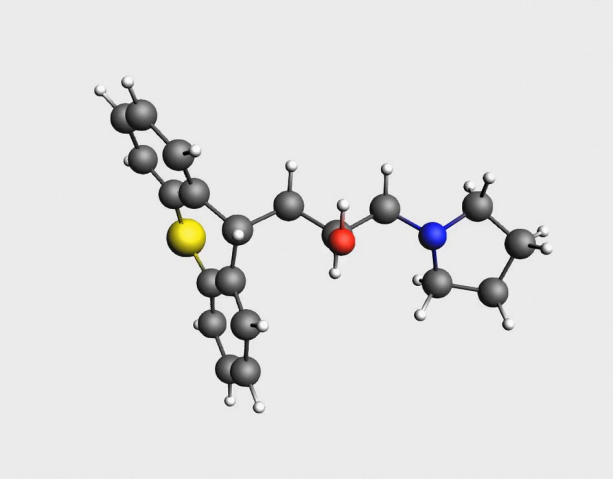
SCM
Software for Chemistry & Materials

Amsterdam Modeling Suite 2023

Making Computational Chemistry Work For You



Conformational search
CREST, any engine

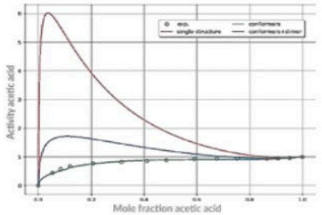
Matti Hellström, Product Manager

hellstrom@scm.com

Full release notes: www.scm.com/2023

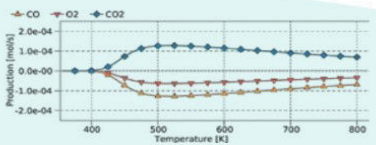
Amsterdam Modeling Suite: AMS

Continuum



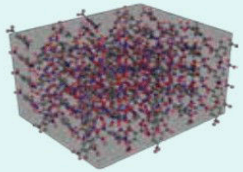
Fluid Thermodynamics
COSMO-RS
COSMO-SAC
UNIFAC

Mesoscale



Kinetics
Kinetic Monte Carlo
Microkinetics

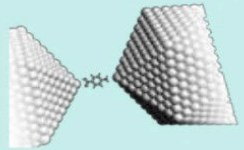
Materials



Force Fields
ReaxFF, GFN-FF
Machine Learning Potentials
Apple & P

QM/MM
FDE, Hybrid Engine

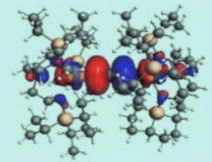
Nano



Tight binding
GFN-xTB, DFTB

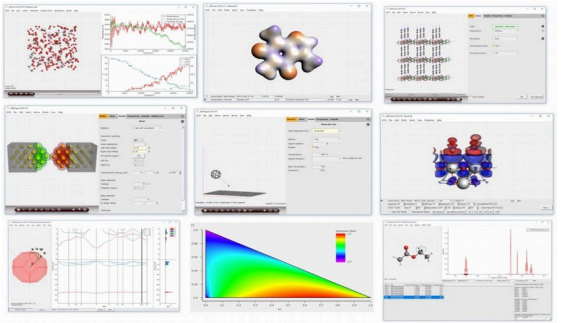
Periodic DFT
BAND, Quantum Espresso

Atomistic

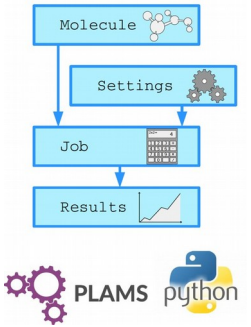


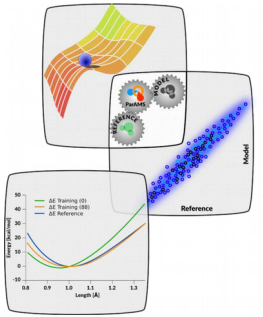
Molecular DFT
ADF

Graphical User Interface



Python scripting, workflows





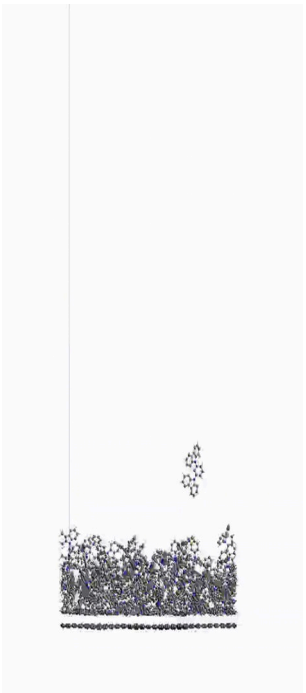
Outline

- Excitations and charge transport
- New methods/functionals in ADF
- M3GNet and ANI-2x machine learning potentials
- Conformers
- APPLE&P polarizable force field
- ACE Reaction Network
- Multiscale Modeling for Heterogeneous Catalysis
- ParAMS for ReaxFF/DFTB parametrization
- New engine: ASE calculators
- New engine: Quantum ESPRESSO (alpha)
- Python tips, PLAMS, Jupyter Lab

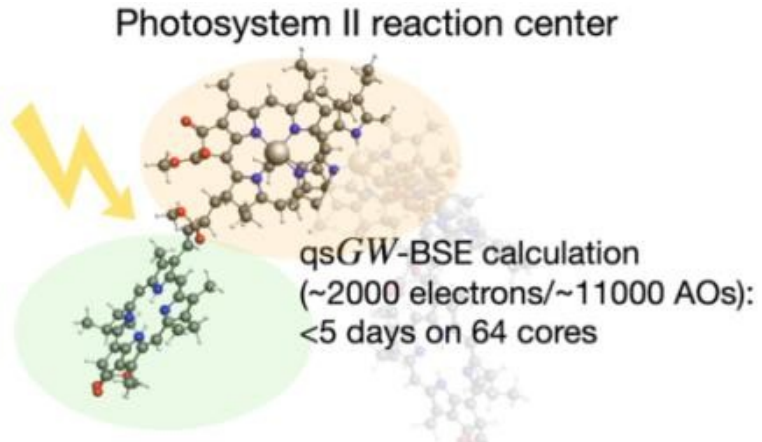
Full release notes: www.scm.com/2023

Excitations and charge transport

- OLED workflow “better and faster”
- GPU acceleration
- Ionization potentials
- Electron affinities
- Exciton energies



- Excitation energies with qsGW-BSE

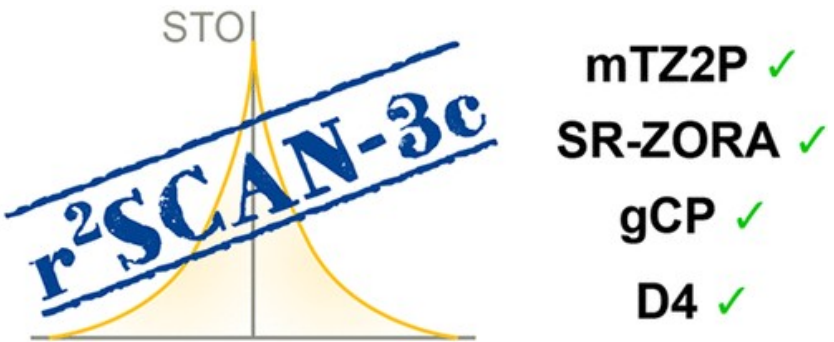


Arno Förster, Lucas Visscher
Quasiparticle Self-Consistent GW-Bethe–Salpeter Equation Calculations for Large Chromophoric Systems
J. Chem. Theory Comput. 2022, 18, 11, 6779–6793

Also with **spin-orbit coupling** (article in progress)

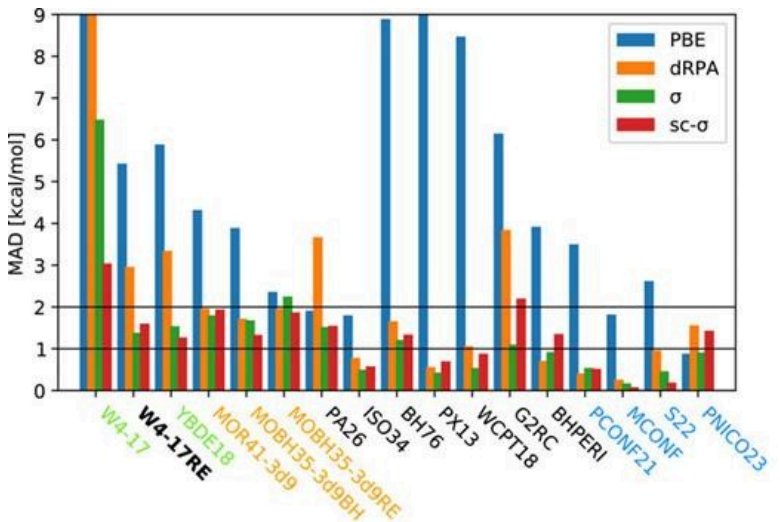
New methods/functionals in ADF

- r²SCAN-3c
  - "Reliable, robust, and accurate"
  - "on par with or more accurate than hybrid M06-2X-D3(0)/TZP"



T. Gasevic, J.B. Stückrath, S. Grimme, M. Bursch
Optimization of the r2SCAN-3c Composite Electronic-Structure Method for Use with Slater-Type Orbital Basis Sets
J. Phys. Chem. A 2022, 126, 23, 3826–3838

- Sigma functional
  - "accuracy of 1 kcal/mol in reaction or transition state energies"



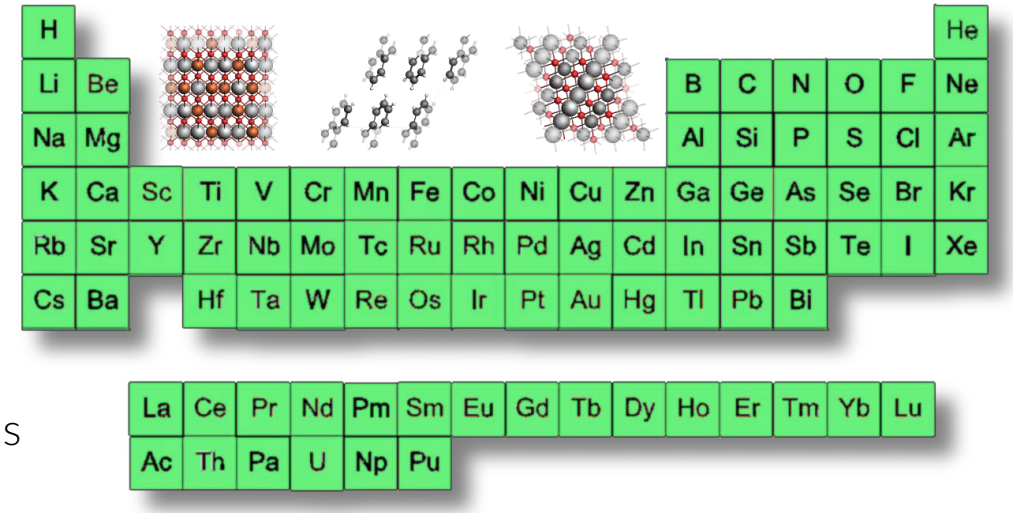
J. Erhard, S. Fauser, E. Trushin, A. Görling
Scaled σ-functionals for the Kohn–Sham correlation energy with scaling functions from the homogeneous electron gas
J. Chem. Phys. 157, 114105 (2022)

M3GNet Machine Learning Potential (1/2)

- Most of the periodic table
- Trained to Materials Project data
  - PBE and PBE+U
  - Can be combined with

    Grimme D3 or D4 dispersion corrections
- A “universal” potential for materials

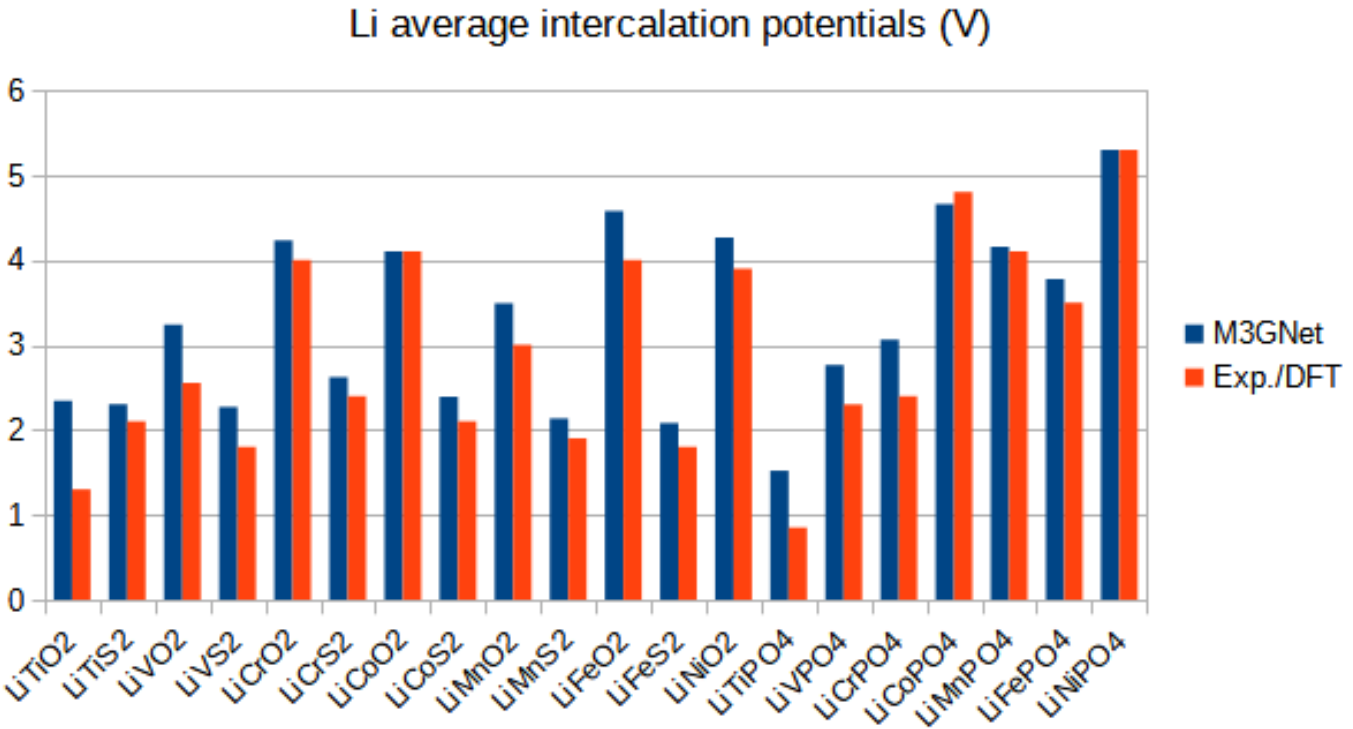
M3GNet-UP-2022 - ML-Potential for the periodic table



C. Chen, S.P. Ong.
A universal graph deep learning interatomic potential for the periodic table
Nat. Comput. Sci. 2, 718-728, (2022)

M3GNet Machine Learning Potential (2/2)

- Equilibrium structures
- Formation energies
- Phase stabilities
- Lattice optimizations
- ML: Do not blindly trust results!



Pre-trained ML Potentials in AMS

M3GNet-UP-2022
Materials
Phase stabilities
Reaction energies
H-Pu

A universal graph deep learning interatomic potential for the periodic table

Chi Chen & Shyue Ping Ong

Nature Computational Science **2**, 718–728 (2022) | Cite this article

ANI-2x
Drug-like molecules
Conformers
Reaction energies
H, C, O, N, F, S, Cl

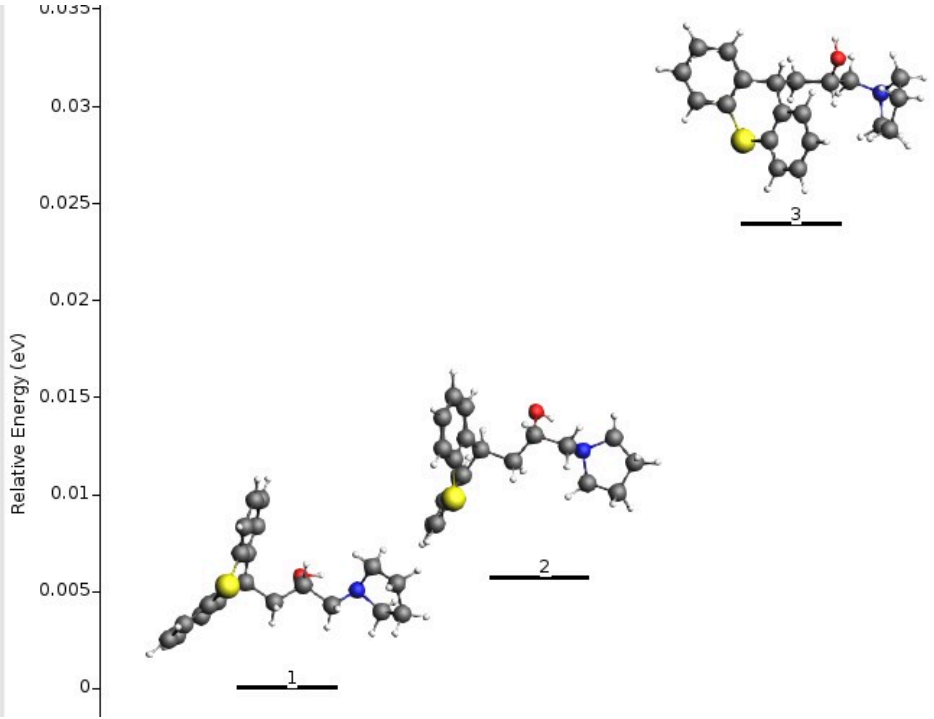
Extending the Applicability of the ANI Deep Learning Molecular Potential to Sulfur and Halogens

Christian Devereux, Justin S. Smith*, Kate K. Huddleston, Kipton Barros, Roman Zubatyuk, Olexandr Isayev*, and Adrian E. Roitberg*

Cite this: *J. Chem. Theory Comput.* 2020, 16, 7, 4192–4202
Publication Date: June 16, 2020
https://doi.org/10.1021/acs.jctc.0c00121

Conformers

- Generate with Rdkit (fast) or CREST (thorough)
- Use ANI-2x, GFN-FF, DFTB, ADF, or any other AMS methods to generate, optimize, and score conformers
- Calculate Boltzmann-averaged properties, for example IR spectra!

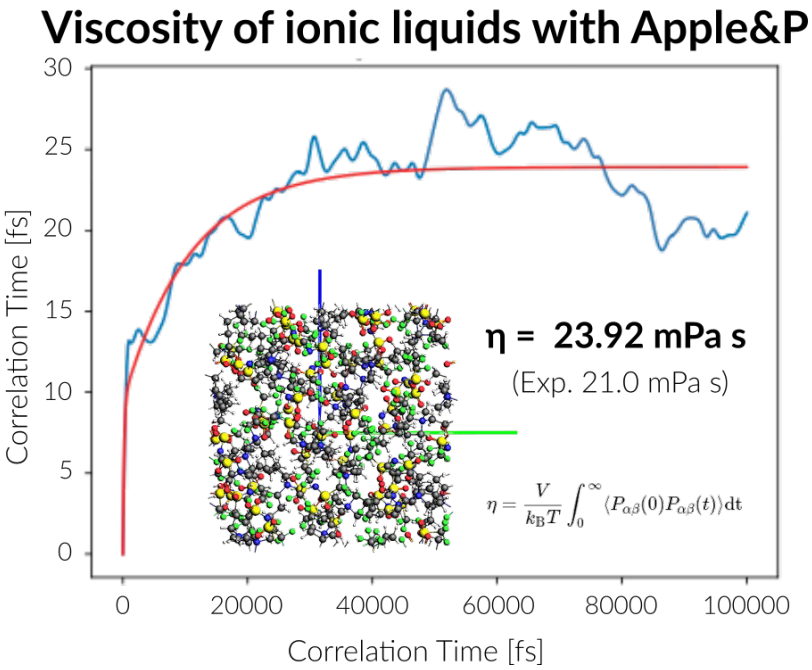


RDKit: Open-source cheminformatics; http://www.rdkit.org

P. Pracht, F. Bohle, S. Grimme.
Automated exploration of the low-energy chemical space with fast quantum chemical methods
Phys. Chem. Chem. Phys. 2020, 22(14):7169-7192

APPLE&P polarizable force field for electrolytes and polymers

- Collaboration with Wasatch Molecular Inc.
- Non-reactive
- Automatic atom typing
- Organic molecules: amides, esters, …
- Solvents: nitriles, carbonates, sulfones, …
- Cations: Li+, hydraziniums, pyrrolidiniums, …
- Anions: hydroxide, TFSI, …

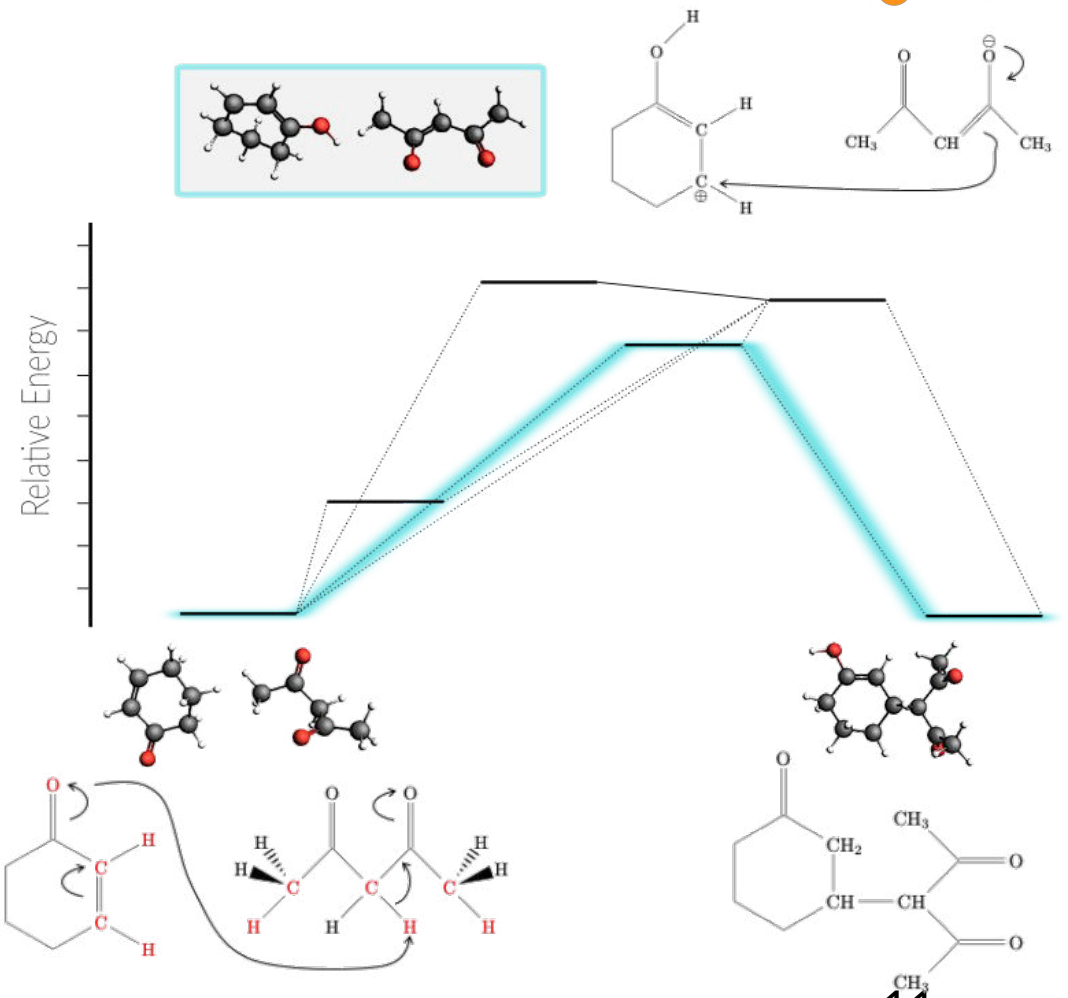


O. Borodin, J. Phys. Chem. B 113, 11463–11478 (2009)
and many subsequent publications

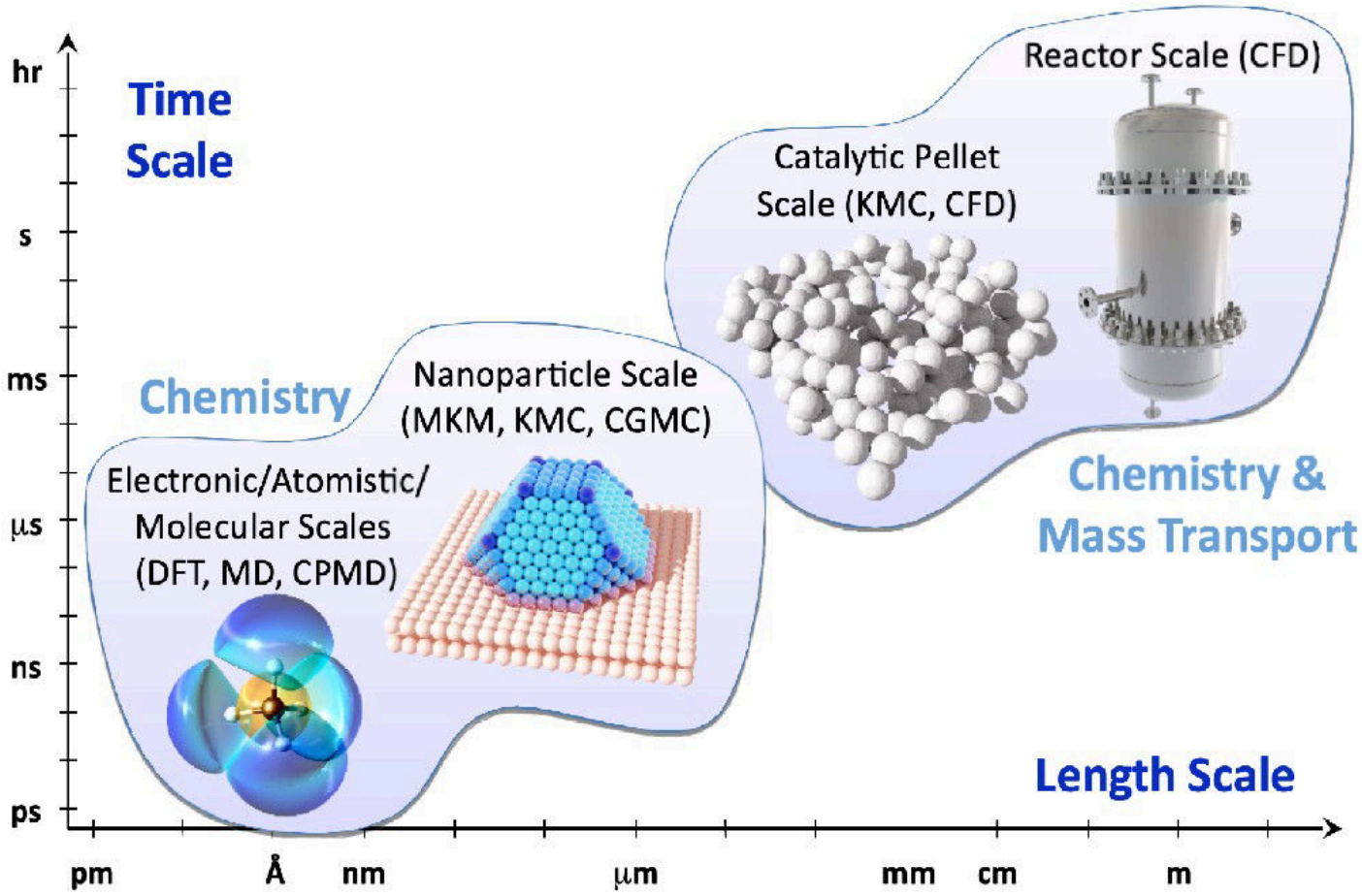
ACE Reaction Network

- Quickly generate and minimize reaction networks
- Find reaction mechanisms

Y. Kim, J.W. Kim, Z. Kim, W.Y. Kim,
Efficient Prediction of Reaction Paths through Molecular Graph and Reaction Network Analysis
Chem. Sci. 2018, 9, 825-835.

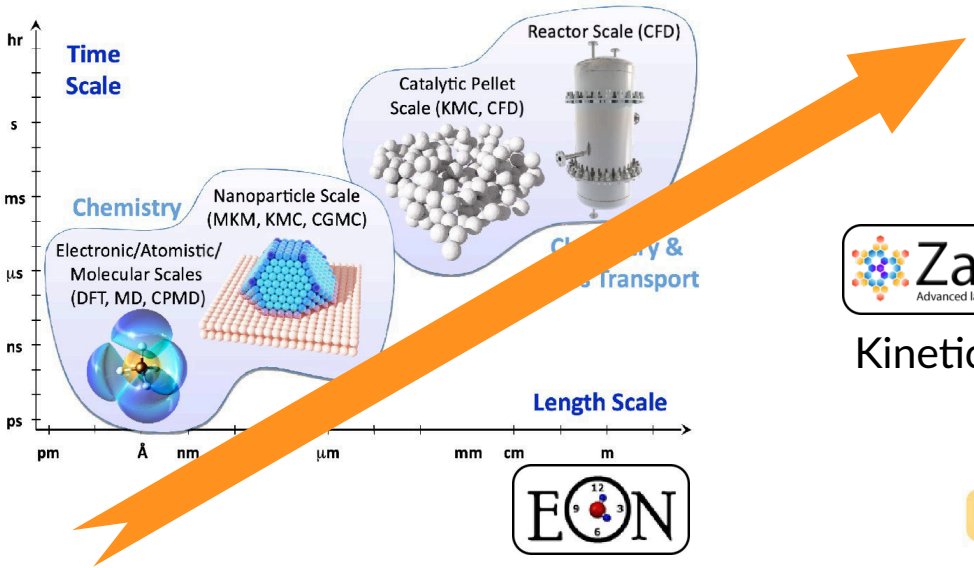


Multiscale Modeling for Heterogeneous Catalysis (1/2)



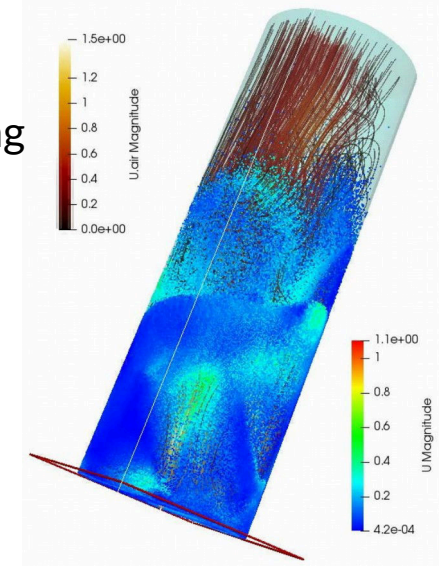
More information:
www.reaxpro.eu

Multiscale Modeling for Heterogeneous Catalysis (2/2)



CatalyticFOAM

Reactor modeling

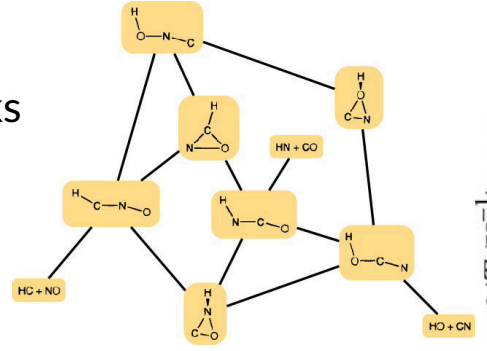


Zacros
Advanced lattice-KMC made easy

Kinetic Monte Carlo

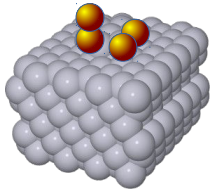
EON

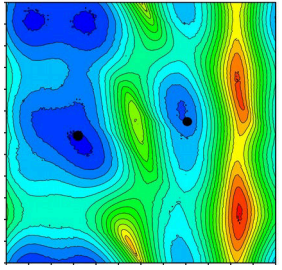
Reaction networks

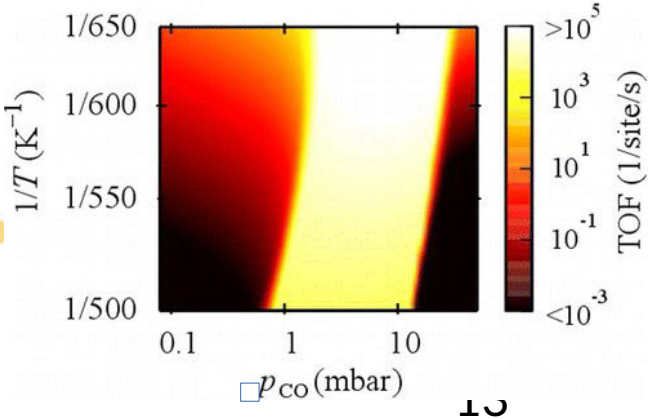


AMS driver

DFT & Force Fields







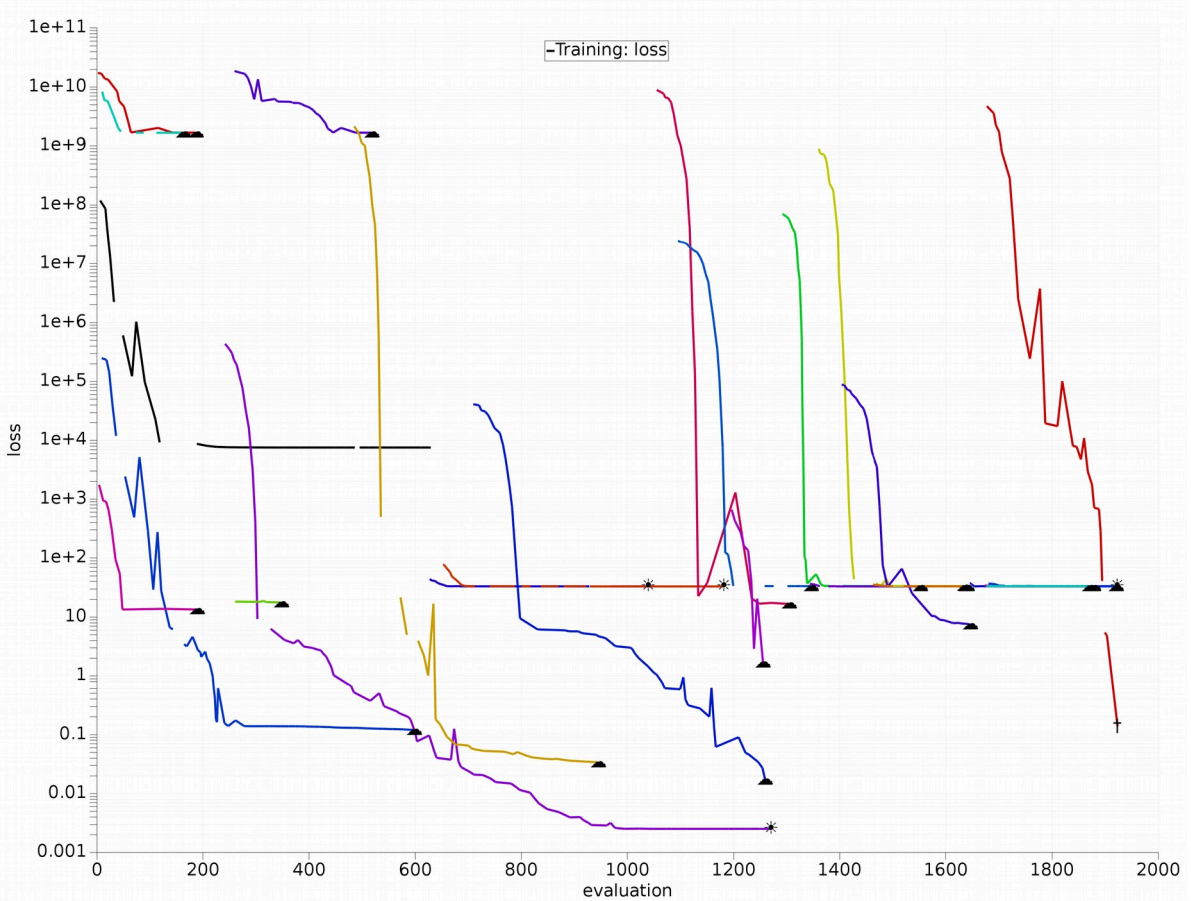
ParAMS for ReaxFF and DFTB parametrizations (1/2)

- Run and control

  multiple optimizers

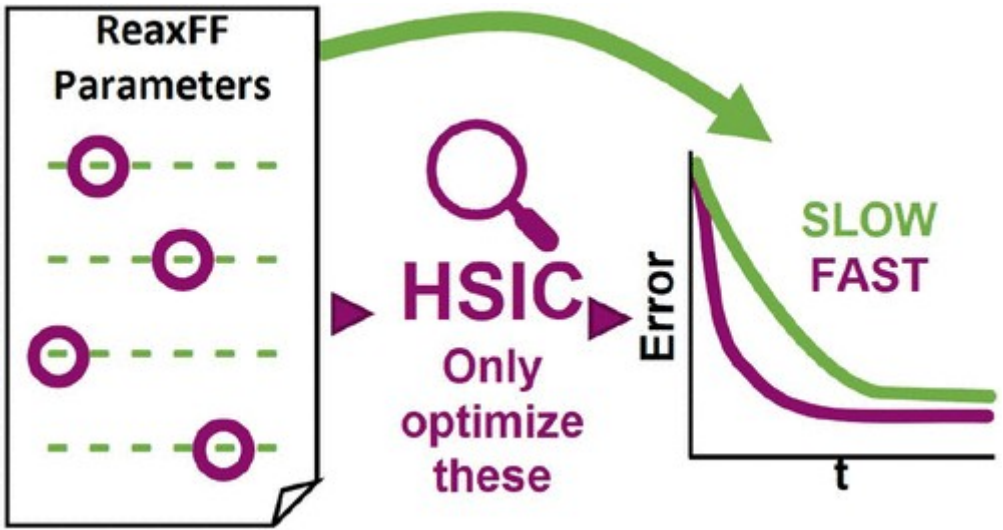
  in parallel

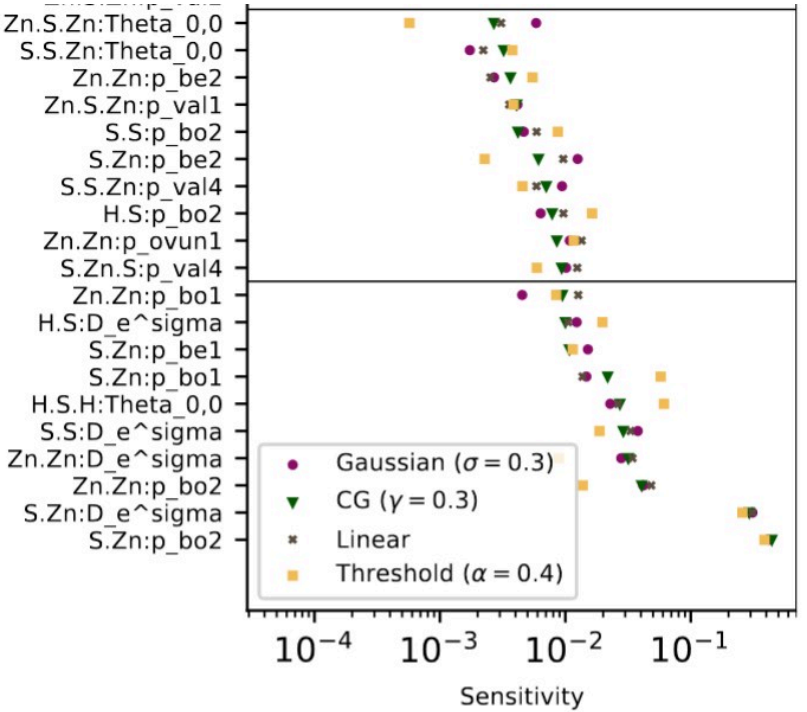
Freitas Gustavo, M., Verstraelen, T.
GloMPO (Globally Managed Parallel Optimization): A tool for expensive, black-box optimizations, application to ReaxFF reparameterizations.
J. Cheminform. 2022, 14, 7.



ParAMS for ReaxFF and DFTB parametrizations (2/2)

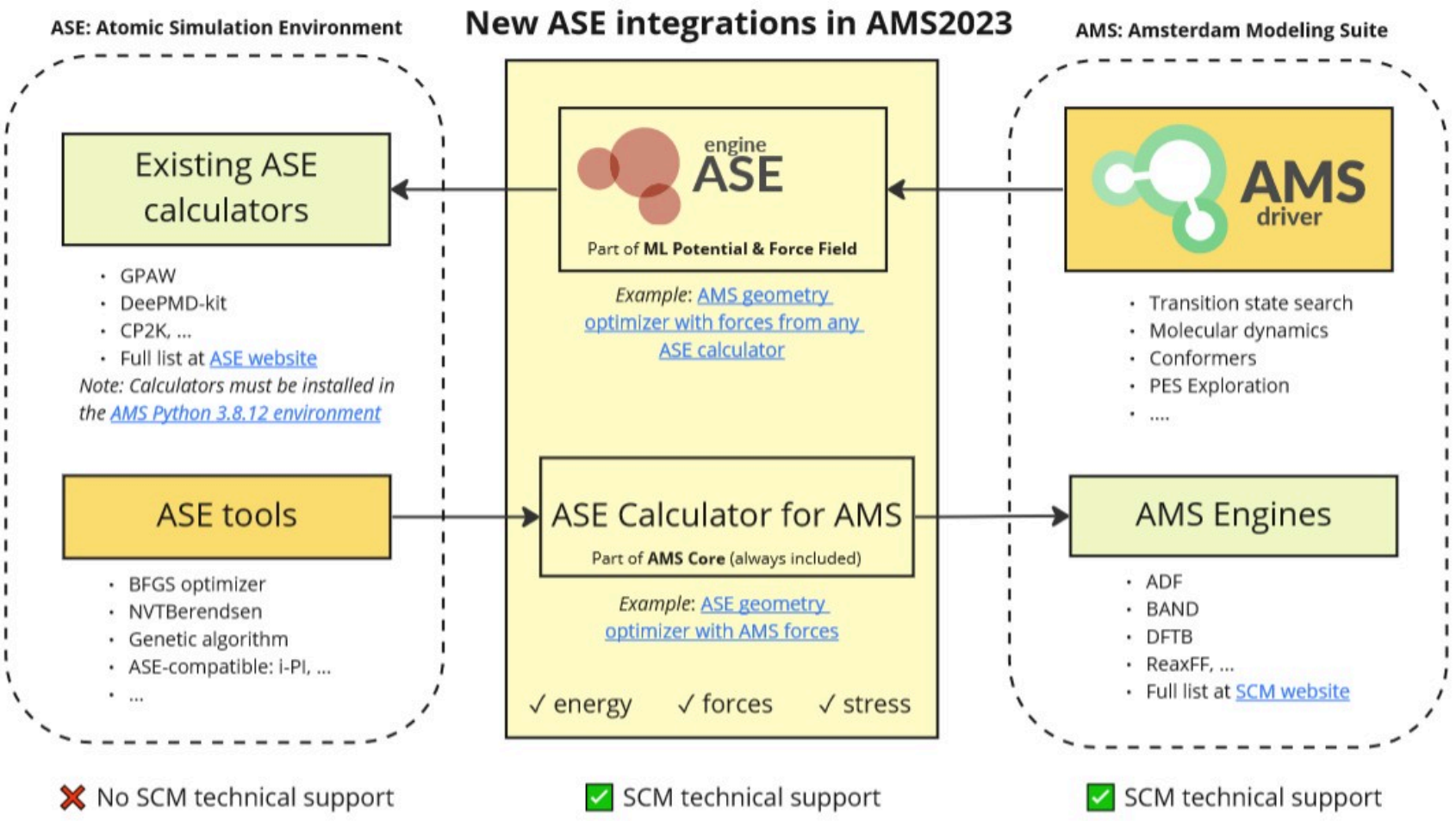
- Parameter sensitivity analysis





M.F. Gustavo, M. Hellström, T Verstraelen.
Sensitivity Analysis for ReaxFF Reparametrization Using the Hilbert–Schmidt Independence Criterion
J. Chem. Theory Comput. 2023, 19, 9, 2557–2573

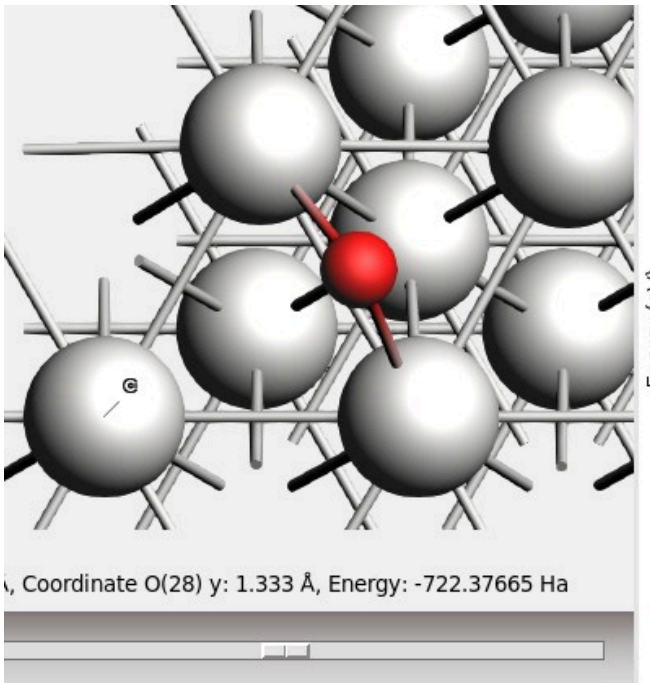
Atomic Simulation Environment (ASE) interface to/from AMS

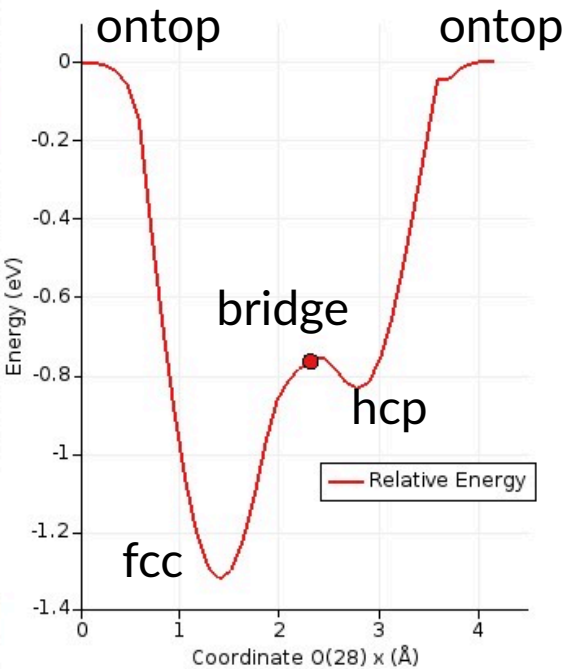


Quantum ESPRESSO (QE) as an AMS engine (alpha, command-line only)

- Expand QE functionality to all AMS Driver tasks
  - Transition state search
  - PES Scan
  - …
- For people who prefer QE. The above is also possible with BAND!

Example PES Scan: O atom diffusion on Pt(111)





Python tips, Jupyter Lab, PLAMS

- Install Jupyter Lab with package manager
- Build, show, and preoptimize structures
- Run simulations
- Plot results or launch AMSmovie

```
print('pure liquid with explicit number of molecules and exact density')
out = packmol(water, n_molecules=64, density=1.0)
printsummary(out)
out.write('water-3.xyz')
show(out)
```

```
pure liquid with explicit number of molecules and exact density
192 atoms, density = 1.000 g/cm^3, box = 12.417, 12.417, 12.417, formula = H128O64
```

Licensing for AMS2023

Functionality	License
OLED workflow	ADF + DFTB + Workflows
qsGW-BSE, r2SCAN-3c, sigma functional	ADF
M3GNet, ANI-2x	MLPot&FF
Conformers	engine
APPLE&P	MLPot&FF + special
ACE Reaction	Workflows (+engine)
Zacros	Workflows + special

Functionality	License
ParAMS	Workflows + engine
ASE Engine	MLPot&FF
ASE Calculator for AMS	engine
Quantum ESPRESSO (AMS Engine)	BAND
Quantum ESPRESSO (standalone)	any
Jupyter Lab, PLAMS	any

Academic collaborators, partners, and contributors for AMS2023

- Woo Youn Kim (Korea Advanced Institute of Science & Technology): ACE-Reaction
- Christine Aikens (Kansas State University): TD-DFT+TB gradients
- Artur Michalak (Jagiellonian University): NOCV functionality
- Mauro Stener (Trieste University): POLTDDFT
- Jochen Autschbach (University at Buffalo): CD with spin-orbit
- Laurent Joubert (Rouen Normandy University): QTAIM additions
- Martin Kaupp (Berlin Institute of Technology): 3D-RISM entropy
- Shyue Ping Ong (University of California San Diego): M3GNet
- Kai Leonhard (RWTH Aachen), ChemTraYzer
- Toon Verstraelen (Ghent University), ParAMS
- Stefan Grimme (Bonn University): r2SCAN-3c, CREST
- Arno Förster, Lucas Visscher (VU Amsterdam): BSE
- Hannes Jónsson (University of Iceland), EON
- Michail Stamatakis (University College London), Zacros
- Mauro Bracconi, Matteo Maestri (Polytechnic University of Milan): CatalyticFOAM

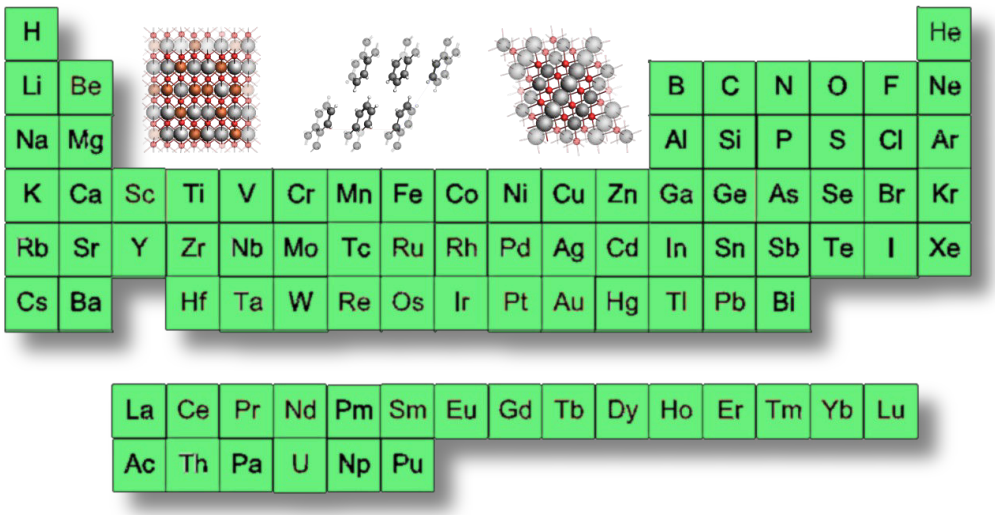
... and many more!

Summary

- AMS2023 released in April, 2023
- Highlights
  - M3GNet universal ML potential
  - APPLE&P polarizable force field
  - qsGW-BSE excitations
  - ParAMS multiple optimizers + sensitivity
  - … and much more!

Full release notes: www.scm.com/2023

M3GNet-UP-2022 - ML-Potential for the periodic table



The End

- Thank you for your attention!
- Release notes: www.scm.com/2023
- Free trial: www.scm.com/free-trial
- YouTube: webinars, tip of the week, ...:

  www.youtube.com/c/AmsterdamDensityFunctional
- Questions?