
- SCM: Spin-off company 1995
- 22 people (15 senior PhD's) + 3 EU fellows
- Many academic collaborators / EU networks
 - ~160 authors
 - New functionality
 - Academia, government & industry users worldwide
- SCM: development, debug, port, optimize, docs & support



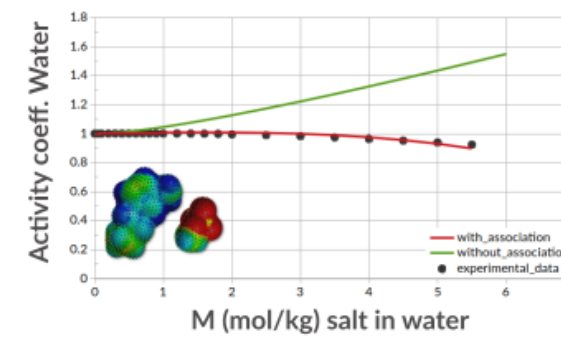
The SCM team in Amsterdam



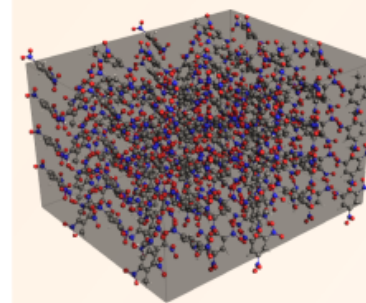
- 15 developers
- 4 support scientists
- 3 office / business
- 3 PhD students (EU)

Amsterdam Modeling Suite

- ADF: powerful molecular DFT
 - Reactivity, spectroscopy
 - Spectroscopy: NMR, EPR, VCD, UV, XAS
- BAND: periodic DFT
 - (2D) Materials, spectroscopy, analysis
 - Interface with QE, VASP
- DFTB & MOPAC: fast electronic structure
- ReaxFF: Reactive MD
 - Dynamics of large complicated systems
- MLPotential
 - Backends SchNetPack, sGDML, PiNN, TorchANI
- COSMO-RS: fluid thermodynamics
 - VLE, LLE, logP, solubility
- AMSdriver: PES exploration, MD, MC
 - Hybrid: multi-layer, QM/MM, QM/QM'
- Integrated GUI, python scripting (workflows)

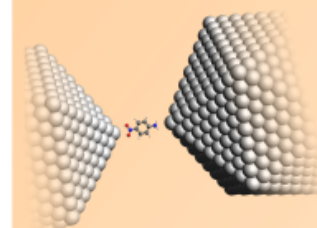


Continuum



COSMO-RS
Fluid Thermodynamics & Property Estimation

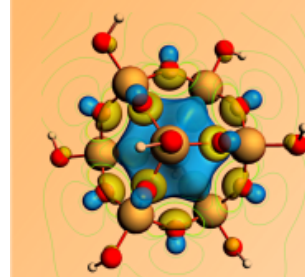
Materials



ReaxFF
Reactive Force Field

MLPotential
Machine Learning Potentials

Nano



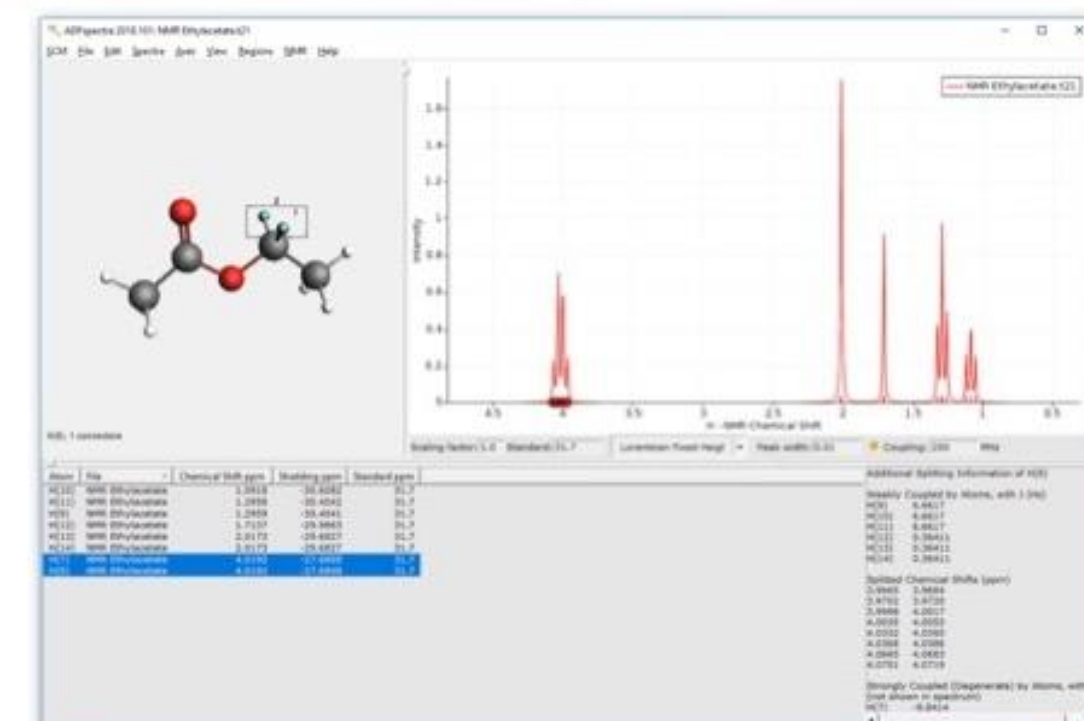
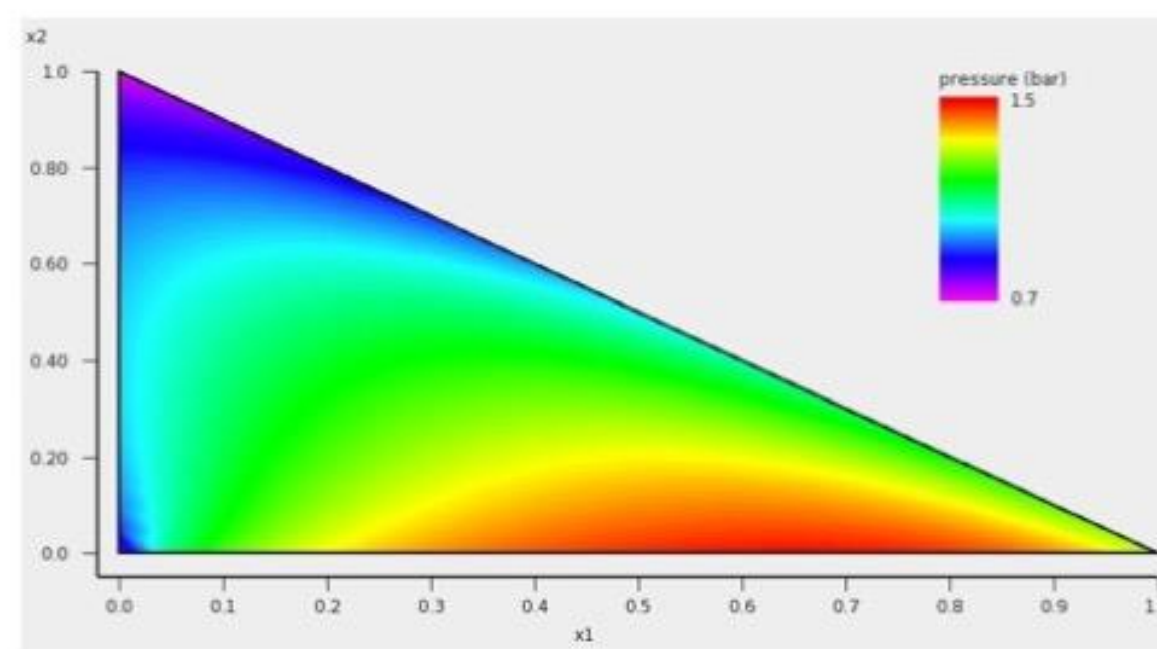
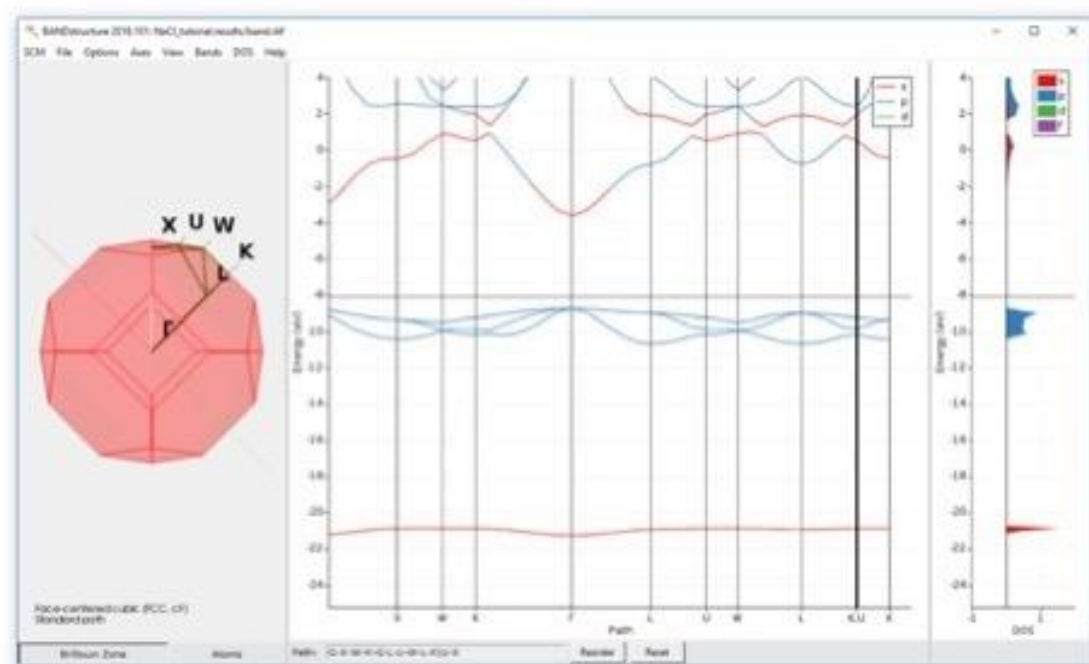
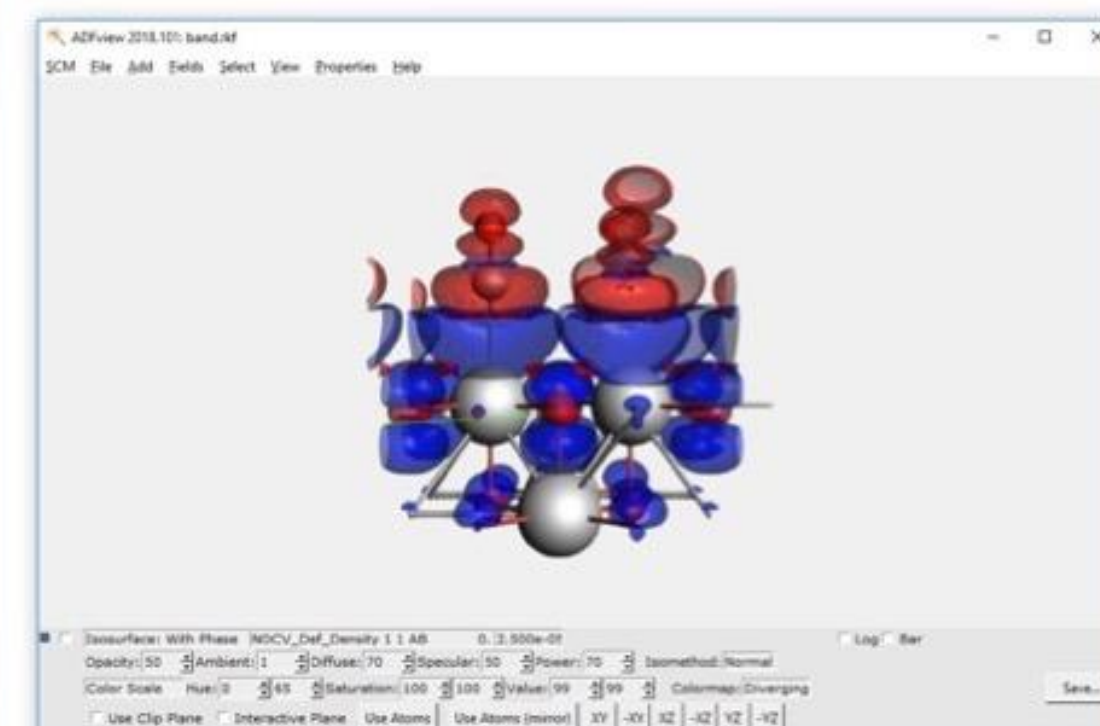
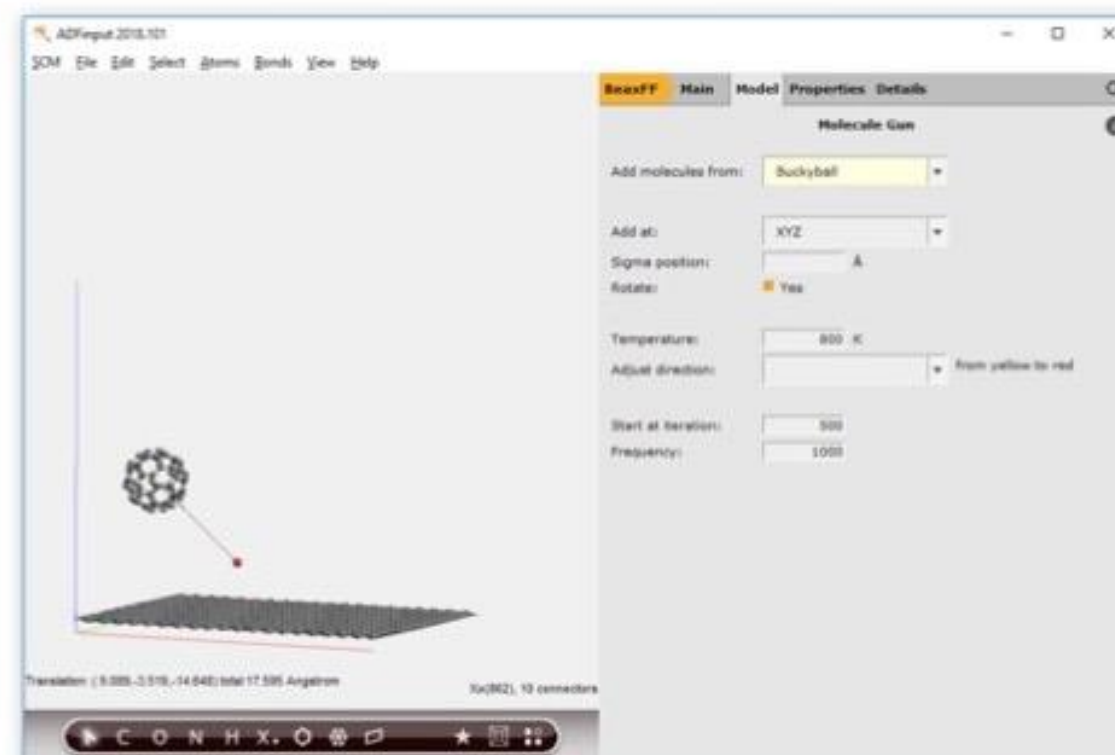
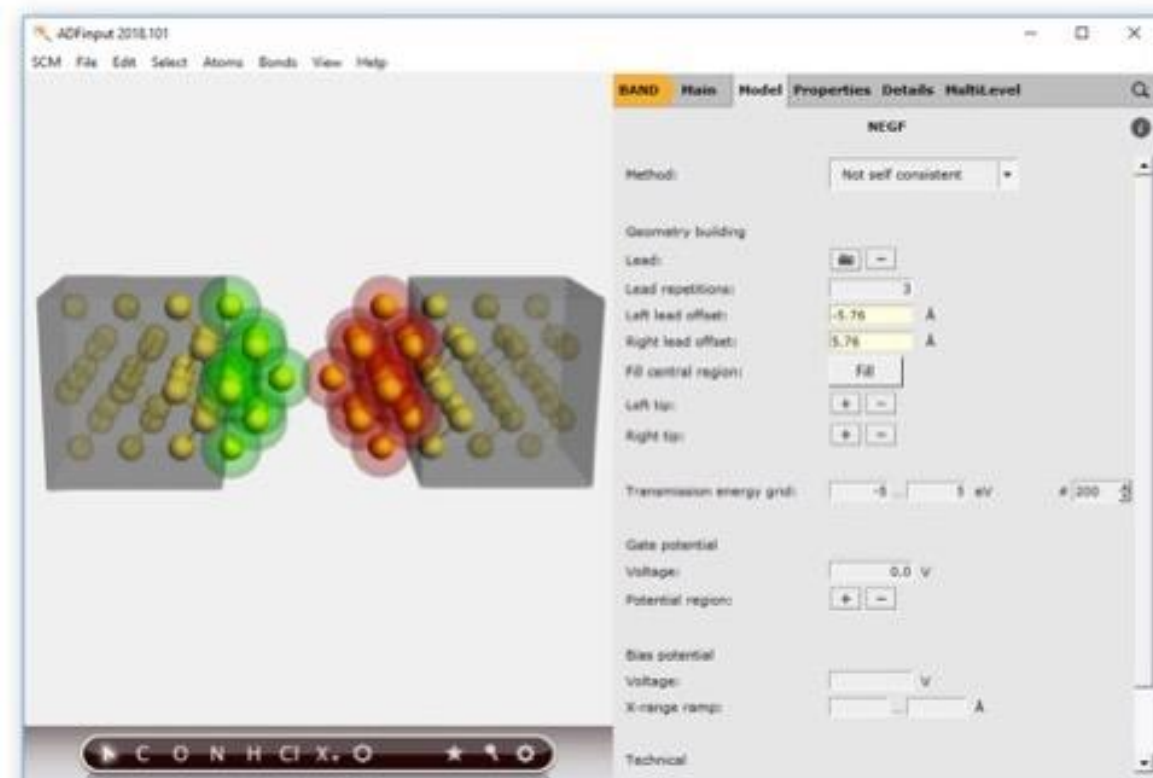
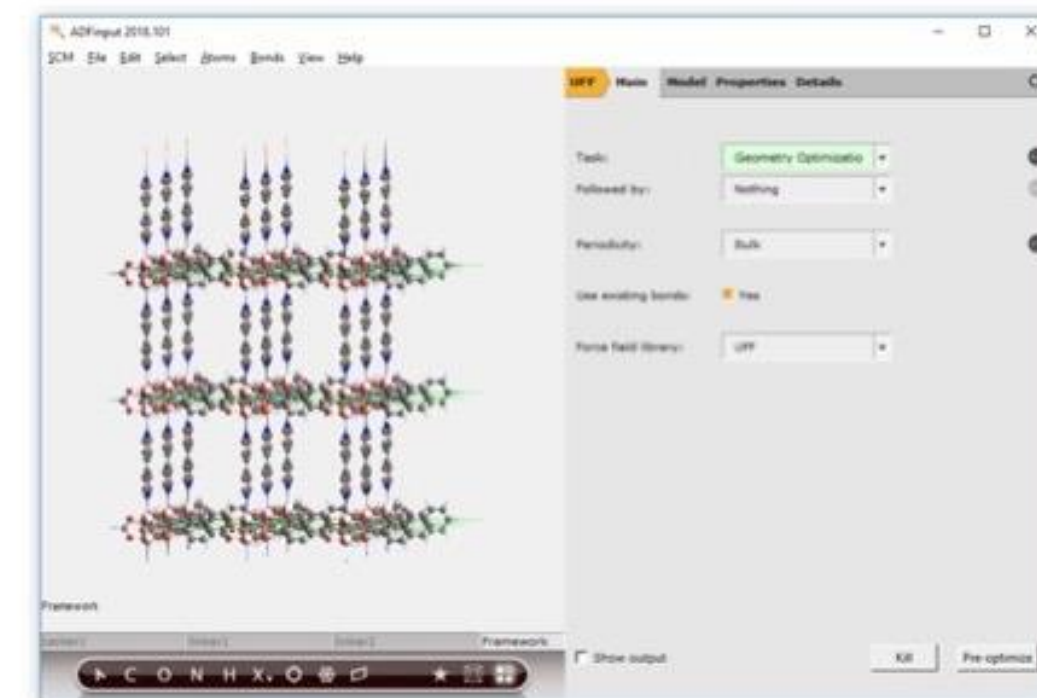
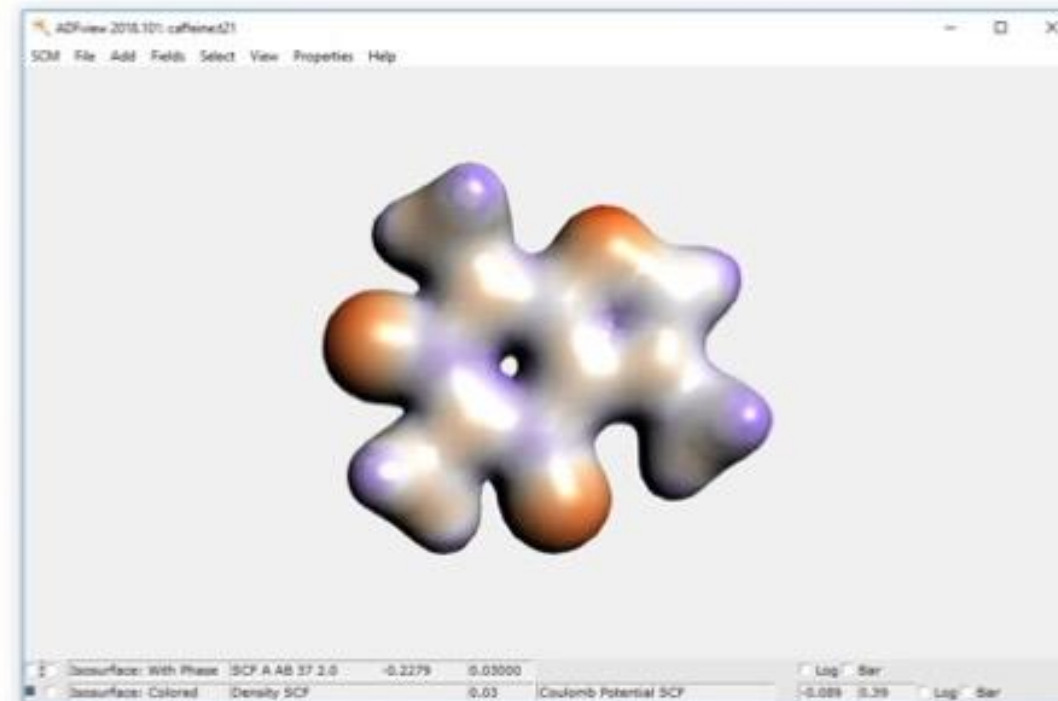
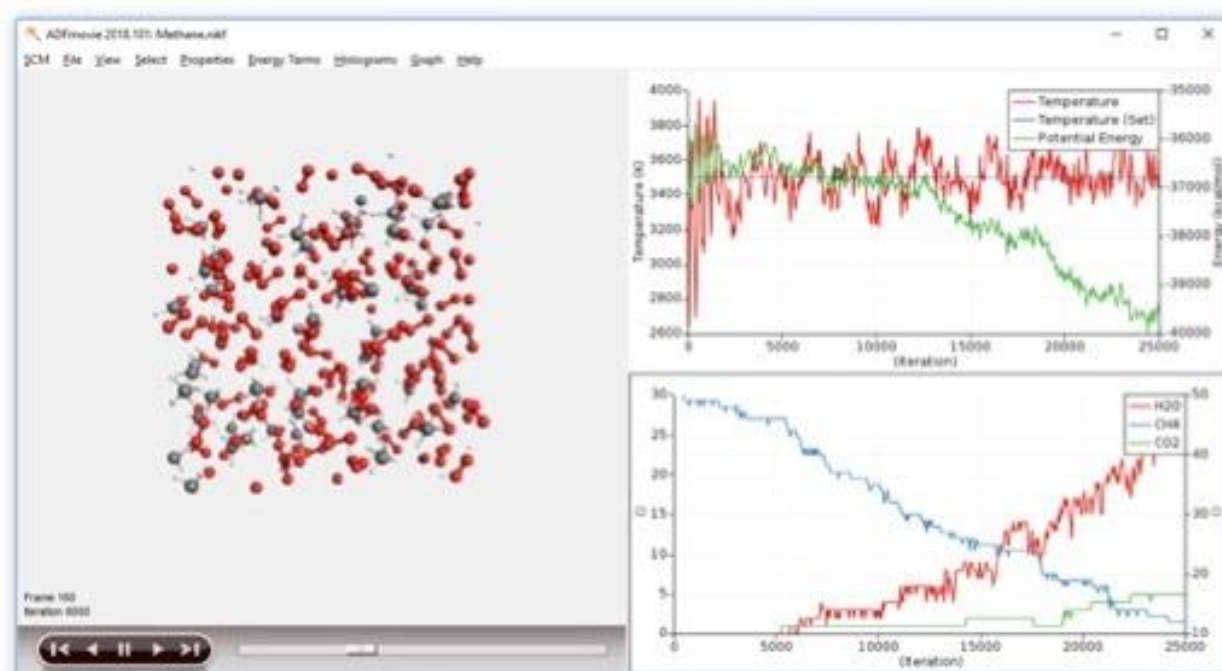
DFTB & MOPAC
Fast approximate DFT
Semiempirical

Atomistic

BAND
Periodic DFT

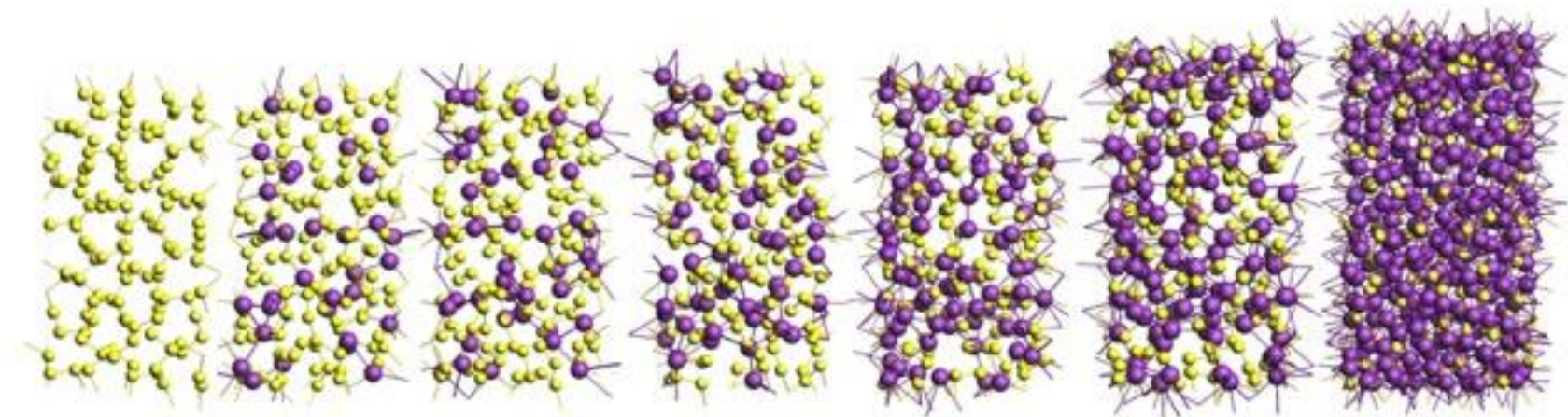
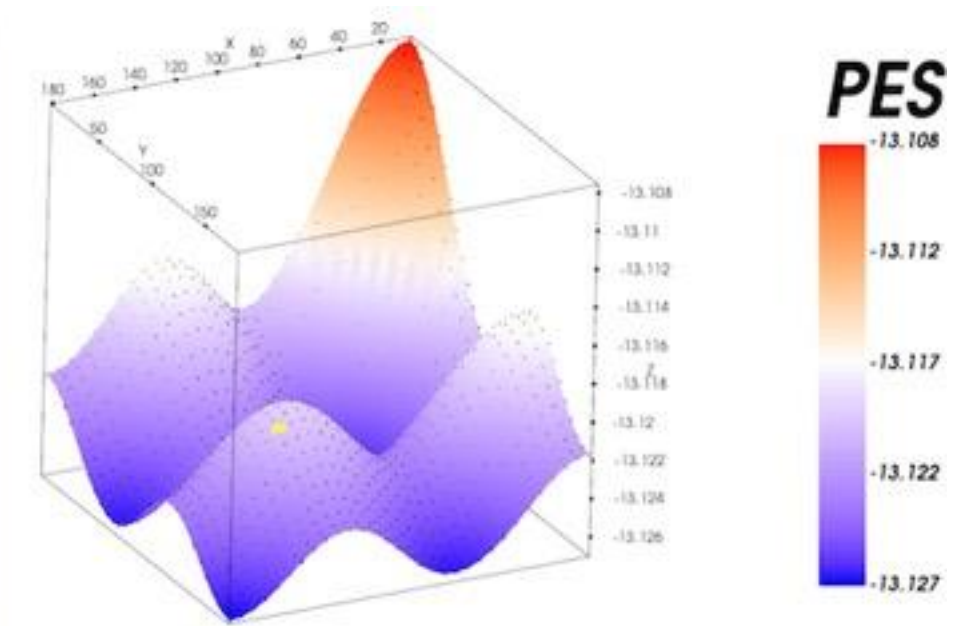
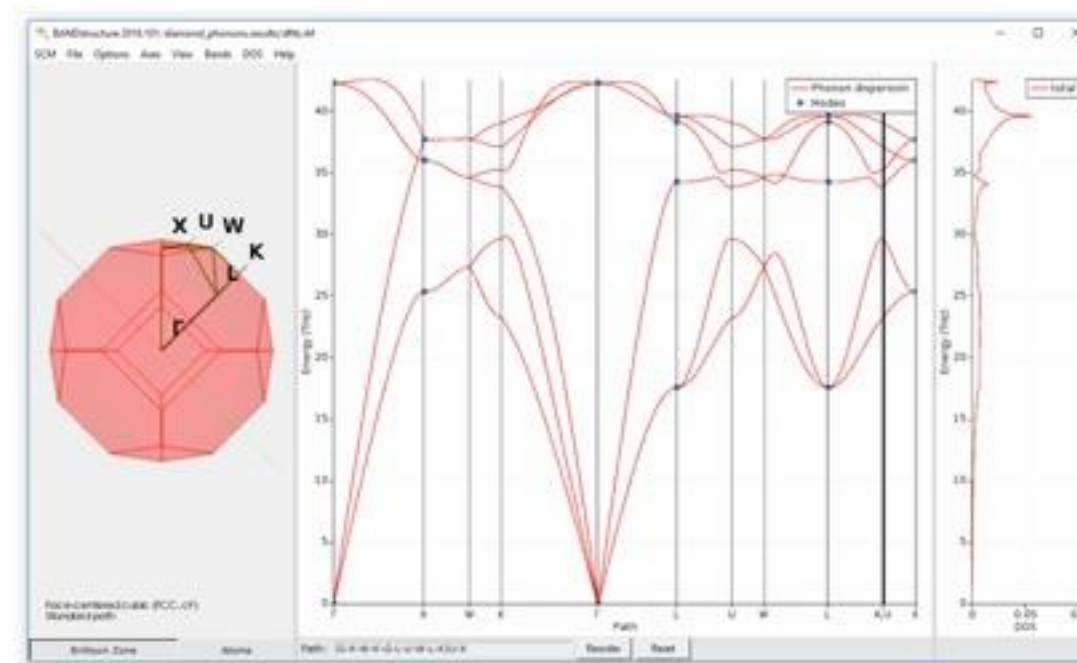
ADF
Molecular DFT

1 GUI: build, run & analyze



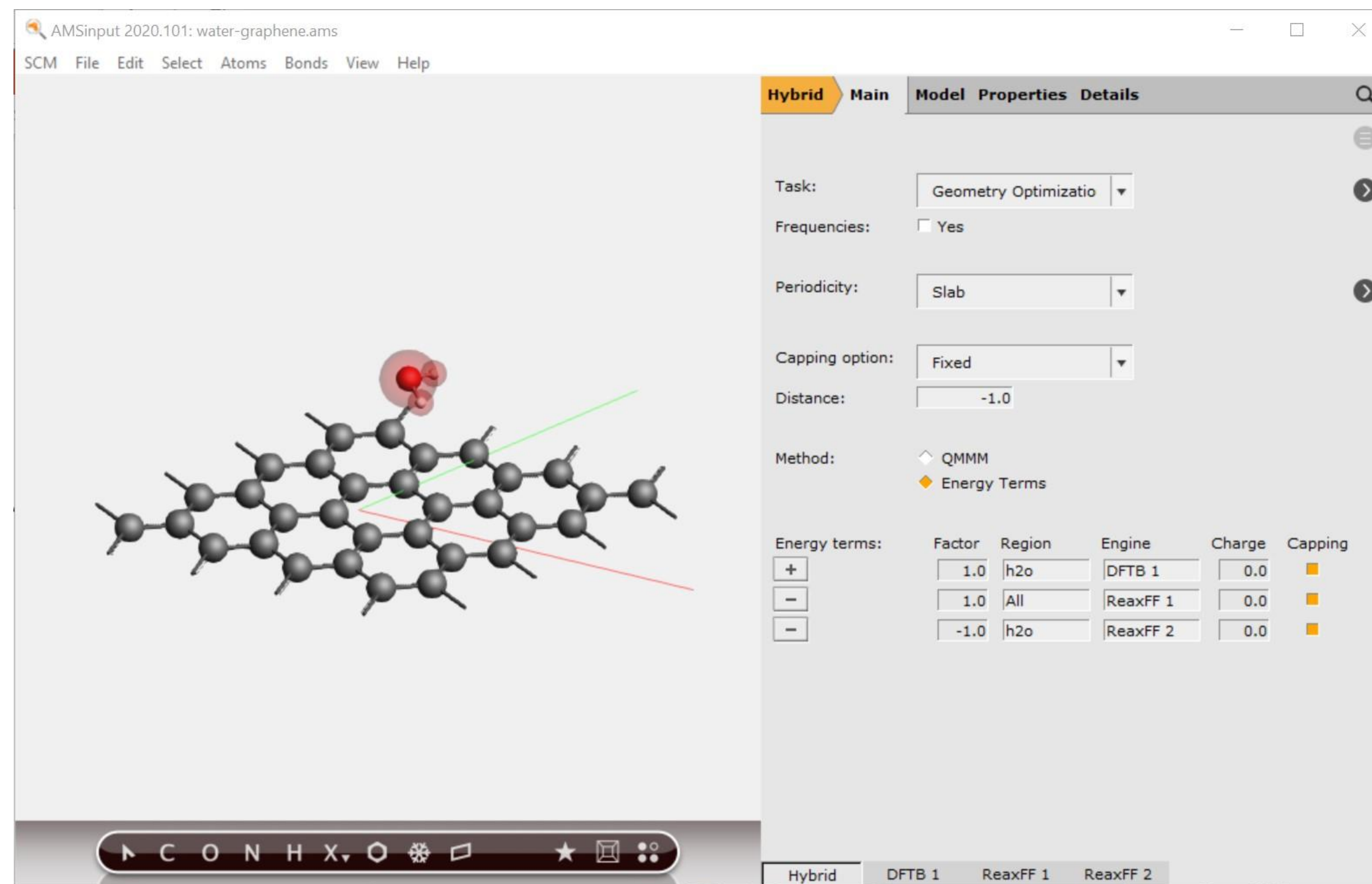
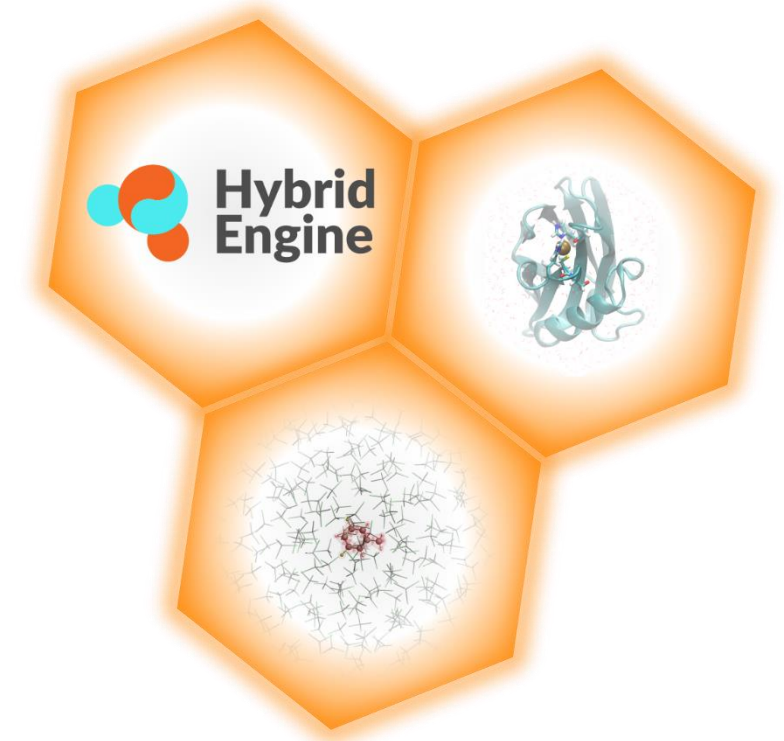
The AMS driver: decouple from Engine

- Frequencies (+ analysis) & phonons
- Stress & elastic tensors
- Scan (multiple) coords, any periodicity
- Geometries, TS, IRC
- Advanced Molecular Dynamics
- (Grand Canonical) Monte Carlo



New in AMS2020: Hybrid Engine

- Multi-layer (subtractive, QUILD, ONIOM)
 - combine **any** periodicity, number of layers, and QM or MM methods
- 2-layer: (additive) QM/MM
 - any periodicity
 - QM: ADF, DFTB, BAND, MM: Force Field engine



The screenshot shows the AMSinput 2020.101: water-graphene.ams interface. The main window displays a 3D model of a water molecule (red and white) interacting with a graphene slab (grey and black). The interface includes a menu bar (SCM, File, Edit, Select, Atoms, Bonds, View, Help) and a toolbar at the bottom. The right-hand side features a 'Hybrid' tab with various settings:

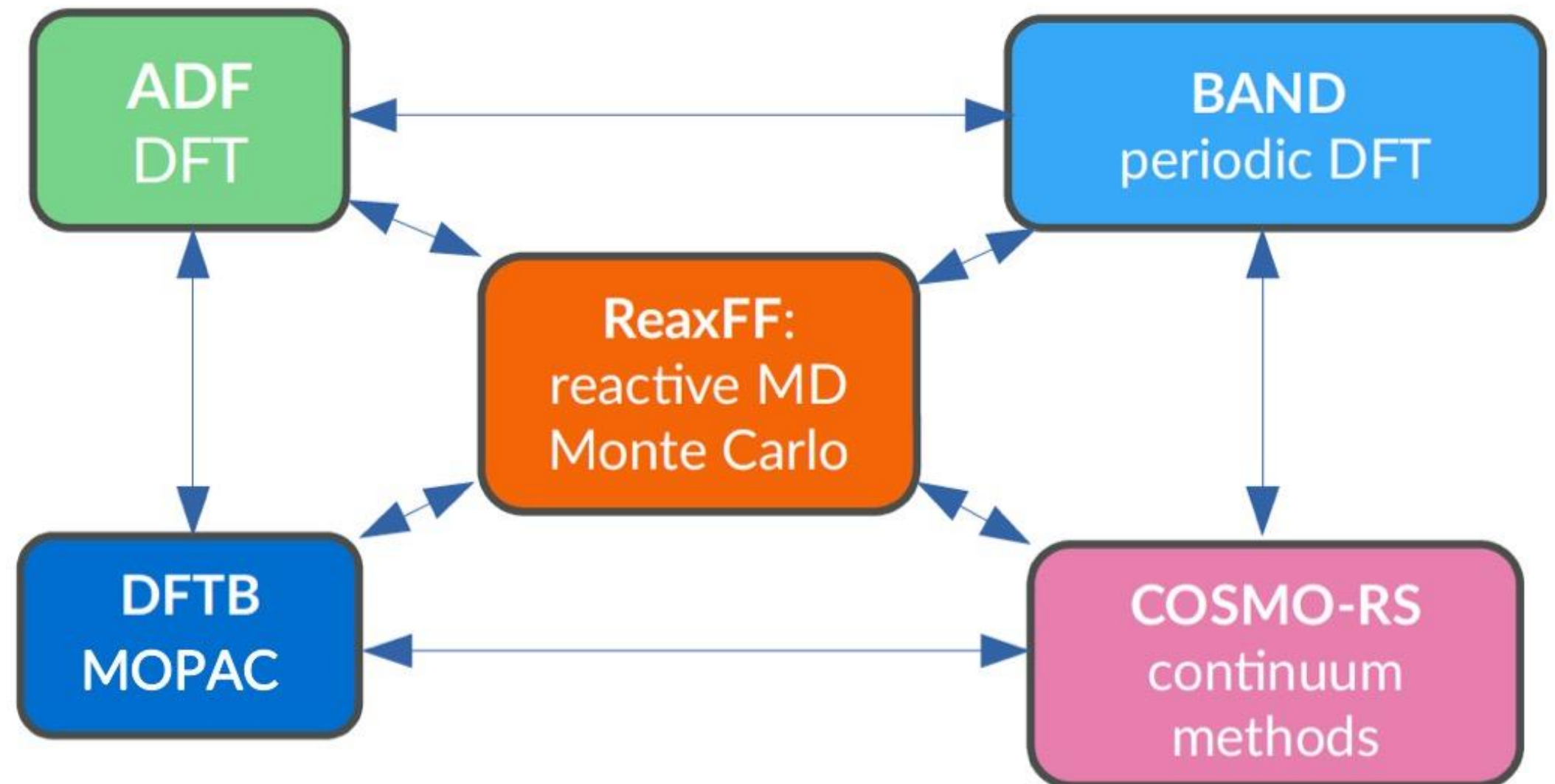
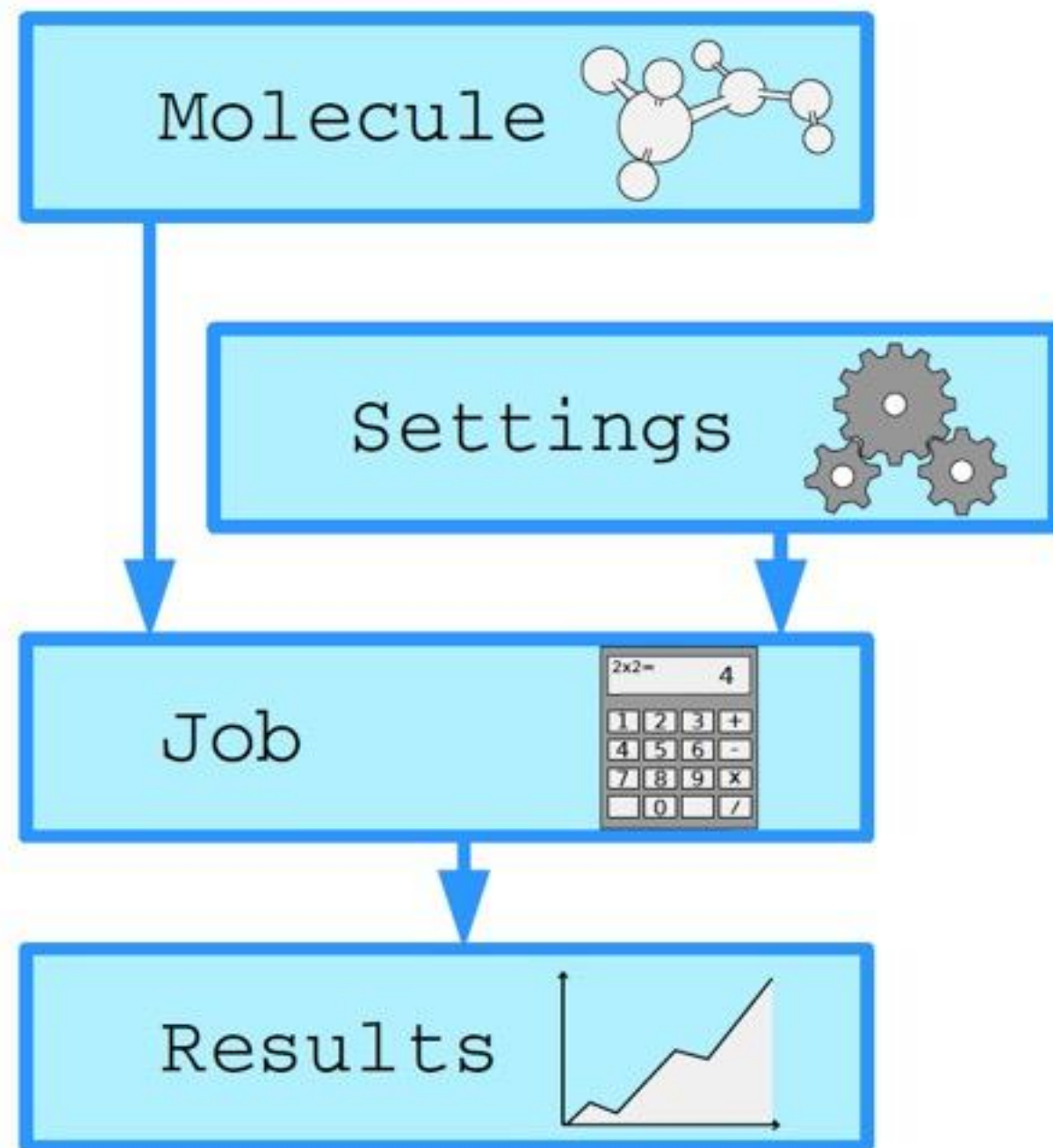
- Task: Geometry Optimizatio
- Frequencies: Yes
- Periodicity: Slab
- Capping option: Fixed
- Distance: -1.0
- Method: QMMM, Energy Terms

Energy terms:	Factor	Region	Engine	Charge	Capping
<input type="checkbox"/> +	1.0	h2o	DFTB 1	0.0	<input type="checkbox"/>
<input type="checkbox"/> -	1.0	All	ReaxFF 1	0.0	<input type="checkbox"/>
<input type="checkbox"/> -	-1.0	h2o	ReaxFF 2	0.0	<input type="checkbox"/>

At the bottom, there is a status bar with 'Hybrid', 'DFTB 1', 'ReaxFF 1', and 'ReaxFF 2' indicators.

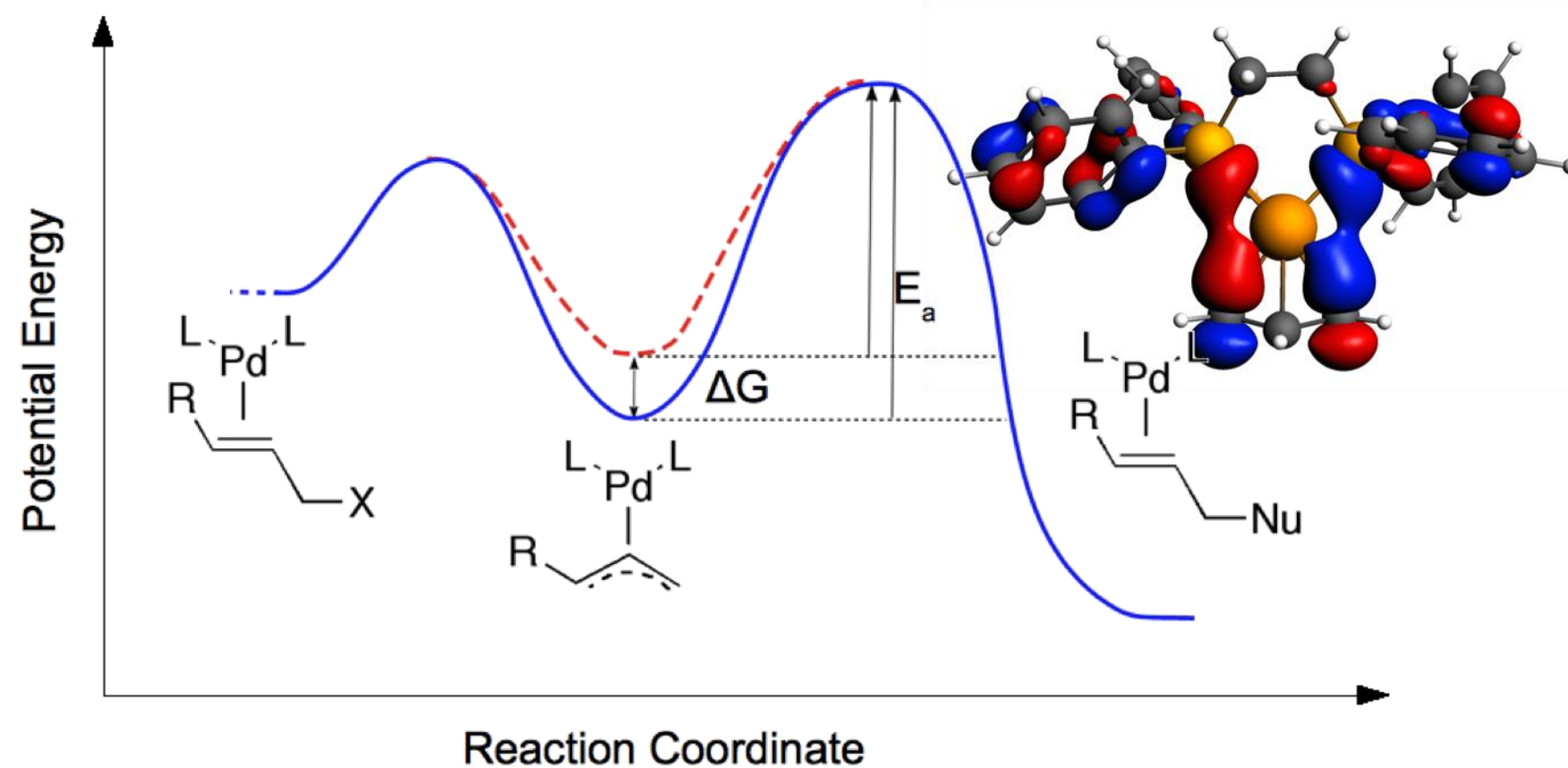
[Demo video](#)

PLAMS: python scripting

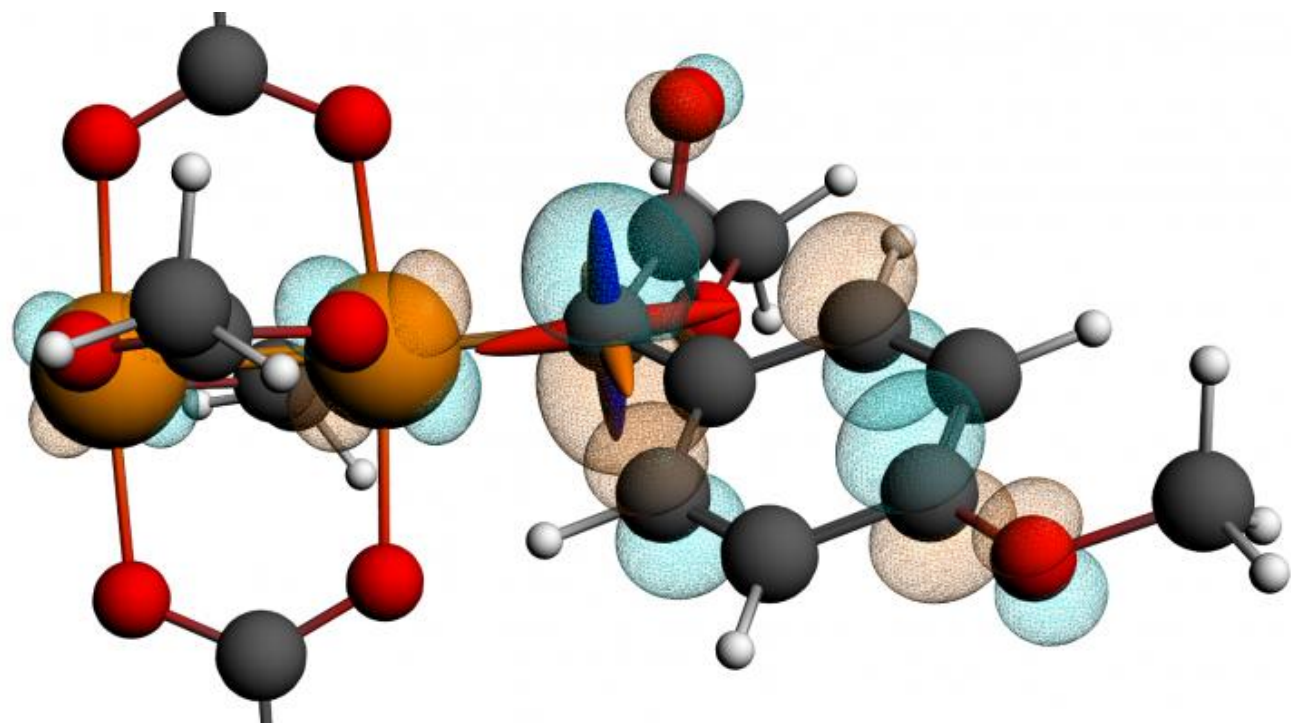


Links all modules + various tools
→ workflows & [screening](#)
→ (custom) post-processing
→ rapid prototyping

ADF: Molecular DFT



Bonding analysis: Understanding Catalyst-Substrate Interactions [Nature Chem. 2, 417 \(2010\)](#)



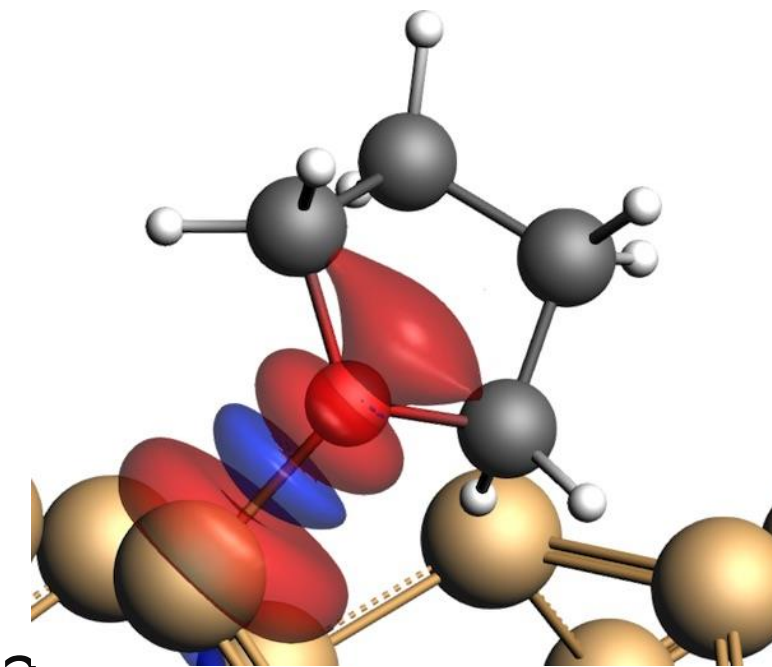
NMR calculations locate ^{13}C di-Rh carbene catalyst intermediate, [Science, 342, 351 \(2013\)](#)

Strong & unique points

- All-electron Slaters, H-Og
- Relativity: ZORA (SR, SOC)
- Reactivity: catalysis
- Spectroscopy
 - EPR, NMR, IR (VCD), UVVIS, XAS
 - Phosphorescence
- Bonding analysis:
 - Fragment-based approach
 - ETS-NOCV, QTAIM, MO diagrams, NCI, ...
 - Transfer integrals (charge mobility)
- Environments
 - Subsystem DFT (FDE), DIM/QM, QM/MM

Periodic DFT: BAND vs Plane Waves

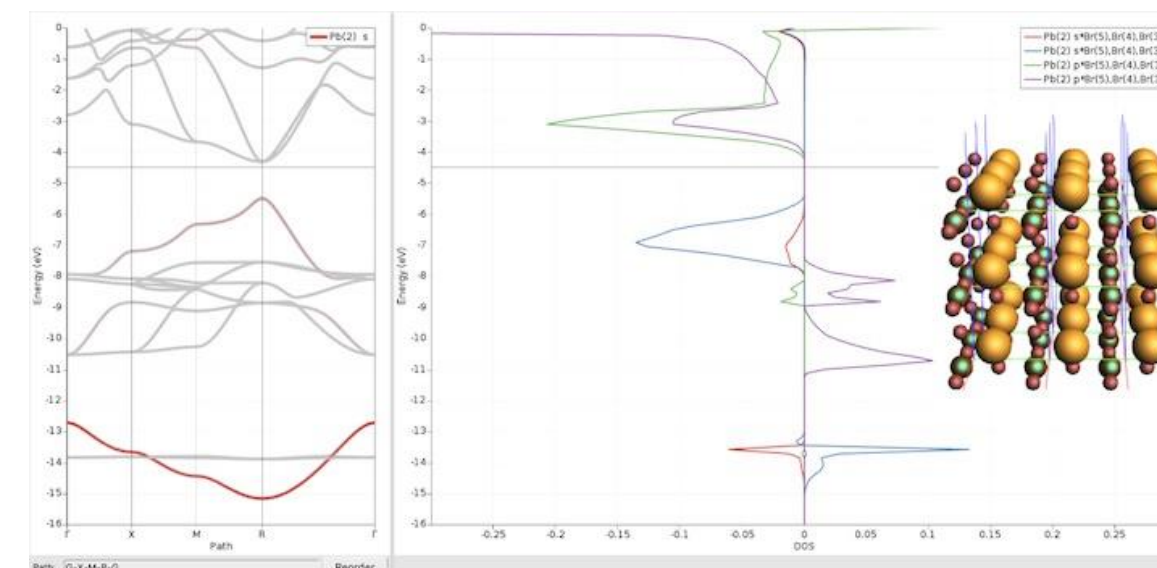
- Atom centered basis functions, STO or NAO
 - Compare cluster with periodic
 - No pseudopotentials, all elements
 - Core spectroscopy (core holes)
 - Easy orbital **analysis**: pDOS, COOP, EDA
 - Fast for empty (1D, 2D, porous)
 - xc: SCAN, MN15-L, HSE06, GLLB-sc, D3(BJ), DFT-1/2
 - Self-consistent NEGF
 - Gate & bias potential
 - Spin transport



periodic energy decomposition analysis (tutorial)

L. Pecher and R. Tonner
[WIREs CMS, \(2018\)](#)

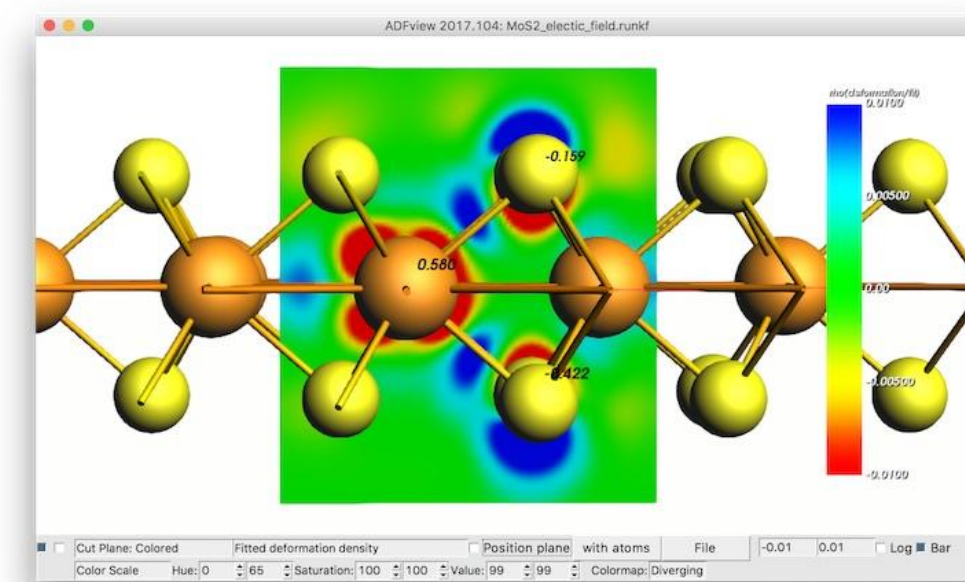
- True 2D surfaces, 1D polymers
 - Het. catalysis: polarization, COSMO, **SM12**
 - 2D electronics (homogeneous E field)
 - Nanotubes
 - QM/MM and QM/QM' for 2D



COOP in perovskites (tutorial)

Goesten & Hoffmann
[JACS \(2018\)](#)

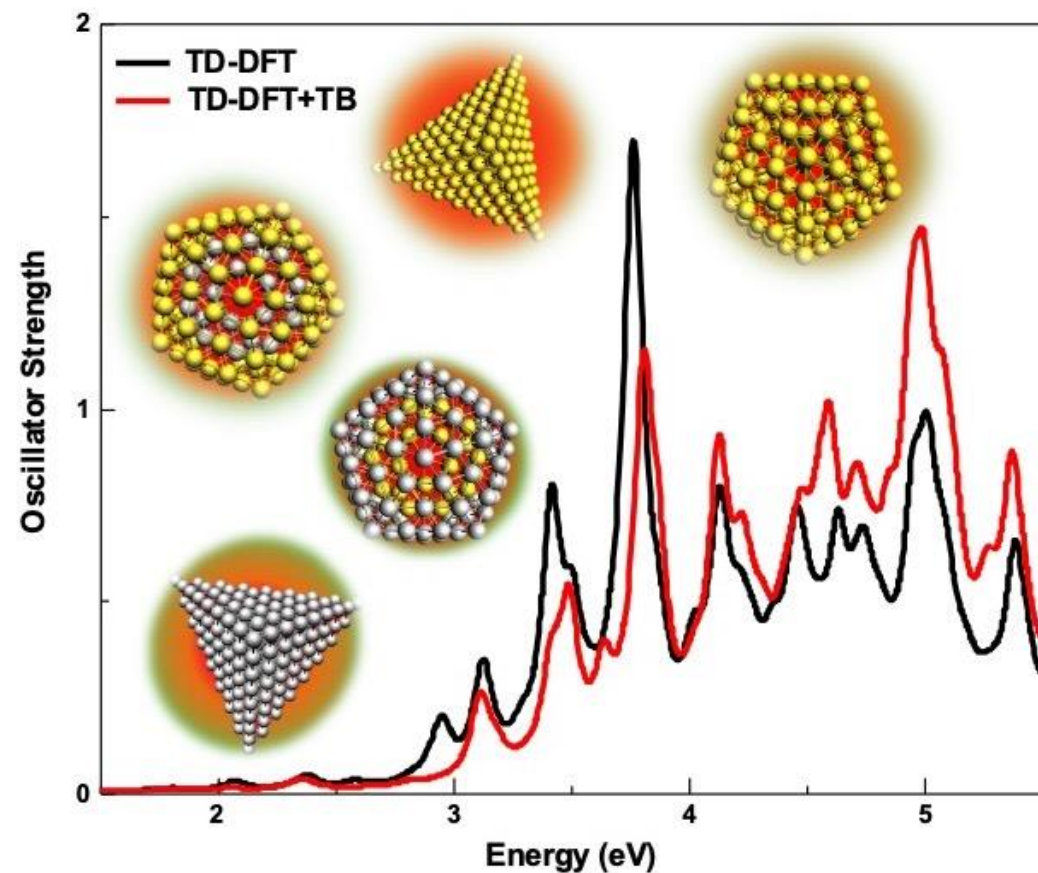
- Integrated Graphical Interface:
 - Easy set up & analysis
 - Switch: ADF, BAND & **Quantum Espresso, VASP**



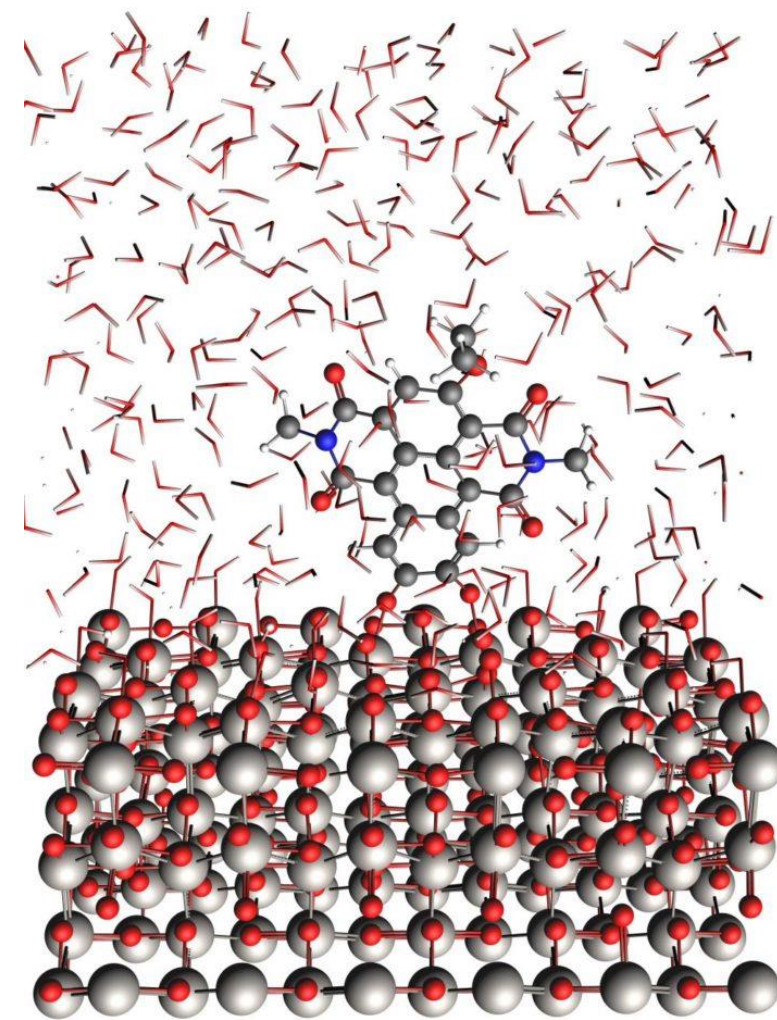
Polarizing 2D semiconductor (tutorial)

N. Zibouche et al.
[PCCP \(2014\)](#)

DFTB: 'fast DFT' for molecules & periodic



Plasmons in nanoparticles
[JPCC 2020, 124, 7946](#)



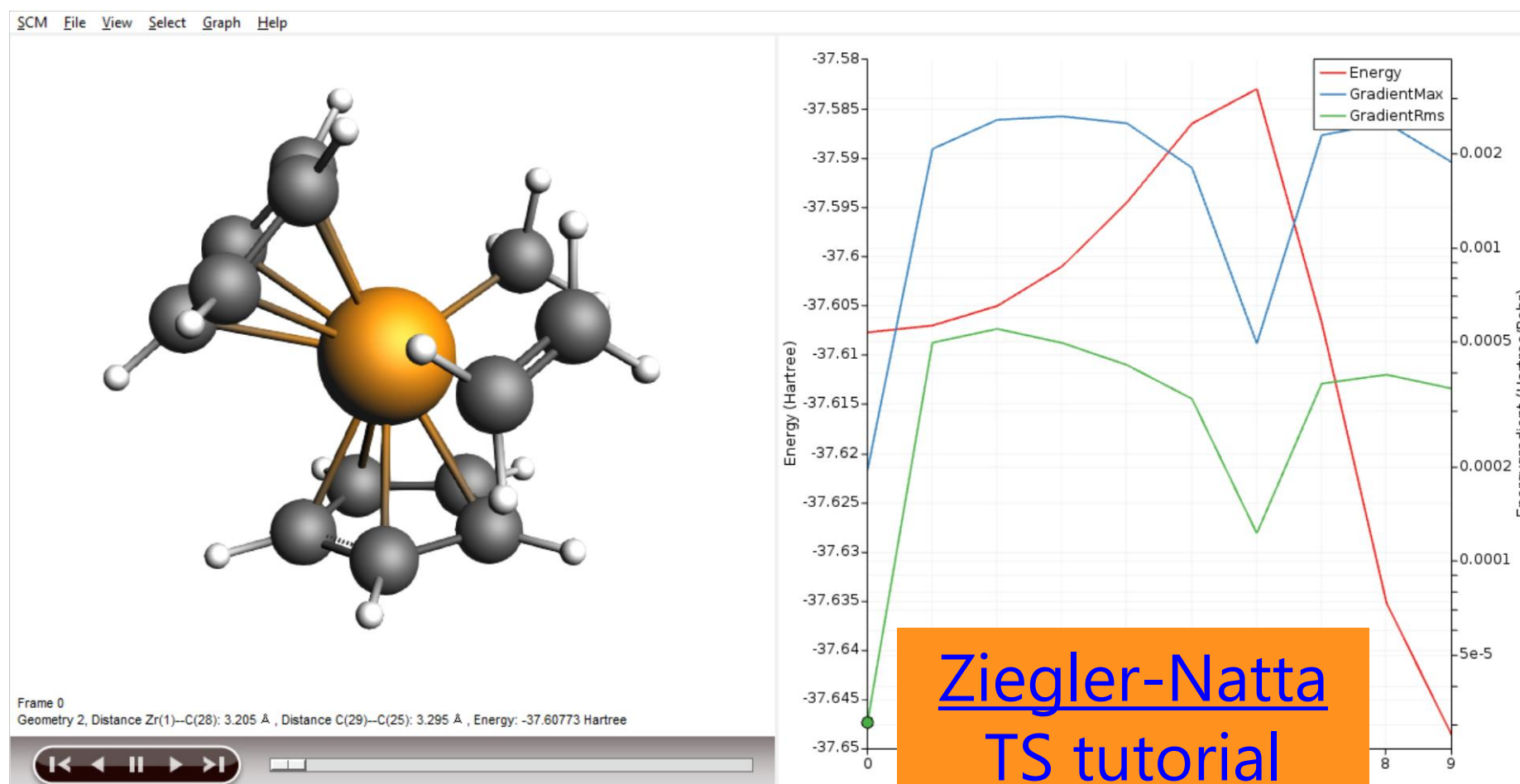
Dye-sensitized solar cell
[JPCC 2020, 124, 27965](#)

Approximated DFT

- Nearest neighbor & minimal basis
- Tabulated elec & rep. parameters:
 - Grimme GFN-xTB (Z = 1-86)
 - **GBSA solvation**
 - QuasiNaNo & DFTB.org

Capabilities & Features

- UV/VIS for molecules (fast!)
- MOs, Band structures, DOS
- 0D, 1D ([CNT](#)), 2D, 3D periodic

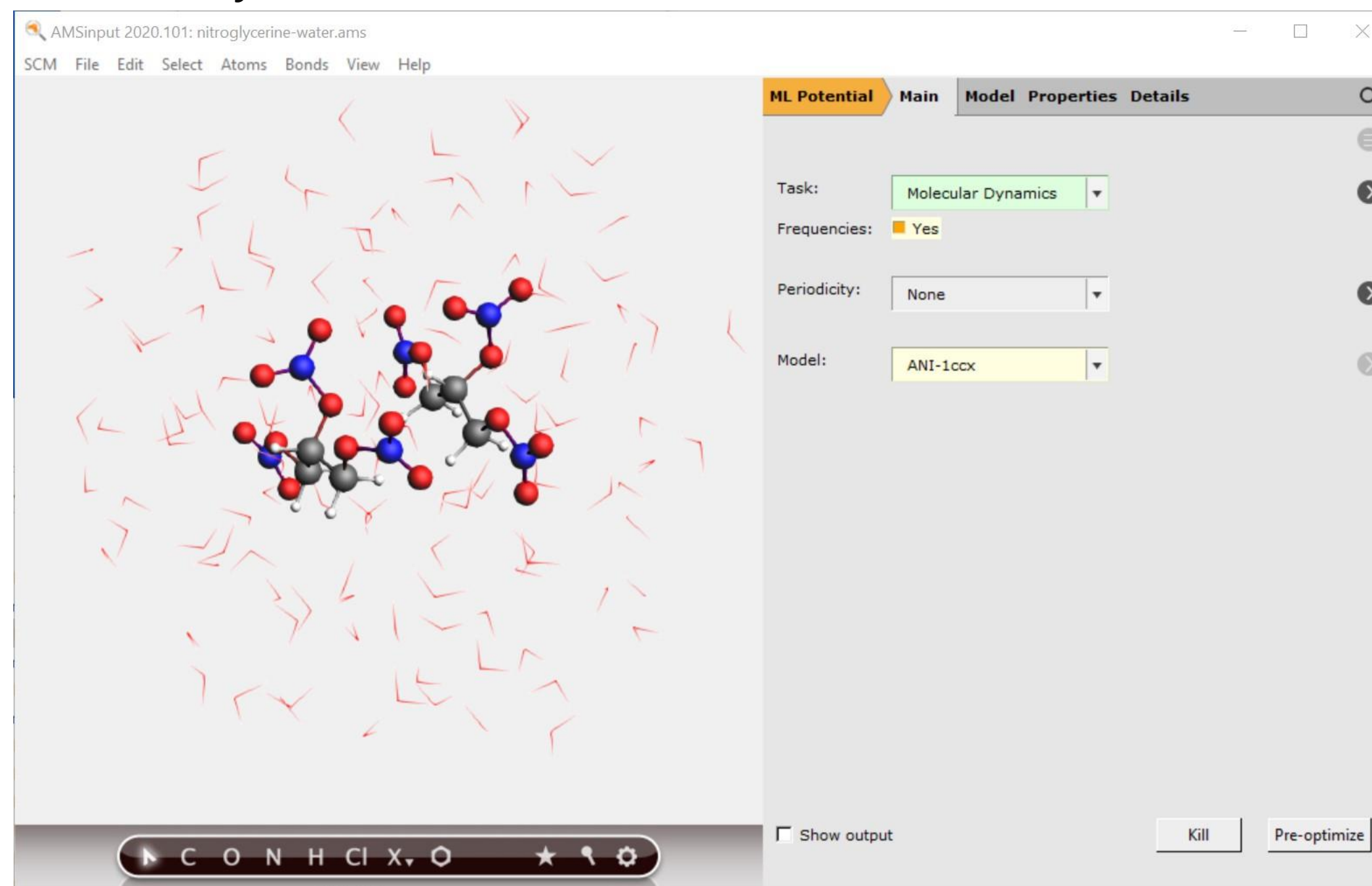


DFTB & MOPAC + AMS driver

- Geometries, frequencies, phonons
- Stress tensors (optimize under p)
- Advanced MD, PES scans
- GCMC, molecule gun

New in AMS2020: MLPotential

- Use machine learning potentials with AMS driver
 - PES scans, conformers, MD, reaction energies, ...
 - Also with Hybrid engine (multi-layer)
- Automatically install popular ML Backends
 - SchNetPack, sGDML, PiNN, TorchANI
 - Pre-parametrized neural network potentials ANI-1ccx, ANI-2x
 - CUDA-enabled PyTorch and Tensorflow can be used



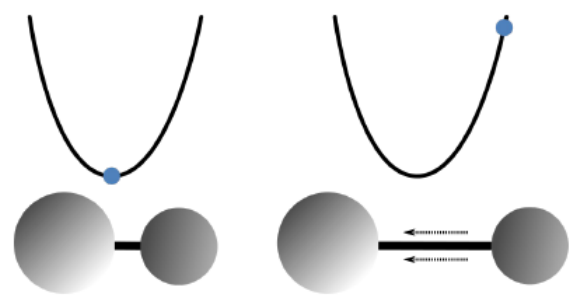
[Demo video](#)

ReaxFF: concept

- Simulate complex systems at realistic scales
 - Atomistic potentials – single atom type (reasonably transferable)
 - Update charges and bond orders at every step

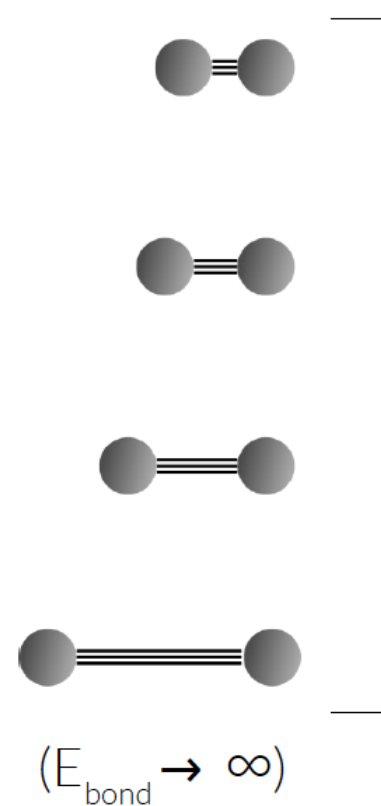
A.C.T. van Duin et al, J. Phys. Chem. A 2001, 105, 9396-9409.

Standard forcefields



Harmonic potentials based on atom distance, bond breaking impossible, e.g.

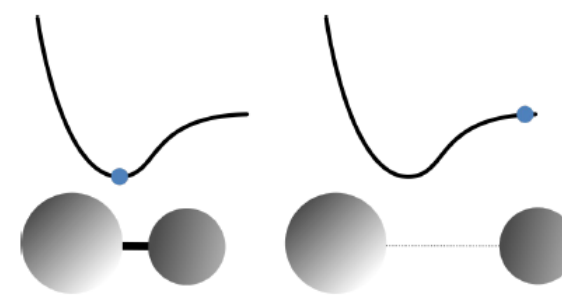
$$E_{\text{bond}} \propto (\text{distance})^2$$



a triple "bond" will always stay a triple "bond"...

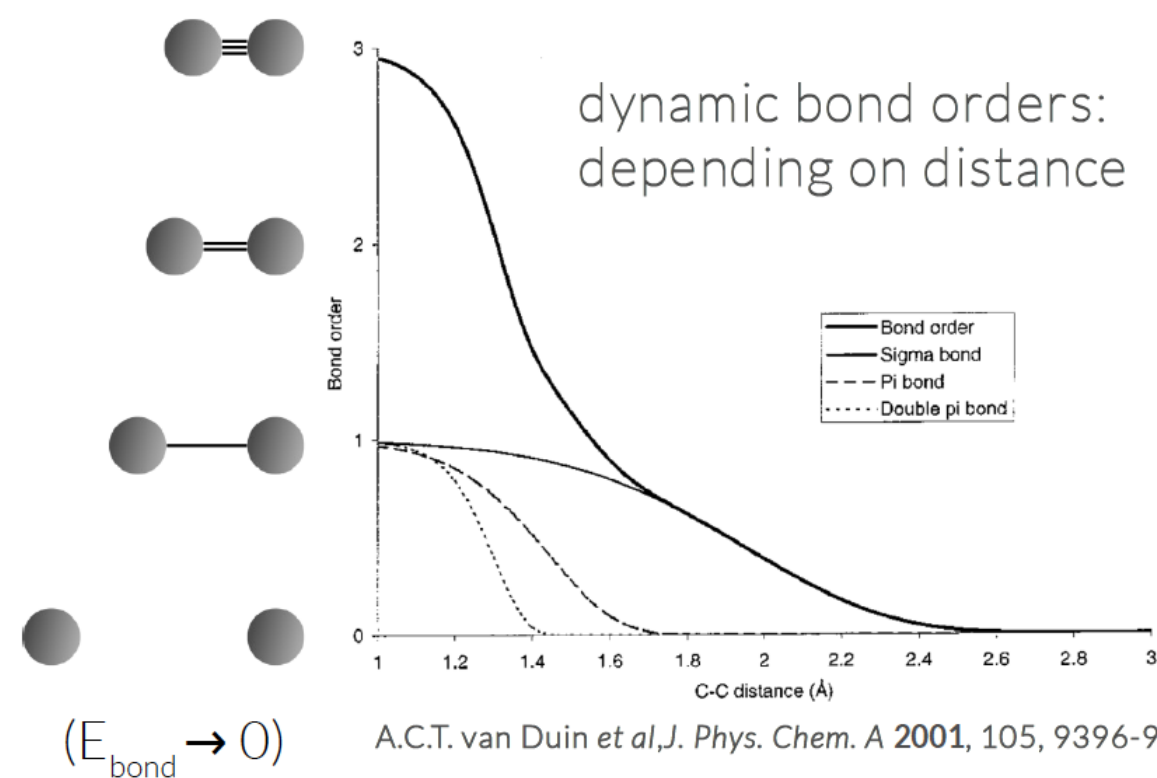
vs

ReaxFF

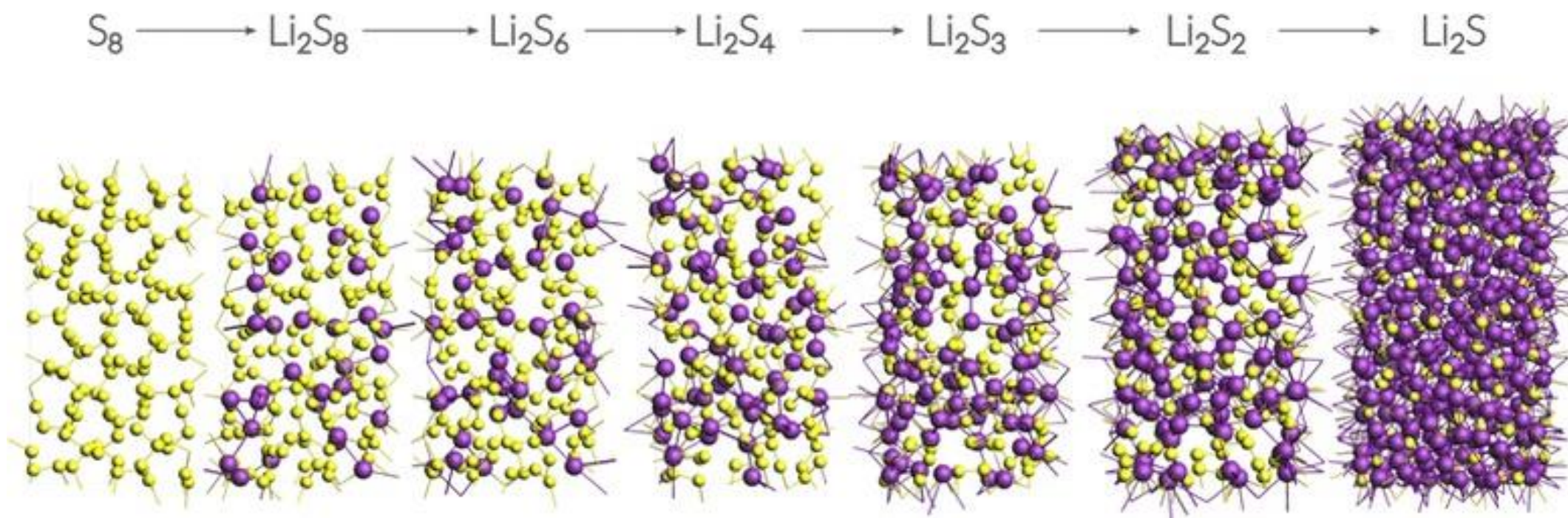


Non-harmonic potentials based on bond orders, bond breaking/forming possible, e.g.

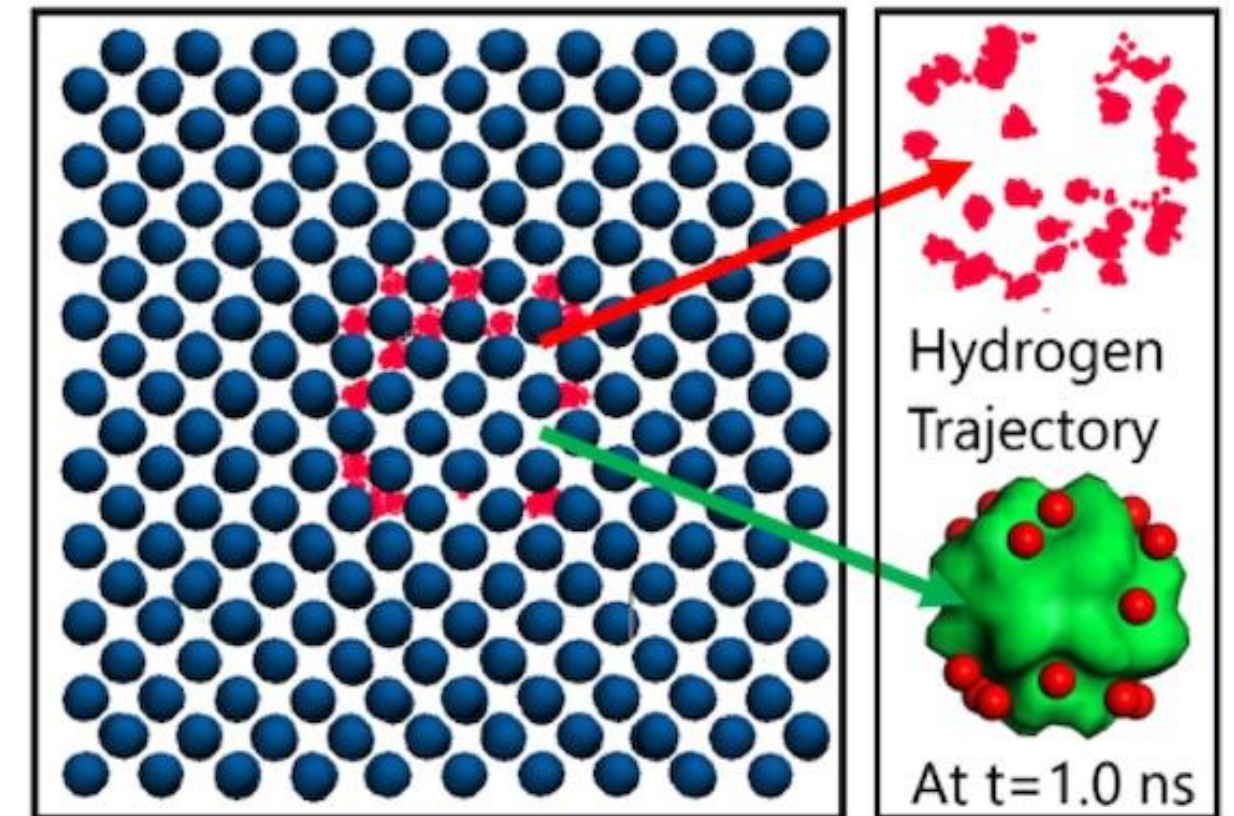
$$E_{\text{bond}} \propto -(\text{bond order}) \times \exp[(1 - \text{bond order})]$$



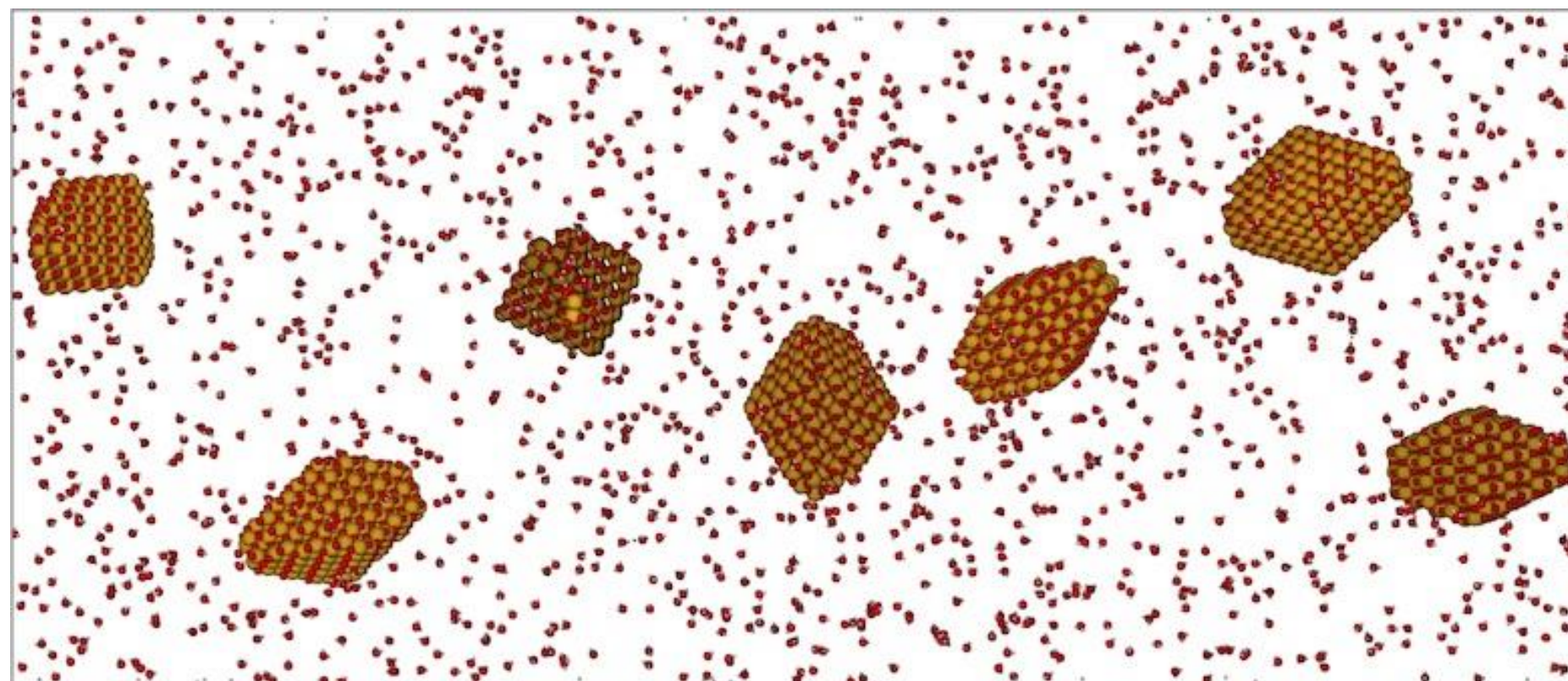
ReaxFF – reactive molecular dynamics



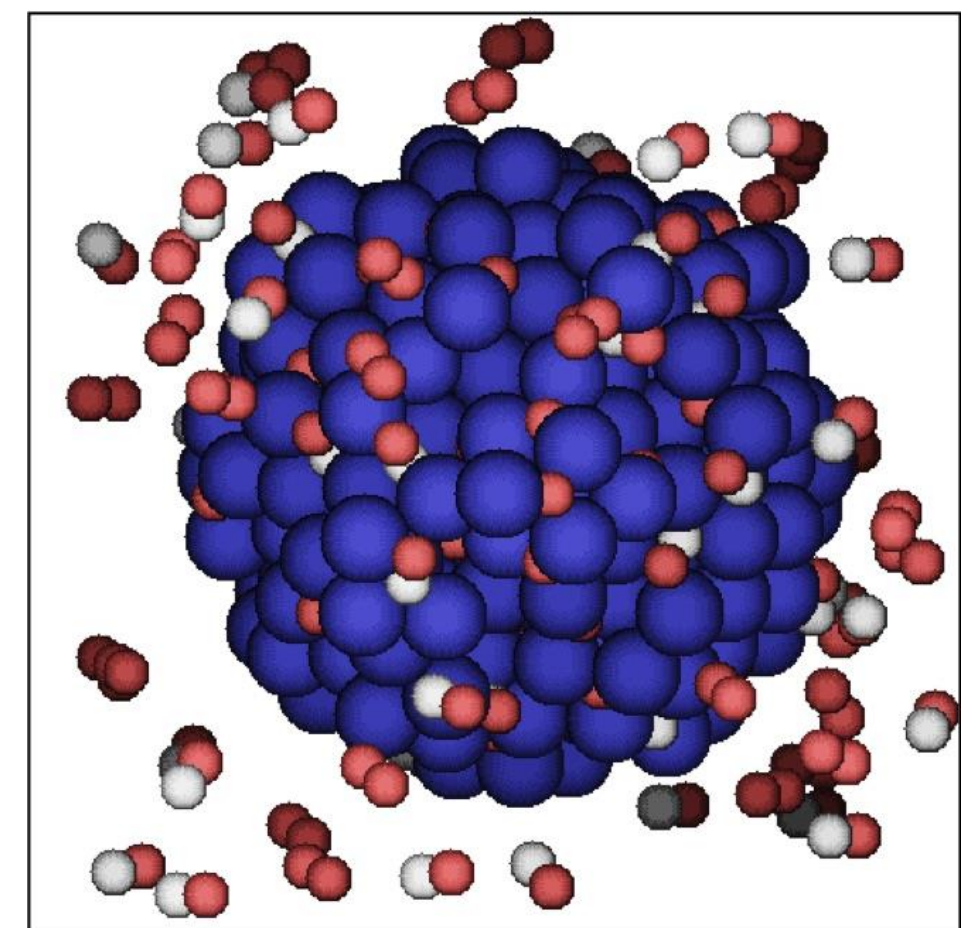
Li battery discharge: J. Electrochem. Soc. **161**, E3009 (2014); PCCP, **17**, 3383 (2015), [tutorial](#)



Hydrogen embrittlement of steels
Phys. Chem. Chem. Phys. **18** 761 (2016)



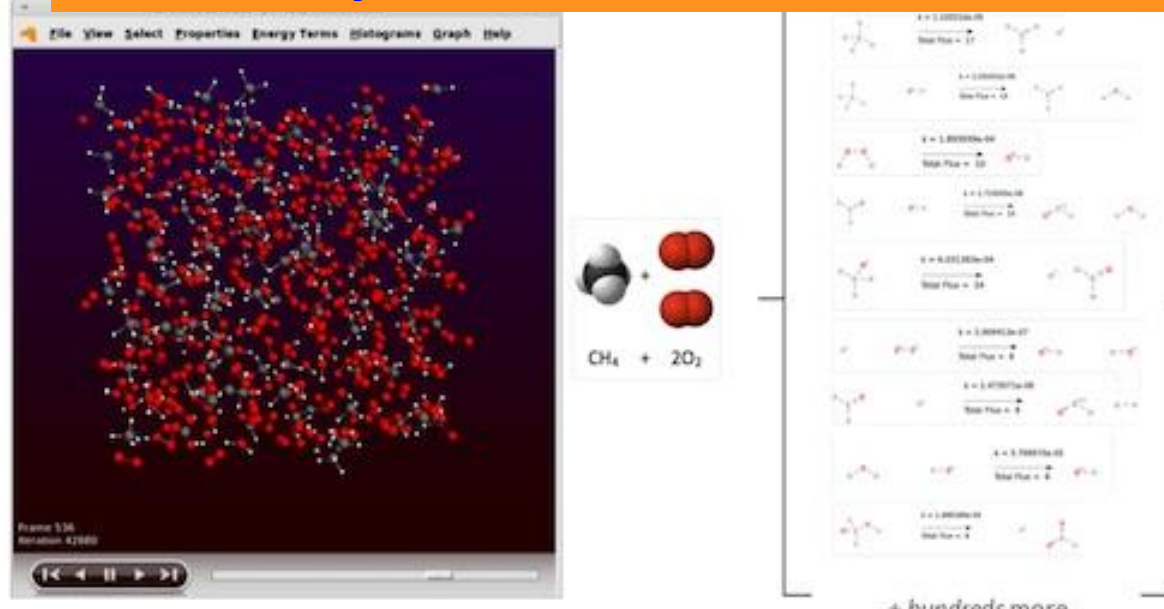
Crystallization TiO_2 nano-particles in water
[Nano Lett. **14**, 1836-1842 \(2014\)](#)



Pd-catalysed CO oxidation GCMC+ReaxFF
J. Chem. Phys., **139** 044109 (2013)

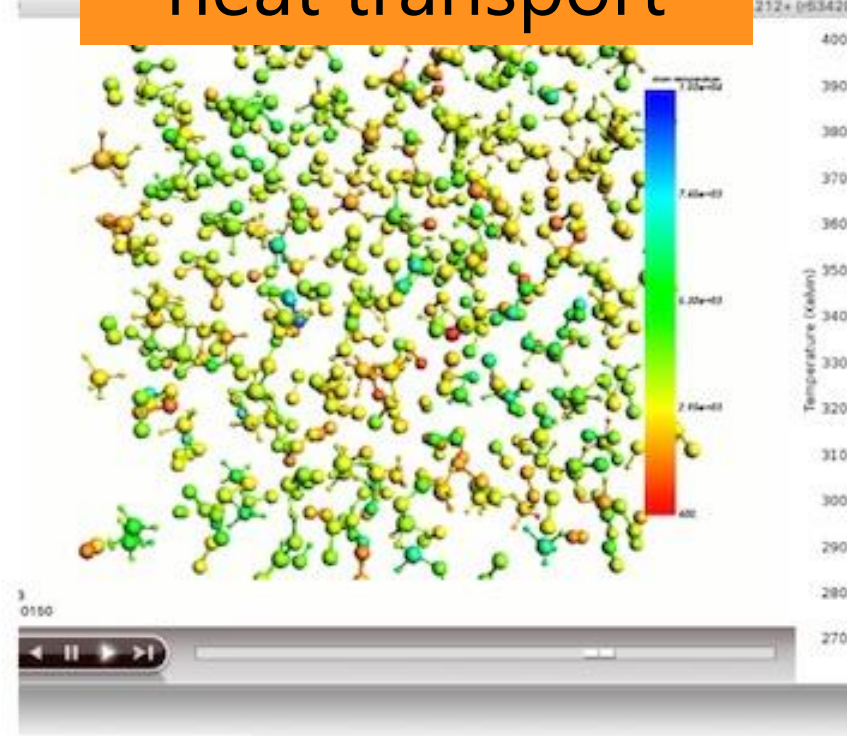
ReaxFF tools in Amsterdam Modeling Suite

Automated rates & pathways
Analyze surface reactions

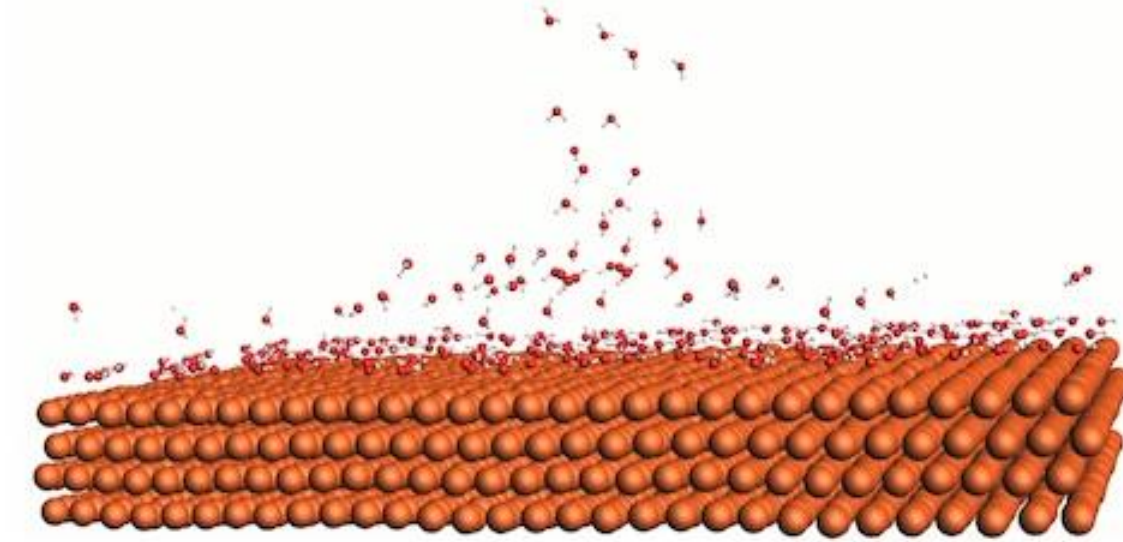


Tools += complete reaction networks
elementary reactions, rate constants, fluxes, timeline

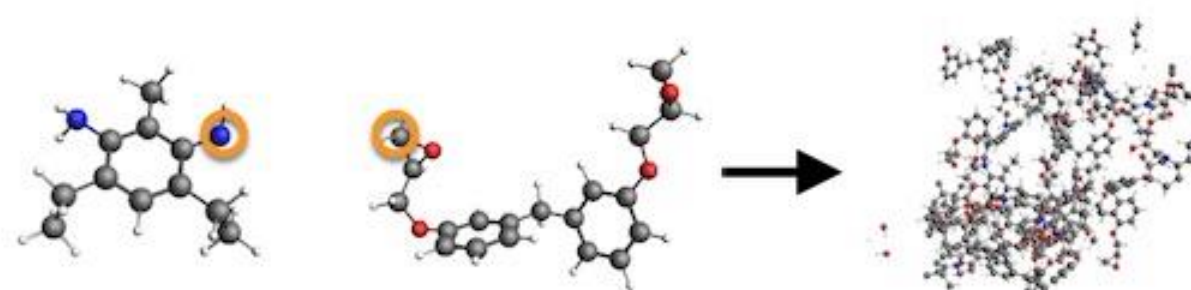
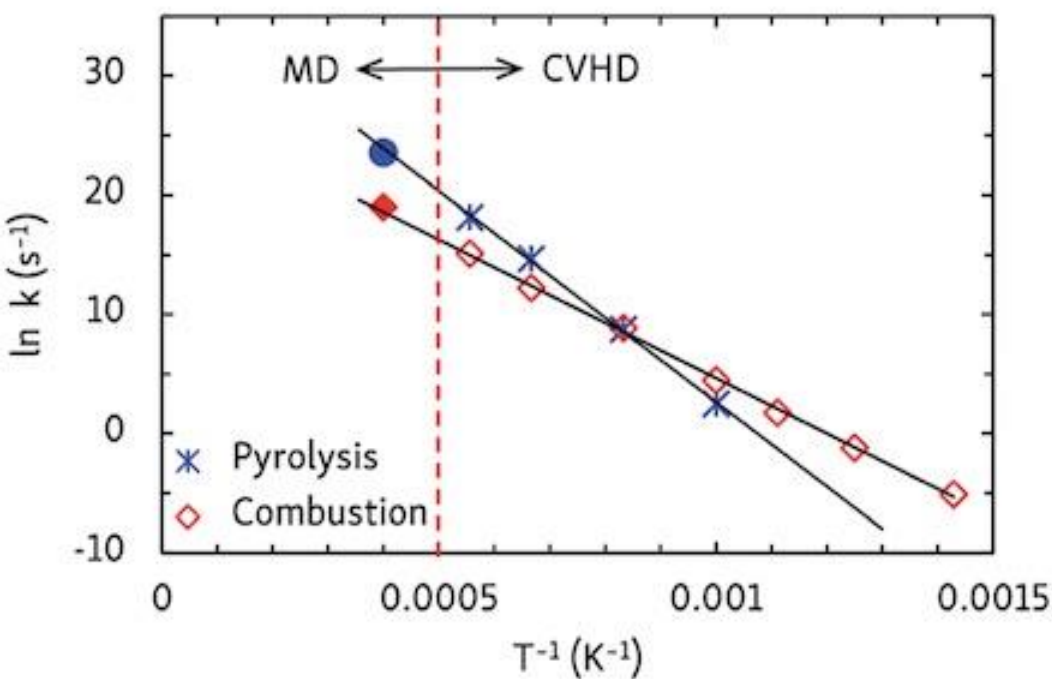
T-NEMD, local T:
heat transport



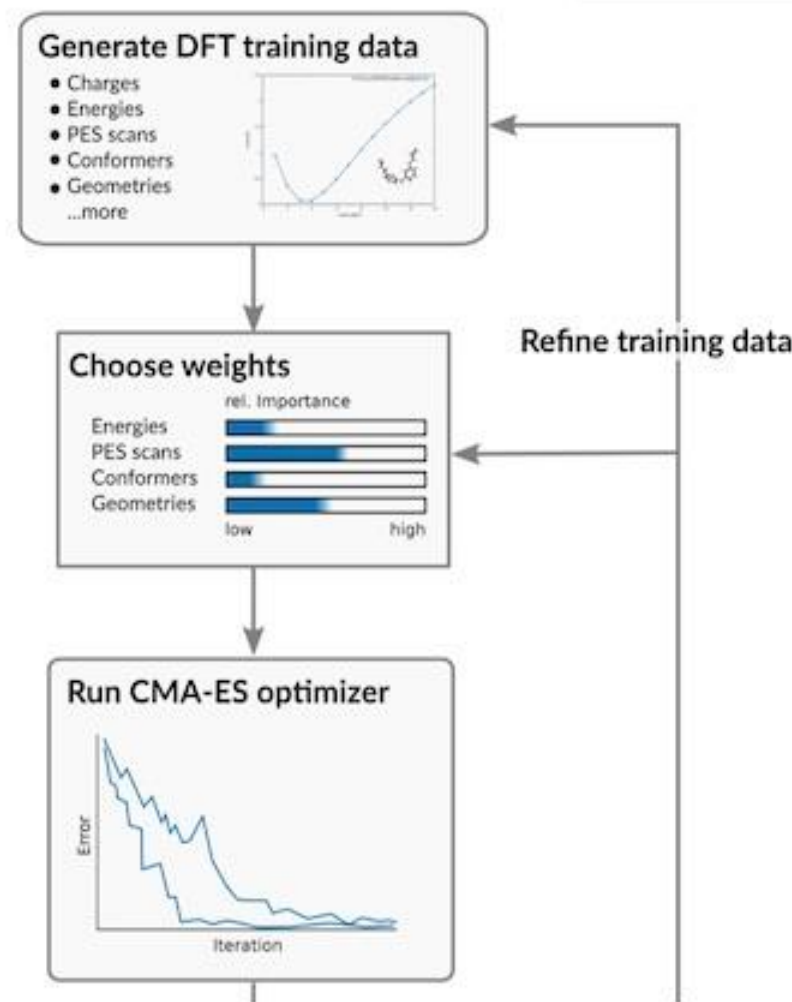
Molecule gun: depositing
molecules on surfaces



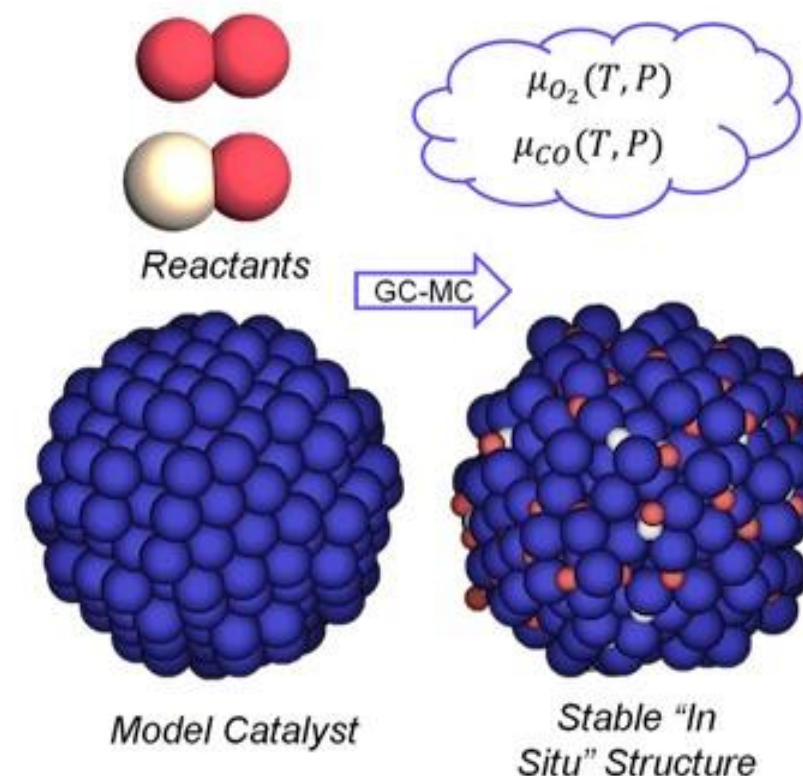
fbMC, CVHD, PRD:
speed up kinetics



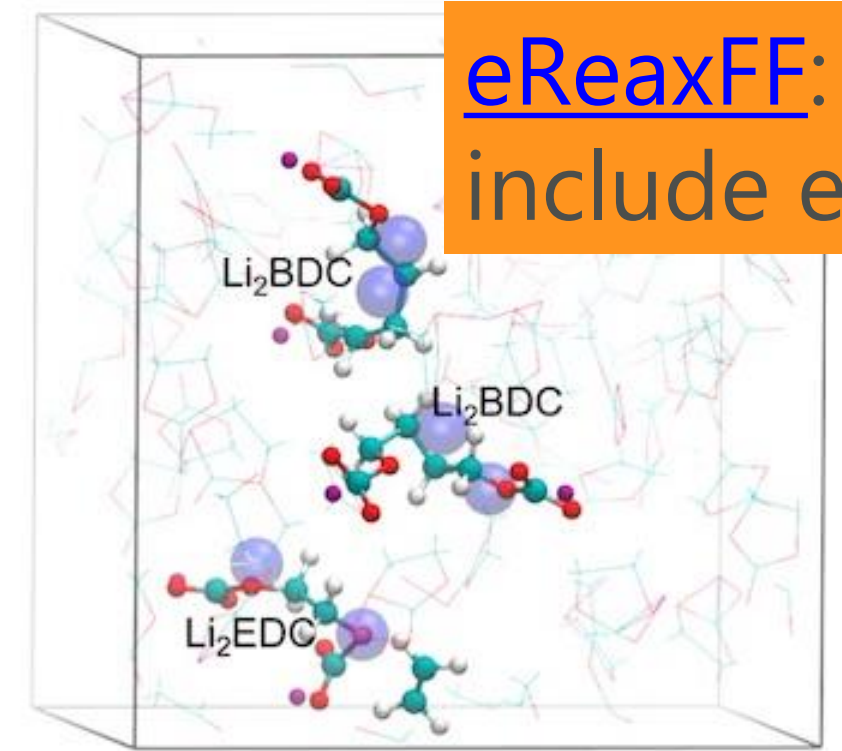
bond boost
build polymers



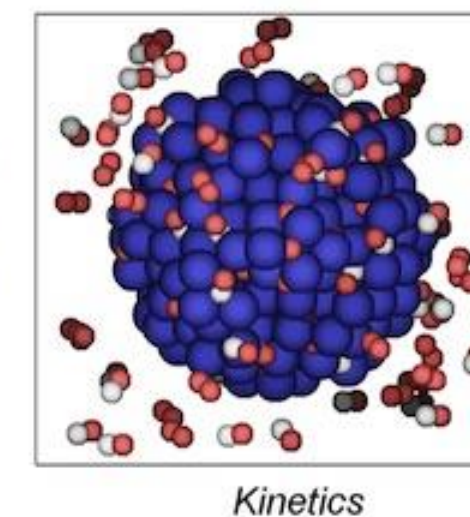
CMA-ES ReaxFF
force field
(re)parameterization



eReaxFF:
include e-



GCMC: speed
up thermo

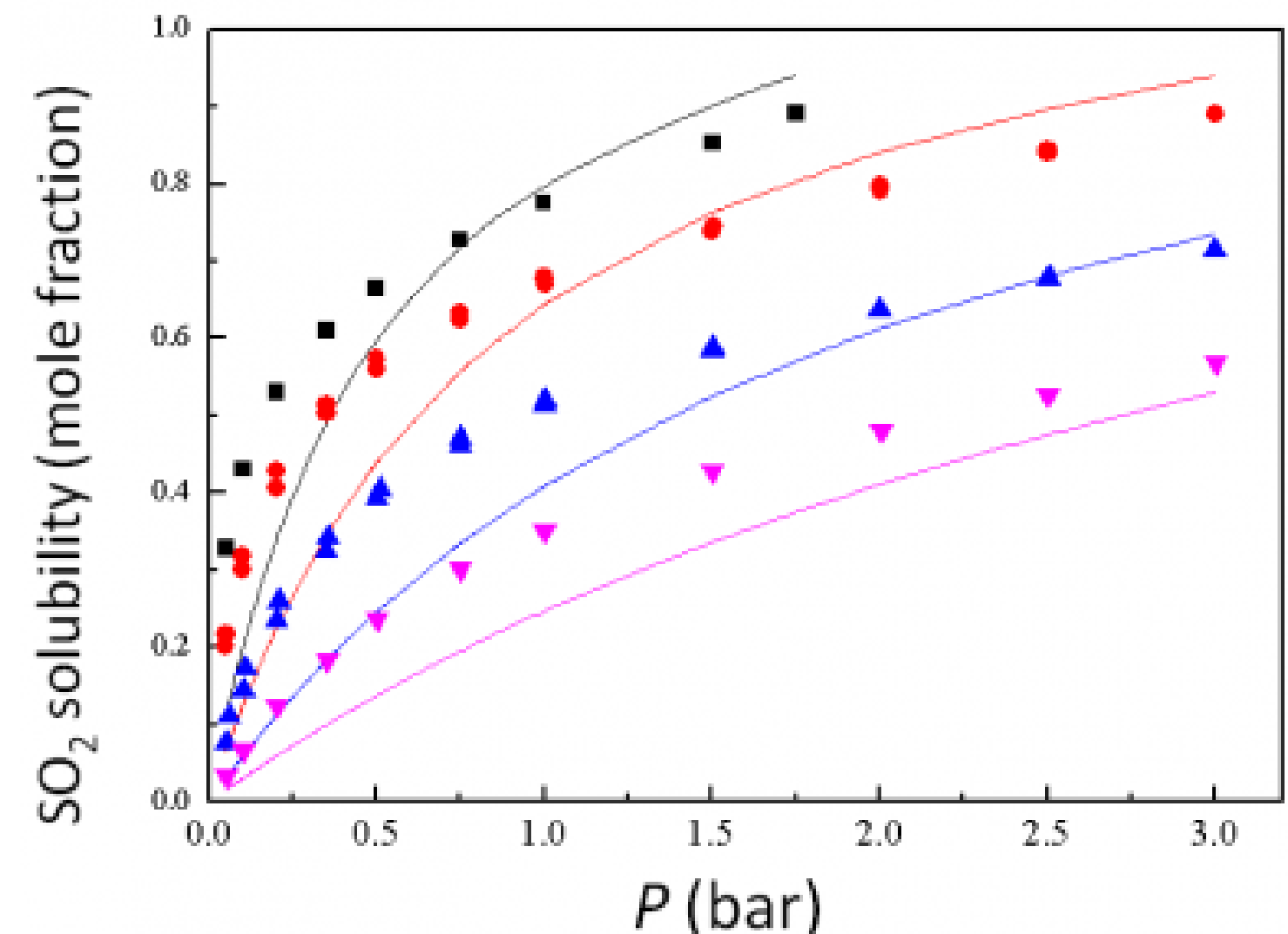
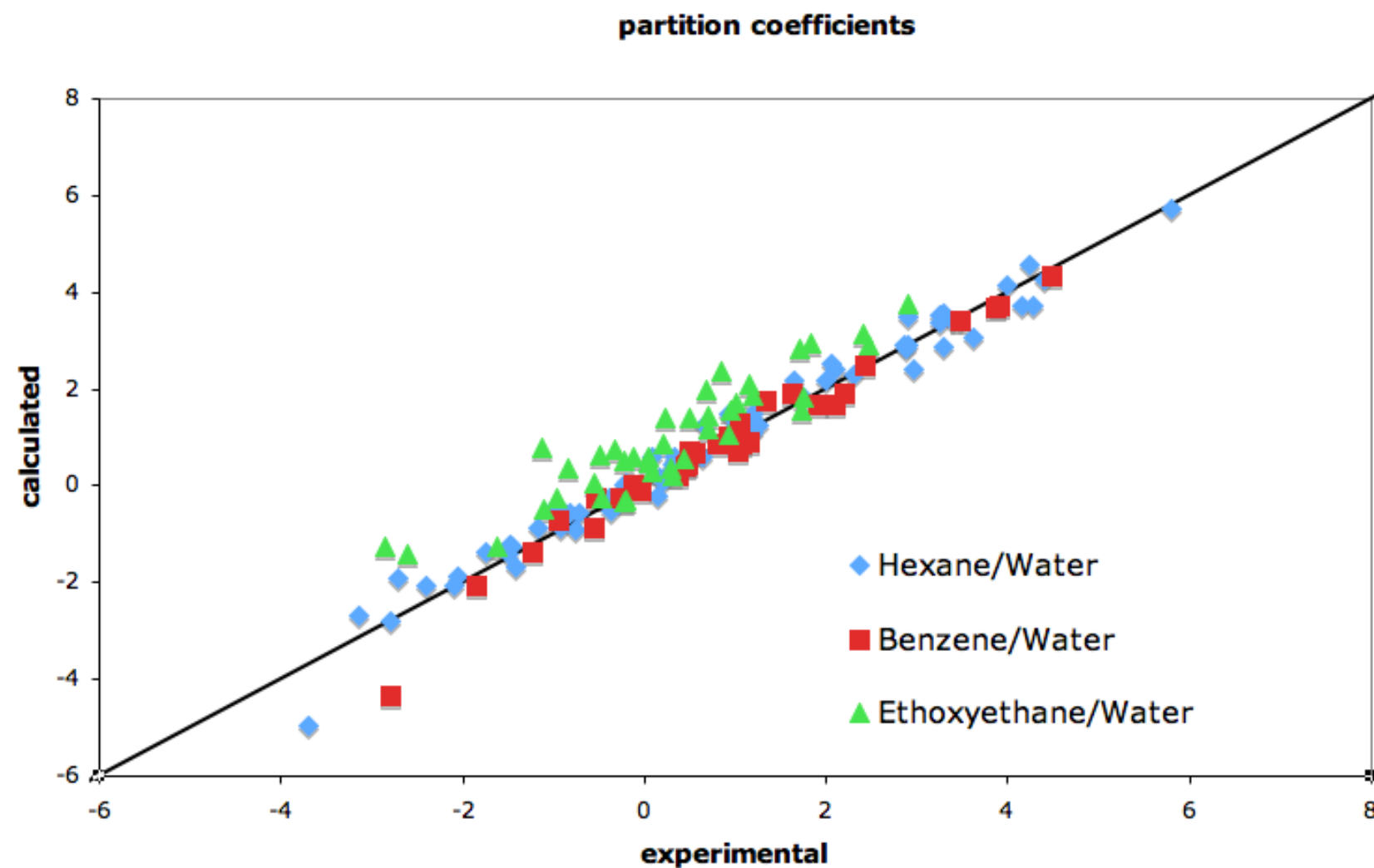
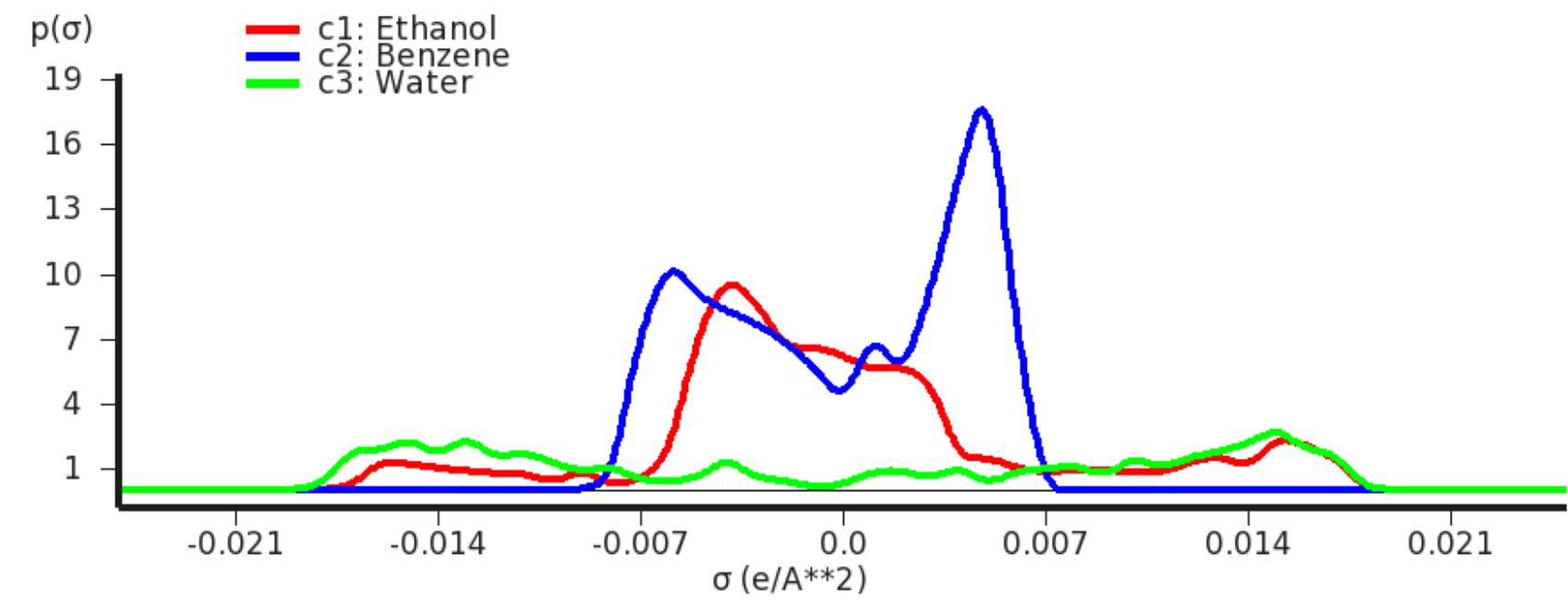


COSMO-RS/SAC: thermodynamic properties of fluids

Quantum Chemistry & QSPR for quick property predictions

COntinuum Solvation MOdel + RS (Klamt), SAC (Sandler)
chemical potential => activity coefficients => instantaneous properties

- Solvation & excess energies, pKa
- Solubilities, LLE, VLE, boiling points
- Optimize mixtures: solubility, LLE
- Polymers: Flory-Huggins X



New in AMS2020: ParAMS (dev)

- Build training sets with AMS
- Define cost function
- Optimize parameters
 - Lennard-Jones
 - ReaxFF
 - DFTB



[documentation](#)

