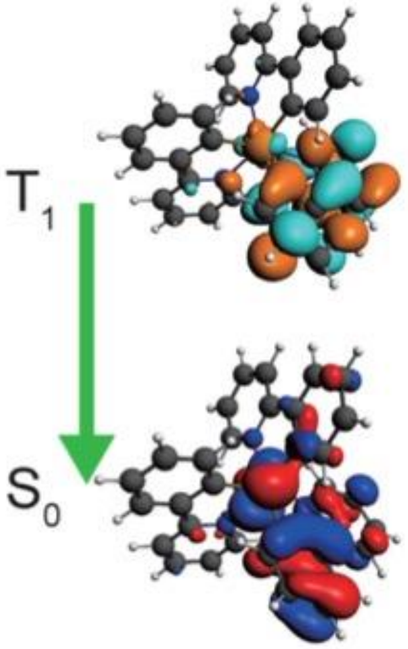
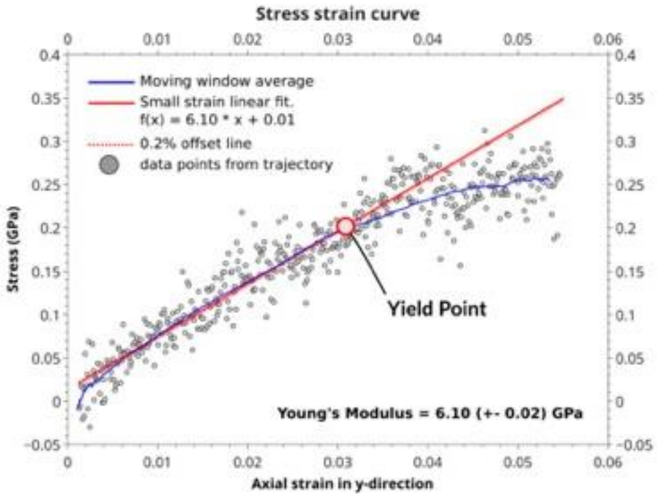
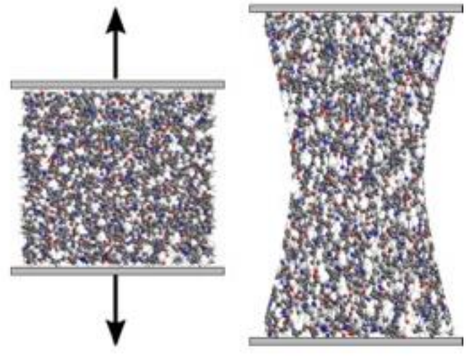
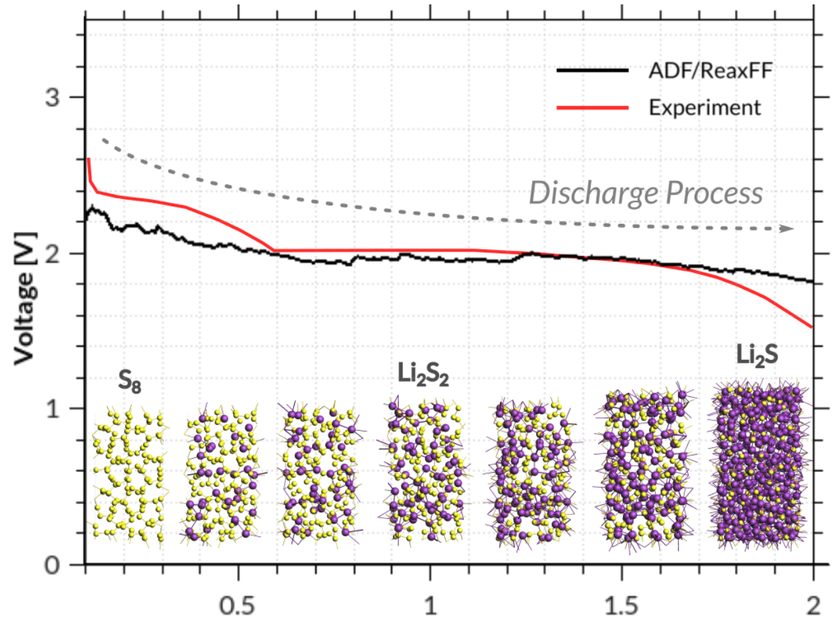
Amsterdam Modeling Suite

Accelerating Chemistry & Materials Research









SCM
Software for Chemistry & Materials

Fedor Goumans, Chief Customer Officer, goumans@scm.com

Seminar / workshop with T&J, Seoul, 19 October 2023 www.scm.com/Korea23

Program

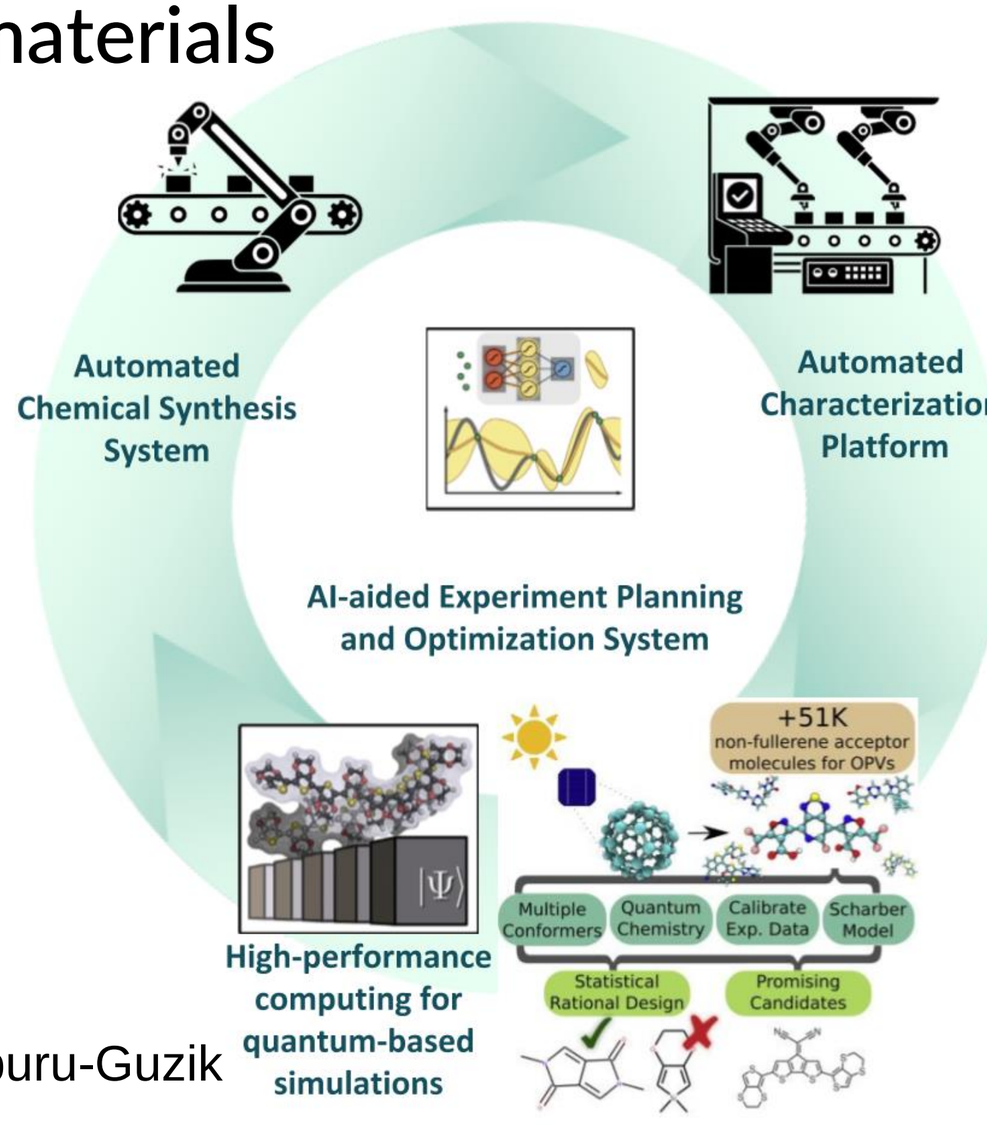
- Motivation, history, background SCM & intro Amsterdam Modeling Suite
- Parametrization of ReaxFF and DFTB with ParAMS
- Modeling OLED materials
  - accurate ionization potentials, electron affinities, and UV/VIS with GW+BSE
  - multiscale device-level modeling
- Modeling battery materials
  - Redox potentials with DFTB, ADF & COSMO-RS
  - Diffusion barriers with the new M3GNet universal ML potential
- Reaction discovery tools
- Other new and upcoming developments in AMS
  - Active learning (on-the-fly ML potentials)
- Files, slides, available to download from: www.scm.com/Korea23

New materials discovery too slow

- 8-19 years to develop materials solutions in new markets
- 80-85% R&D programs fail
- >50% R&D spending only incremental improvement
- **Catch 22**: slow discovery ⇔ few new materials

https://www.mckinsey.com/industries/chemicals/our-insights/chemical-innovation-an-investment-for-the-ages

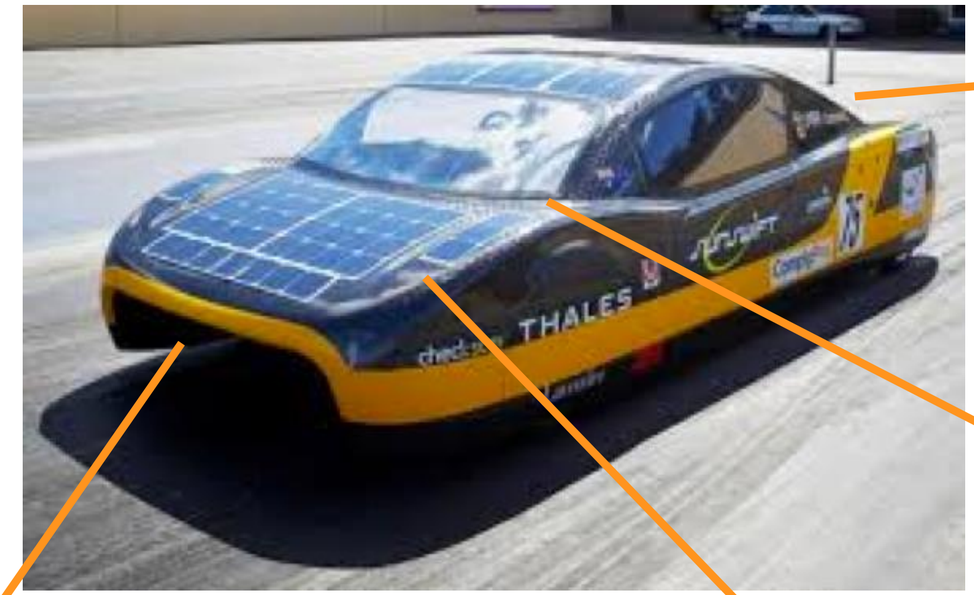
Simulations -> predict new materials
Robots -> make new materials
AI -> improve simulations and DOE



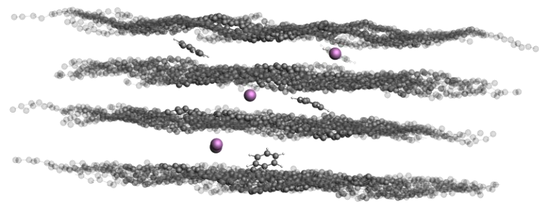
the Matter Lab - Aspuru-Guzik

Bottom up Property Prediction

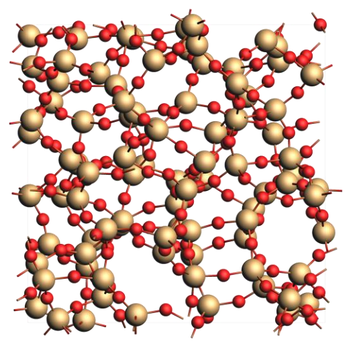
Properties are determined at the atomistic level => predict, understand & improve through modeling



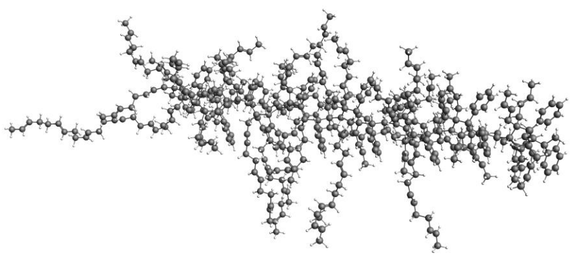
Batteries: fast recharge, high capacity

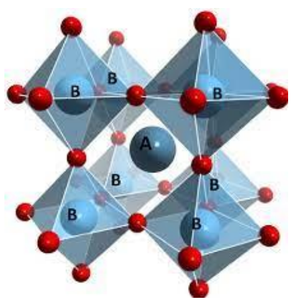


Chassis: light & durable, coating
Glass: optical properties, electronics



Tires: Reduce wear &friction

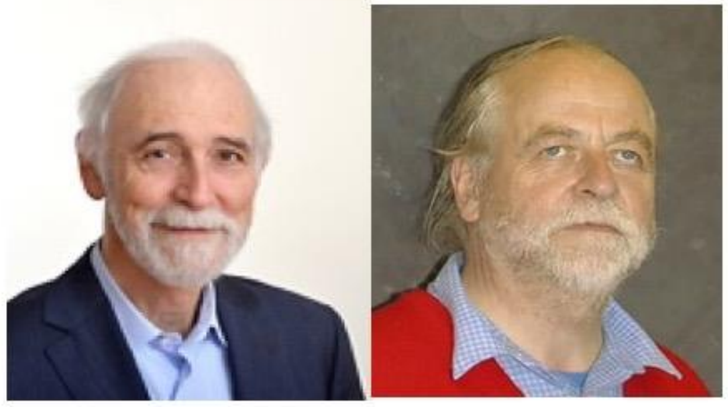


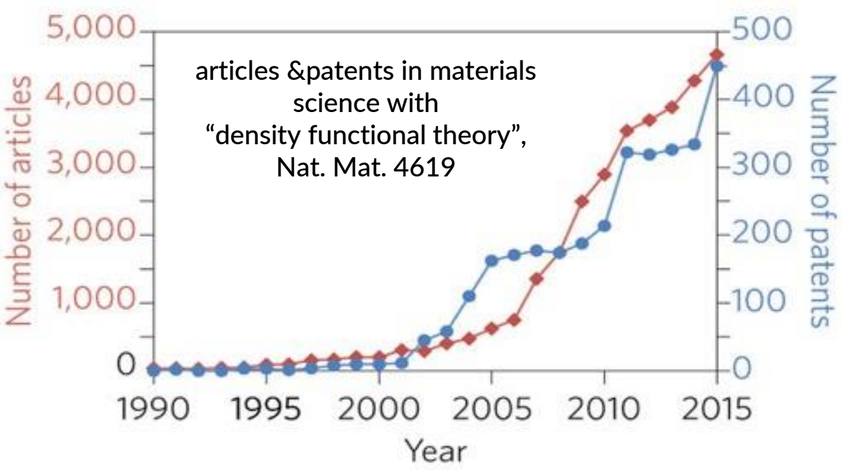


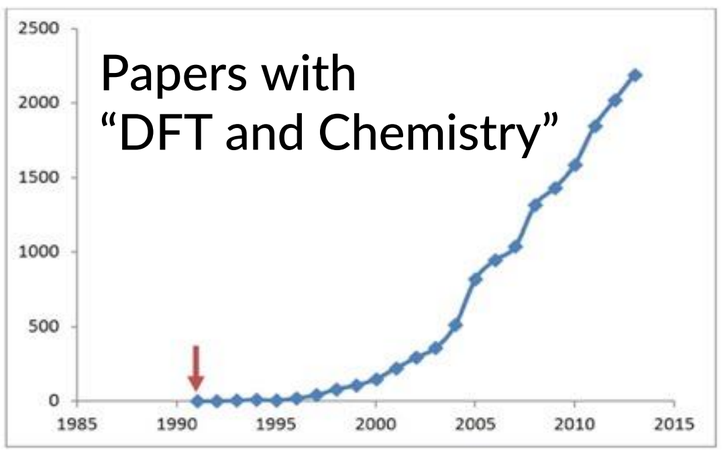
Solar cells: long lifetime & high efficiency

Background: SCM, ADF & AMS

- **ADF: first DFT code to understand chemistry (1970s)**
  Baerends@VU (>'73), Ziegler@Calgary(+) (>'75)
- **1980s: support from Mitsui, Shell, Akzo, Unilever**
- **SCM: Spin-off company 1995**
- **2010s: DFTB, ReaxFF, COSMO-RS (Albemarle, DSM)**
- **2019: Multi-scale: ReaxPro (BASF, Dow, Shell, JM)**
- **29 people (21 senior PhD's) + 2 EU fellows**
- **Many academic collaborators & EU networks**
- **SCM: development, debug, port, optimize, & support**







The SCM team in Amsterdam

Prof. Evert Jan Baerends
Founder and Scientific Adviser

Dr. Stan van Gisbergen
CEO

Mrs. Kitty Kleinlein
Office Manager

Mrs. Sorana Burcusel
Custom Support Officer

Dr. Fedor Goumans
Chief Customer Officer

Dr. Robert Rüger
Software Architect

Dr. Nicolas Onofrio
Technical Sales Representative

Dr. Maria Aliaga
Technical Sales Representative

Dr. Ole Carstensen
Application Engineer

Dr. Sergio López López
Scientific Partner Manager

Dr. Matti Hellström
Product Manager

Dr. Nick Austin
Software Developer

Dr. Franco Egidi
Software Developer

Dr. Olivier Visser
Software Developer

M. Sc. Laurens Groot
Software Developer

Dr. Erik van Lenthe
Software Developer

Dr. Alexei Yakovlev
Software Developer

Dr. Rosa Bulo
Software Developer

M. Sc. Mirko Franchini
Software Developer

Dr. Pier Philipsen
Software Developer

Dr. Tomáš Trnka
Software Developer

Dr. Nestor Aguirre
Software Developer

M. Sc. Hans van Schoot
Software Developer

Dr. Wei-Lin Chen
Software Developer

Dr. Paul Spiering
Software Developer

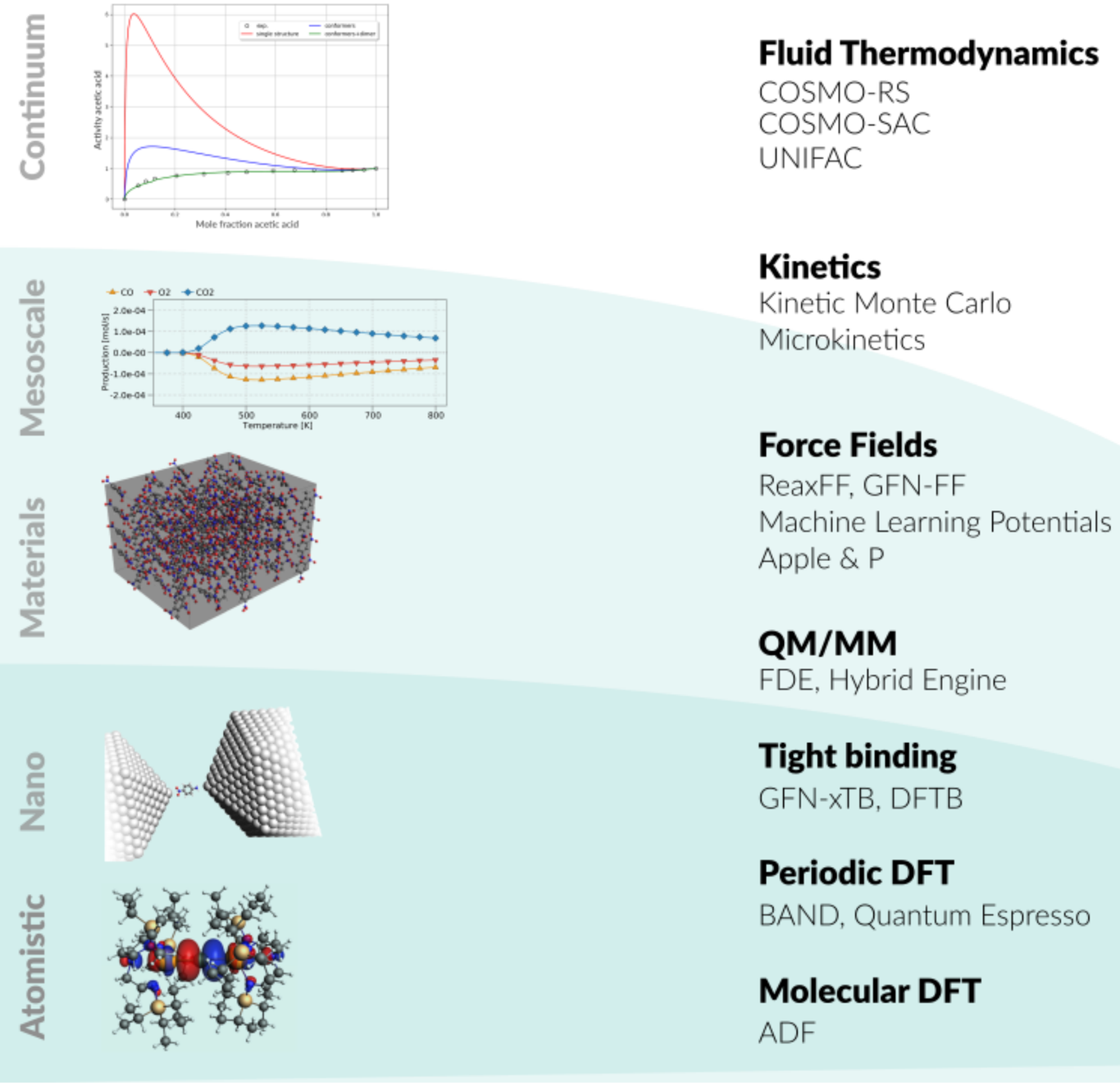
Dr. Bas Rustenburg
Software Developer

M. Sc. Edoardo Spadetto
EU Fellow

M. Sc. Giulio Benedini
EU Fellow

Amsterdam Modeling Suite

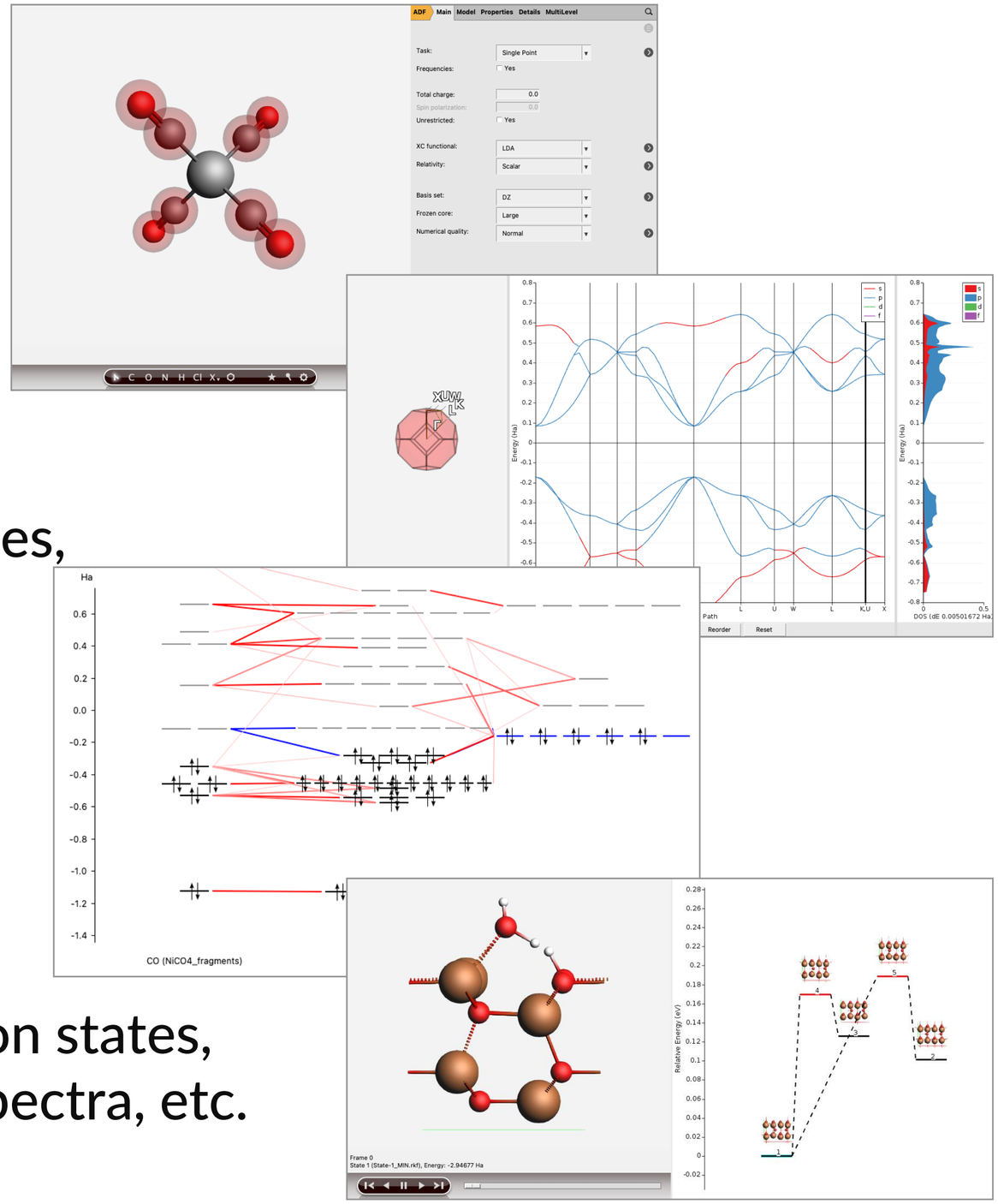
- ADF: powerful molecular DFT
  - Reactivity, spectroscopy
  - Spectroscopy: NMR, EPR, VCD, UV, XAS
- BAND: periodic DFT
  - (2D) Materials, spectroscopy, analysis
  - Interface with QE, VASP
- DFTB, MOPAC: fast electronic structure
- ReaxFF: Reactive MD
  - Dynamics of large complicated systems
- MLPotential, force fields
  - Several backends, ANI-2x, M3GNet
- COSMO-RS: fluid thermodynamics
  - VLE, LLE, logP, solubility
- **AMSdriver**: PES exploration, MD, MC
  - Hybrid: multi-layer, QM/MM, QM/QM'
- Integrated **GUI**, **python scripting**
- **ParAMS**: parametrize ReaxFF & xTB



The graphical user interface (GUI)

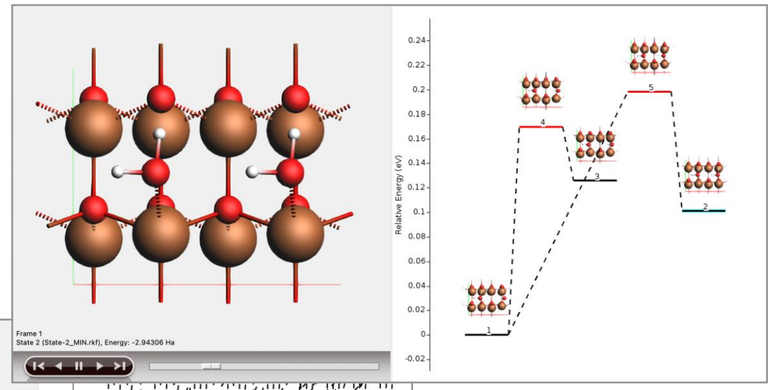
Setup & analyze calculations

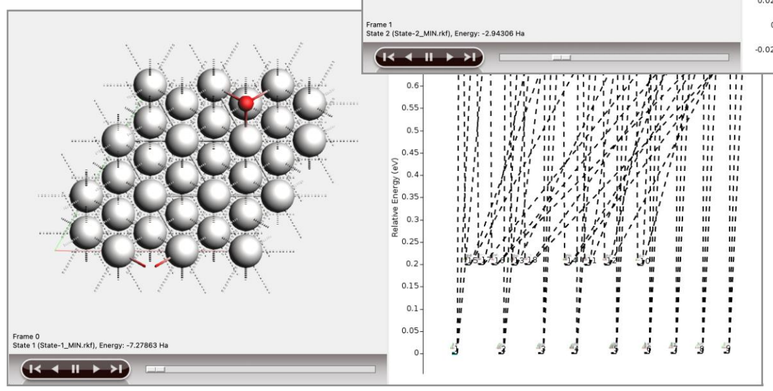
- AMSjobs
  - manage jobs, locally or remotely
  - extract summaries
- AMSinput
  - build molecules, periodic systems, surfaces, polymers, etc.
  - import structures from many formats
- AMSview, AMSlevels, AMSspectra, etc.
  - analyze results
  - visualize trajectories, structures, transition states, orbital densities, DOS, band structure, spectra, etc.



AMS driver: MD with ‘anything’

A unified driver to explore the Potential Energy Surface (PES)





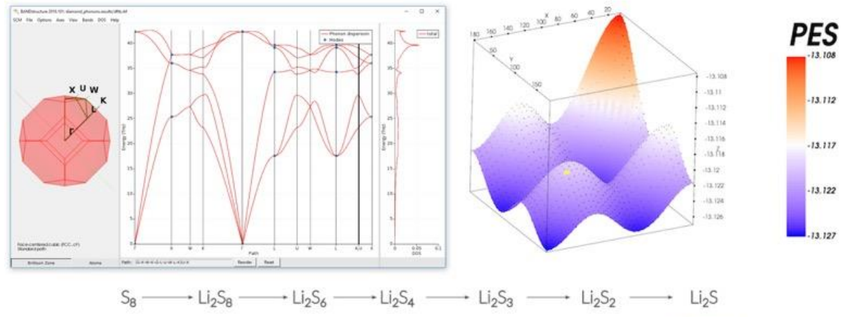
Tasks

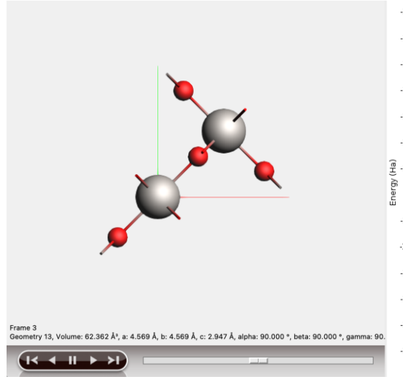
- Molecular dynamics
- Frequencies & phonons
- Stress & elastic tensors
- Scan coordinates & constraints
- Monte Carlo, etc.
- Reaction discovery

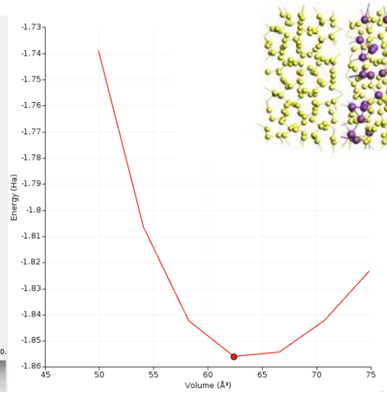
AMS driver

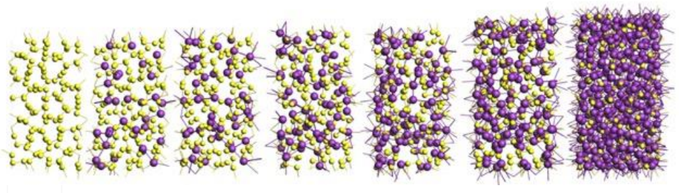
Engines

- ADF
- BAND
- DFTB
- ReaxFF
- MLP, FF
- External

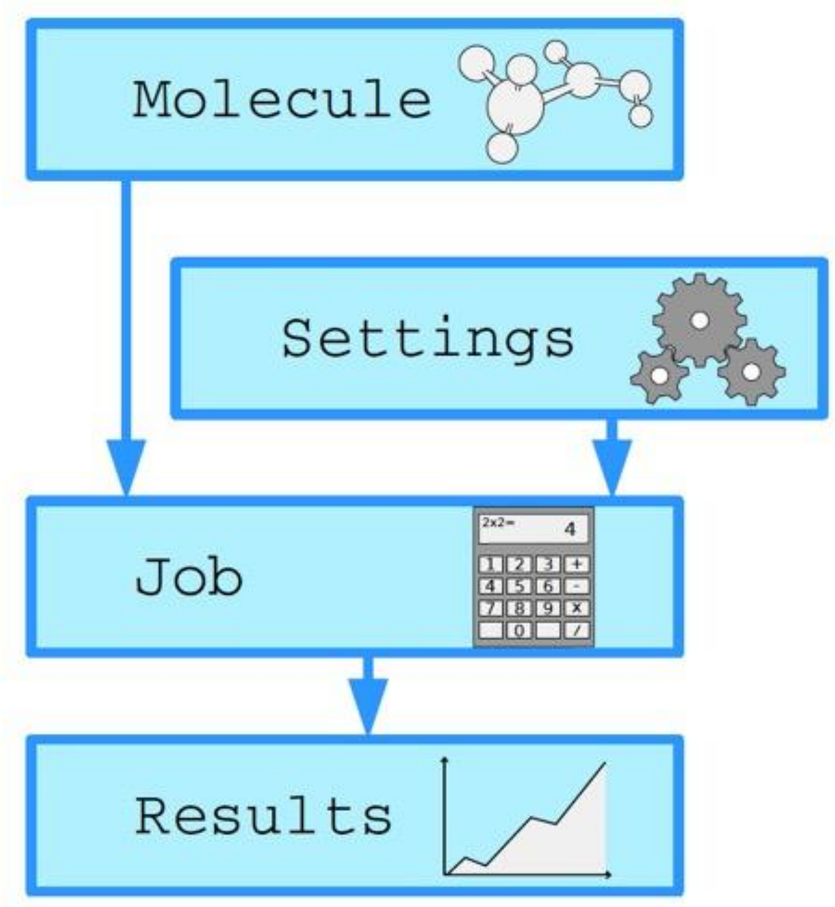








PLAMS: python scripting

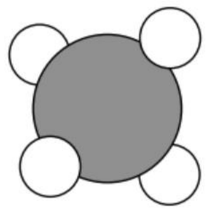


PLAMS python

Create a box of methane

First, create a gasphase methane molecule:

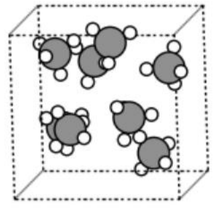
```
single_molecule = from_smiles('C', forcefield='uff') # or use Molecule('your-own-file.xyz')
show(single_molecule)
```



You can easily create a box with a liquid or gas of a given density. For more advanced options, see the Packmol example.

```
box = packmol(
    single_molecule,
    n_molecules=8,
    region_names='methane',
    density=0.4, # g/cm^3
)
print("Lattice vectors of the box:\n{}".format(box.lattice))
show(box)
```

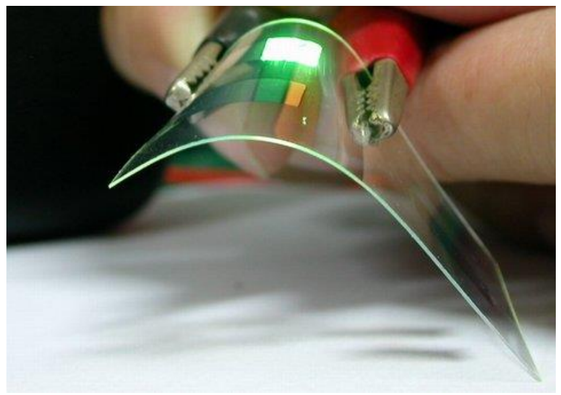
```
Lattice vectors of the box:
[[8.106820570931148, 0.0, 0.0], [0.0, 8.106820570931148, 0.0], [0.0, 0.0, 8.106820570931148]]
```



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

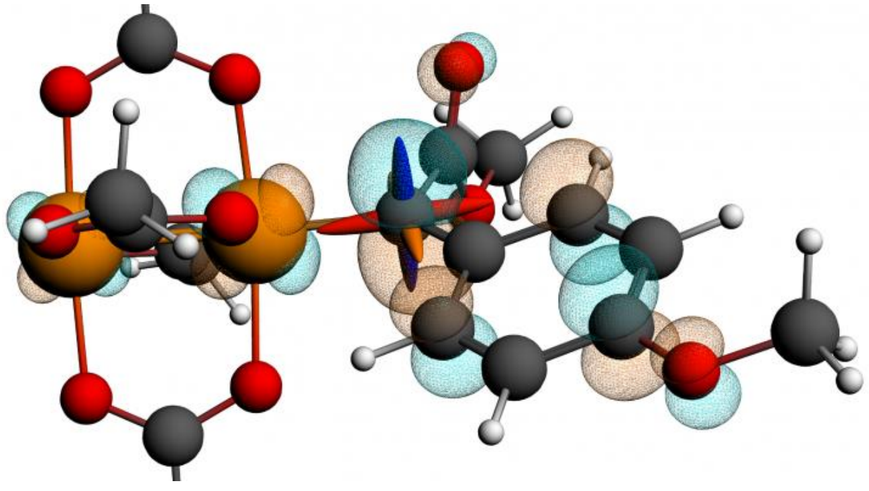
ADF: Molecular DFT

Organic electronics



Strong & unique points

- All-electron Slaters, H-Og
- Relativity: ZORA (SR, **SOC**)
- Spectroscopy
  - EPR, NMR, IR (VCD), UVVIS, XAS
  - qsGW+BSE
  - Phosphorescence

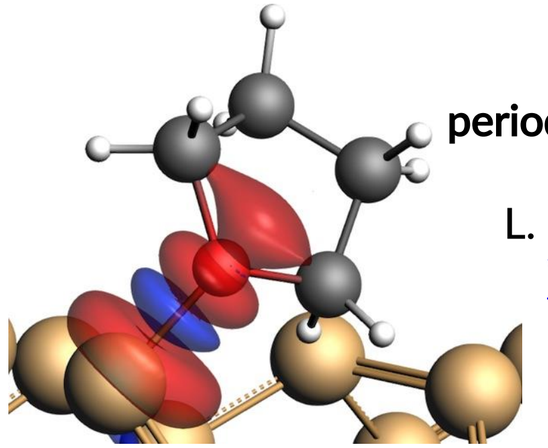


NMR calculations locate ^{13}C di-Rh carbene catalyst intermediate, Science, **342**, 351 (2013)

- Bonding analysis:
  - Fragment-based approach
  - ETS-NOCV, QTAIM, MO diagrams, NCI, ...
  - Transfer integrals (charge mobility)
- Environments
  - Subsystem DFT (FDE), DIM/QM, QM/MM, QM/FQ, 3D-RISM, COSMO, SM12

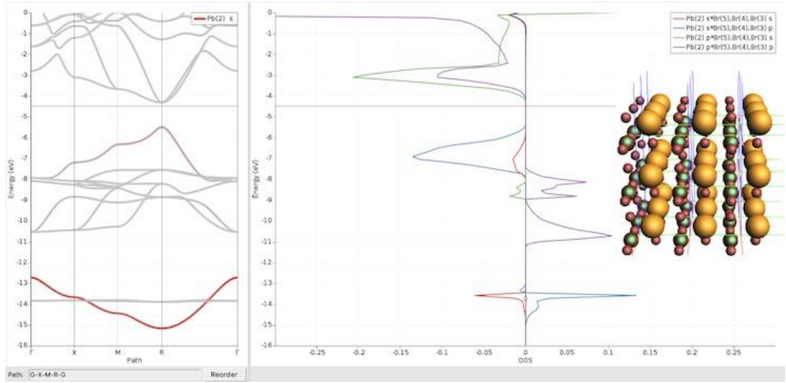
Periodic DFT: BAND vs Plane Waves

- Atom centered basis functions, STO or NAO
  - Compare cluster with periodic
  - No pseudopotentials, all elements
  - Core spectroscopy (core holes)
  - Dielectric function, refractive index, susceptibility
  - Easy orbital **analysis:** pDOS, COOP, EDA
  - xc: r2SCAN, MN15-L, HSE06, GLLB-sc, D3(BJ), D4, DFT-1/2
  - Self-consistent NEGF: Gate & bias potential, spin transport



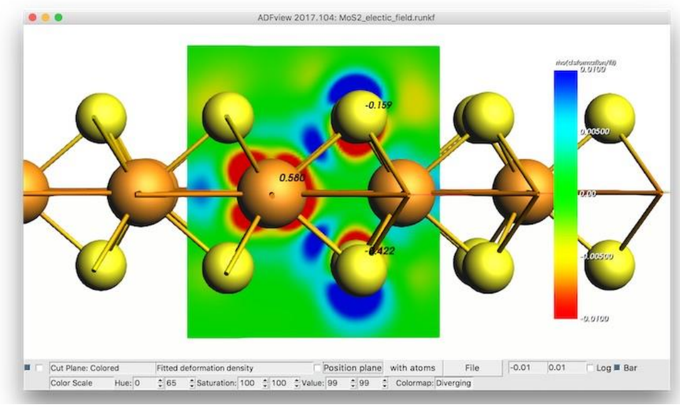
periodic energy decomposition analysis (tutorial)
L. Pecher and R. Tonner
WIREs CMS, (2018)

- True 2D surfaces, 1D polymers
  - Catalysts: polarization, solvation
  - 2D electronics (homogeneous E field)
  - Easy access to **Work function**
  - QM/MM and QM/QM' for 2D



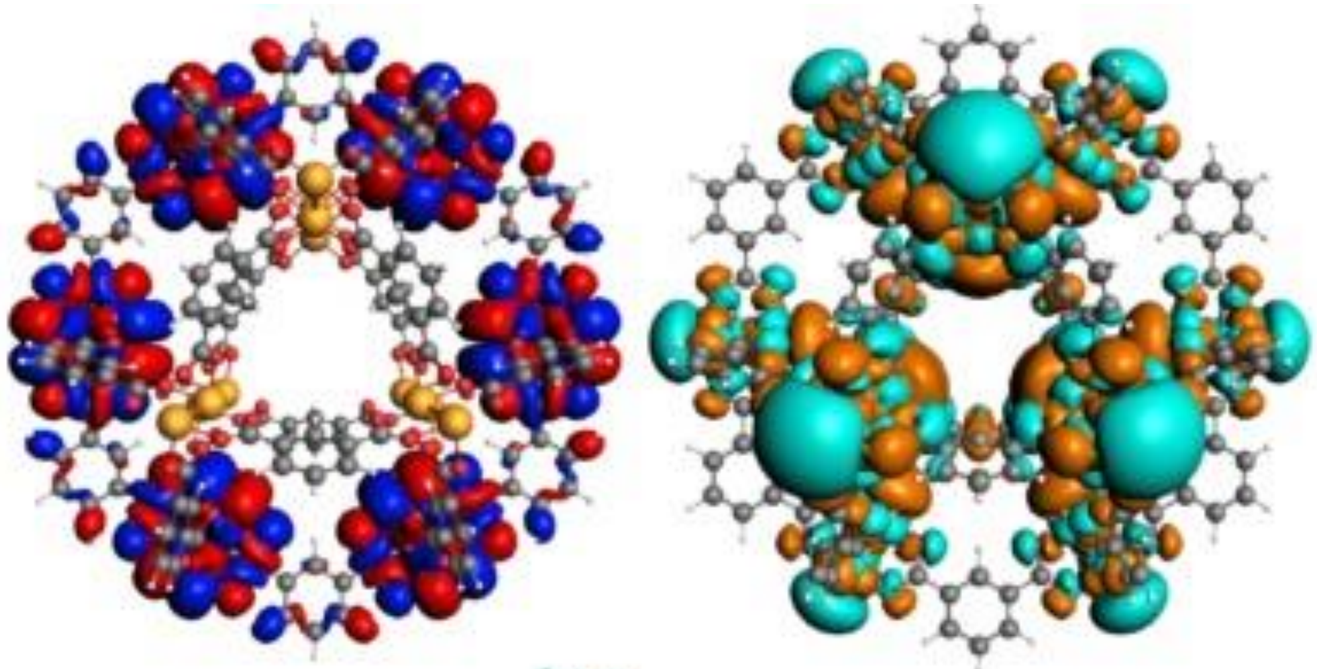
COOP in perovskites (tutorial)
Goesten & Hoffmann
JACS (2018)

- 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



Approximated DFT

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

Capabilities & Features

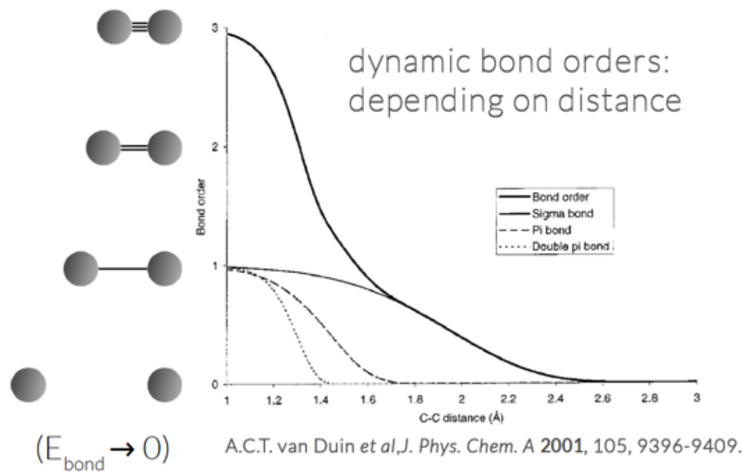
- UV/VIS (fast!)
- MOs, band structures, DOS

Through AMS

- Geometries, frequencies, phonons
- Stress tensors (optimize under p)
- Advanced MD, PES scans
- GCMC, molecule gun
- Multi-layer, QM/MM, QM/QM’
- Reparametrize xTB

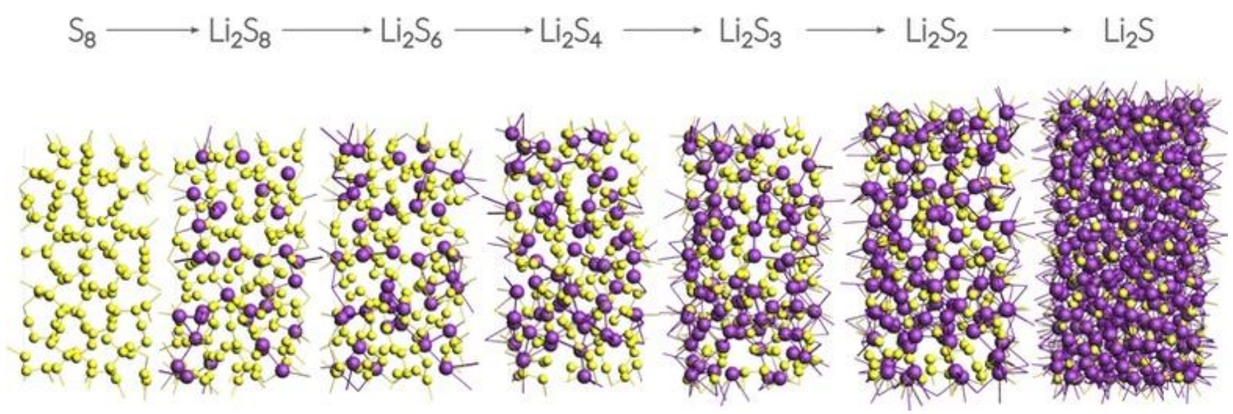
ReaxFF – reactive molecular dynamics

- No discontinuities in energy or forces
- No pre-defined reaction sites or types
  - Dynamic bond orders, charge equilibration
  - Only 1 atom type per element

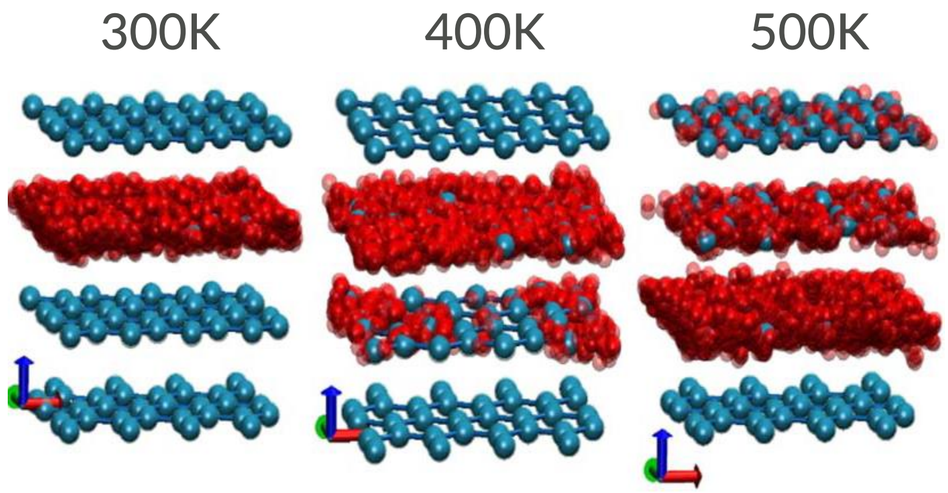


A.C.T. van Duin *et al*,*J. Phys. Chem. A* **2001**, 105, 9396-9409.

$$E_{\text{system}} = E_{\text{bond}} + E_{\text{lp}} + E_{\text{over}} + E_{\text{under}} + E_{\text{val}} + E_{\text{pen}} + E_{\text{coa}} + E_{\text{C}_2} + E_{\text{tors}} + E_{\text{conj}} + E_{\text{H-bond}} + E_{\text{vdWaals}} + E_{\text{Coulomb}}$$



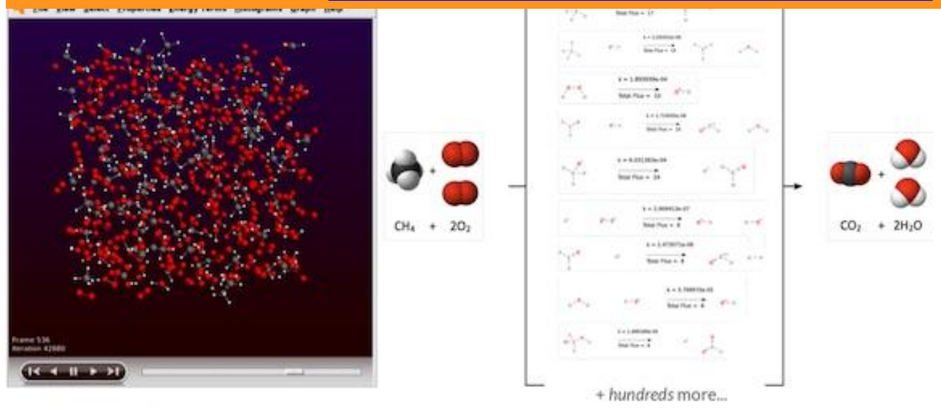
Li battery discharge: J. Electrochem. Soc. **161**, E3009 (2014); PCCP, **17**, 3383 (2015), tutorial



eReaxFF to study electron mobility & Li ion reduction, explicit electrons & electric field, *J. Electrochem. Soc.* **169** ,110540 (2022)

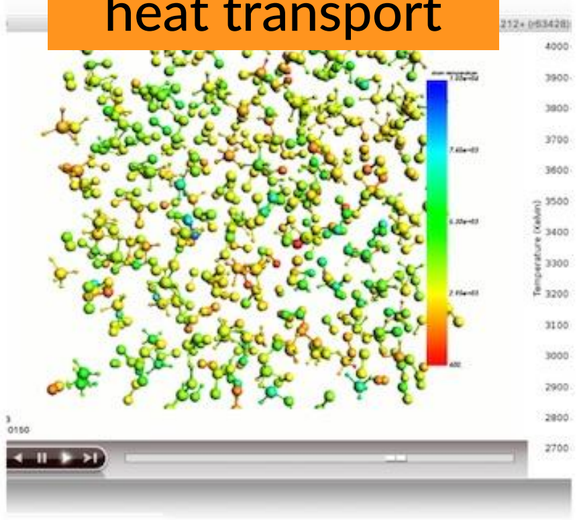
Reactive MD tools Amsterdam Modeling Suite

ChemTraYzer: Automated rates & pathways
New: Analyze surface reactions

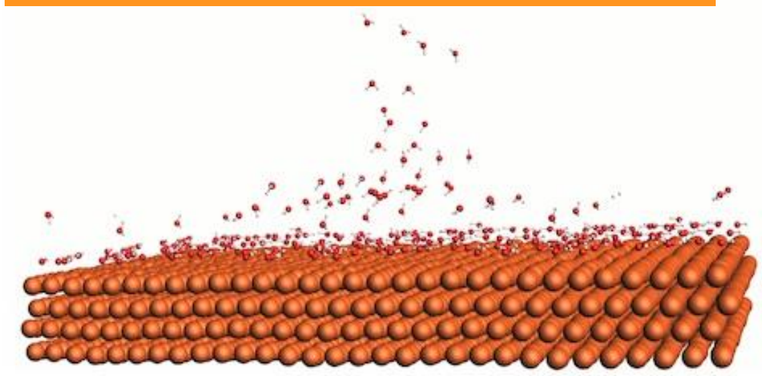


Tools += complete reaction networks
elementary reactions, rate constants, fluxes, timeline

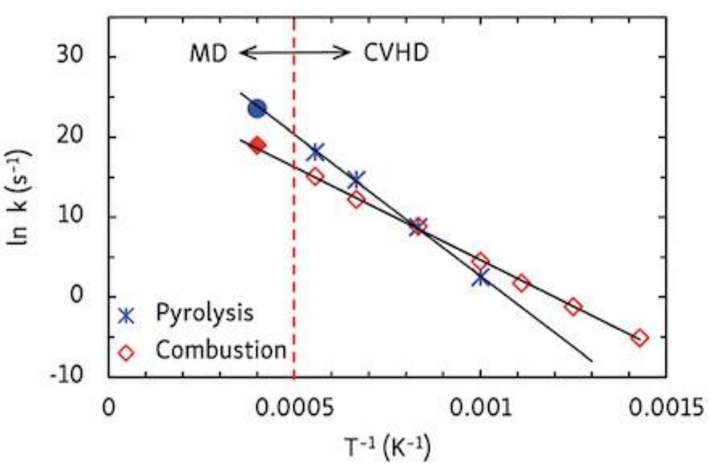
T-NEMD, local T:
heat transport

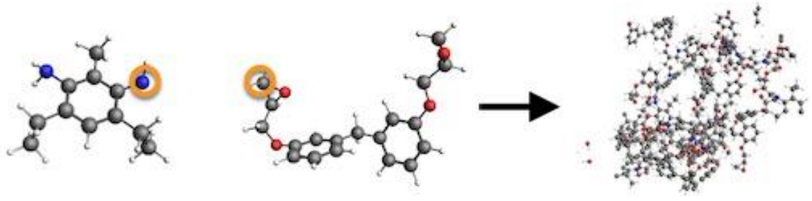


Molecule gun: depositing molecules on surfaces

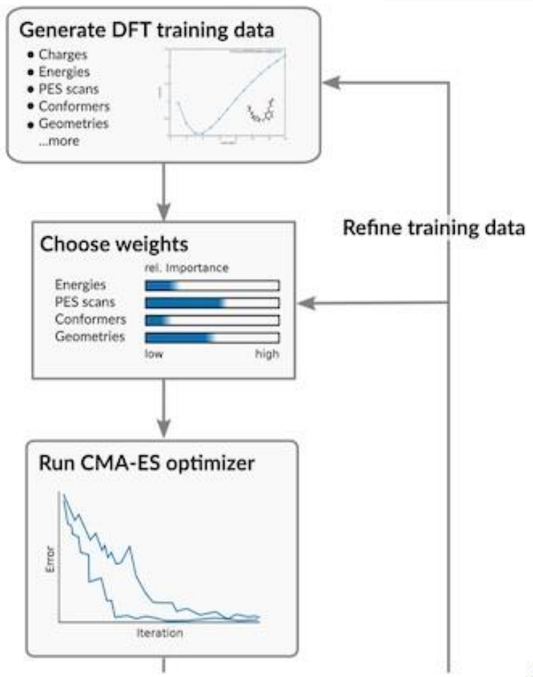


fbMC, CVHD, PRD:
speed up kinetics

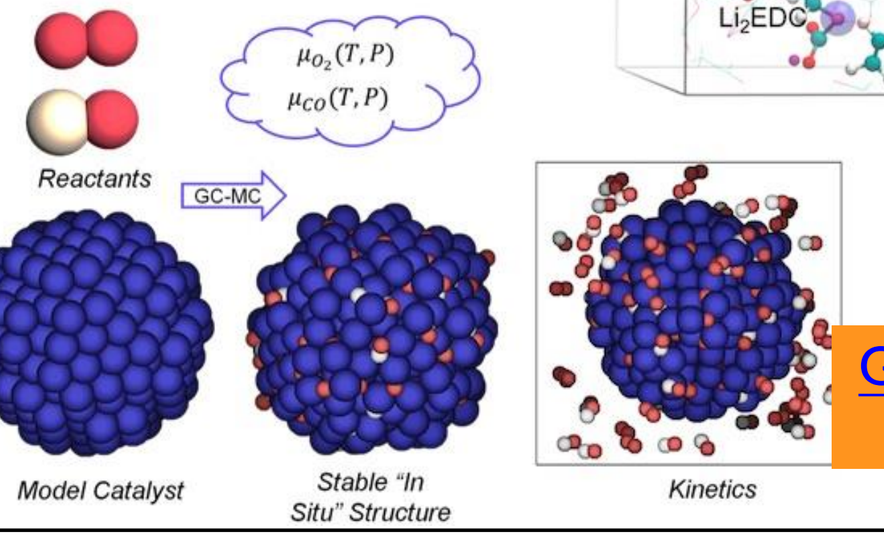


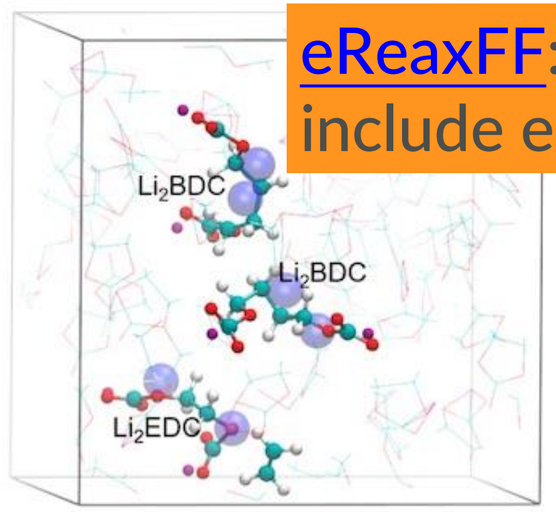


bond boost
build polymers



ParAMS - easy ReaxFF & DFTB (re)parameterization



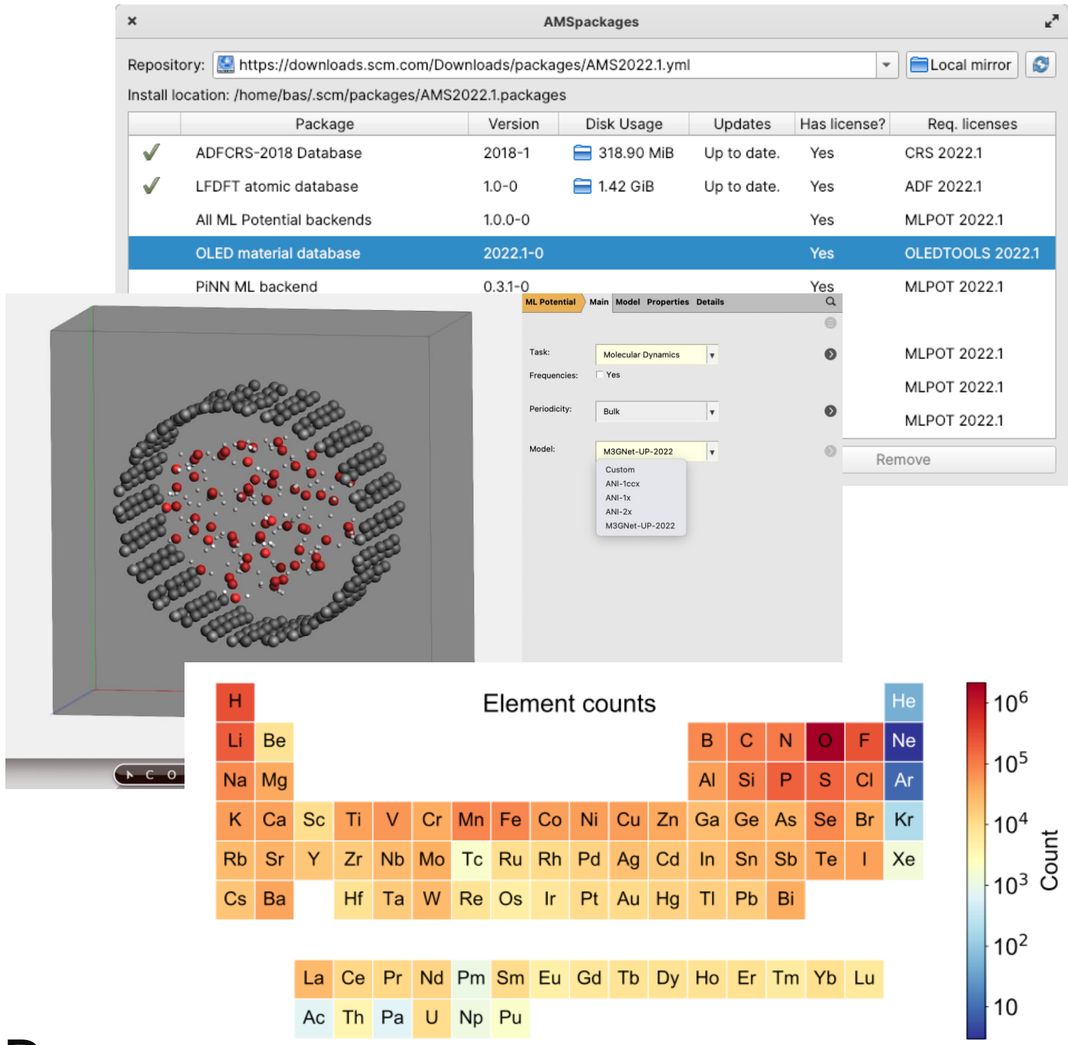


eReaxFF: include e-

GCMC: speed up thermo

Machine Learning Potentials

- Automatically install popular ML Backends
  - Pre-parametrized
    - i) ANI-1x and 2x (H, C, N, O, F, S, Cl)
    - ii) M3GNet (“Universal”)
  - Backends, via ASE
    - iii) NEquIP, FLARE (on-the-fly)
    - iv) sGDML
    - v) SchNet
    - vi) CHGNet
- Use MLP with all the tasks in the AMS driver
  - PES scans, reaction discovery, conformers, IR, phonons, MD, MC etc.
  - Hybrid (multi-layer): combine with other methods
- CUDA-enabled PyTorch and Tensorflow



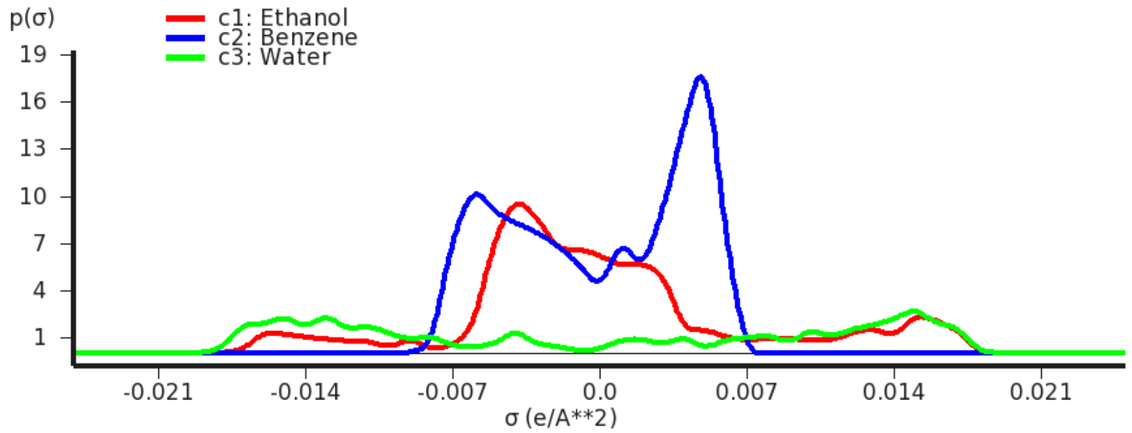
i) O. Isayev et al. Chem. Sci., 2017, 8, 3192–3203
ii) C. Chen, S.P. Ong., Nature Comp. Sci. 2, 718–728 (2022)
iii) S. Batzner et al. Nature Comm. 13: 2453 (2022)
iv) S. Chmiela et al. Comp. Phys. Commun. 240 (2019) 38-45
v) K. T. Schütt et al., J. Chem. Theory Comput. 15 (2019) 448-455

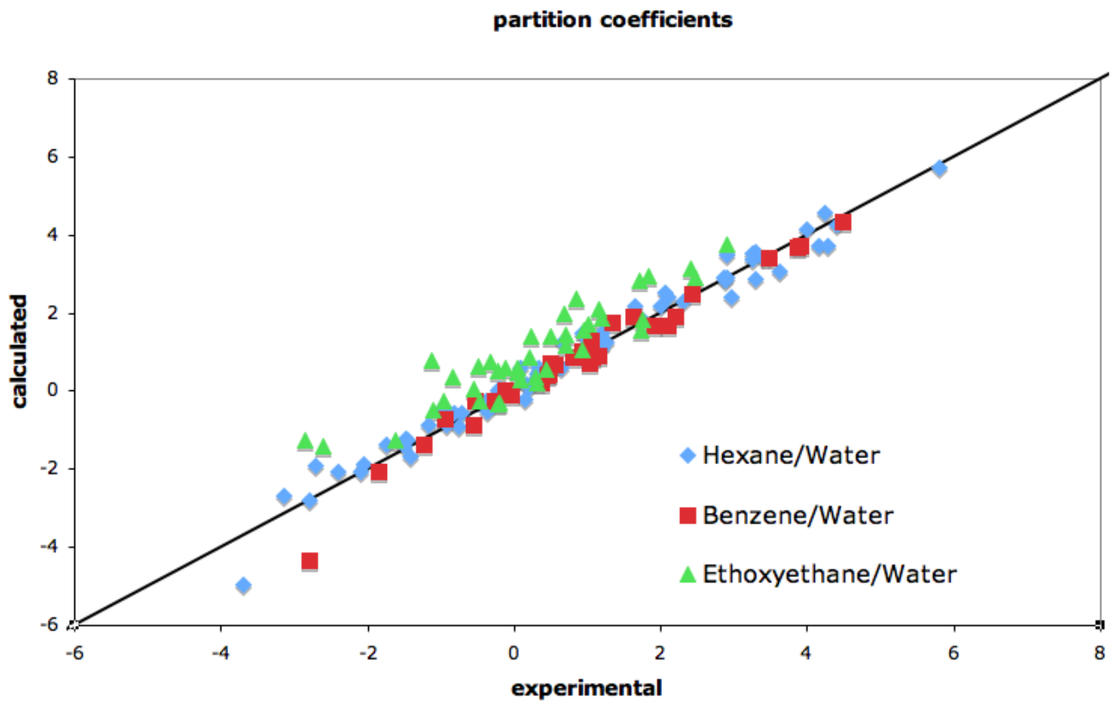
COSMO-RS/SAC: thermodynamic properties of fluids

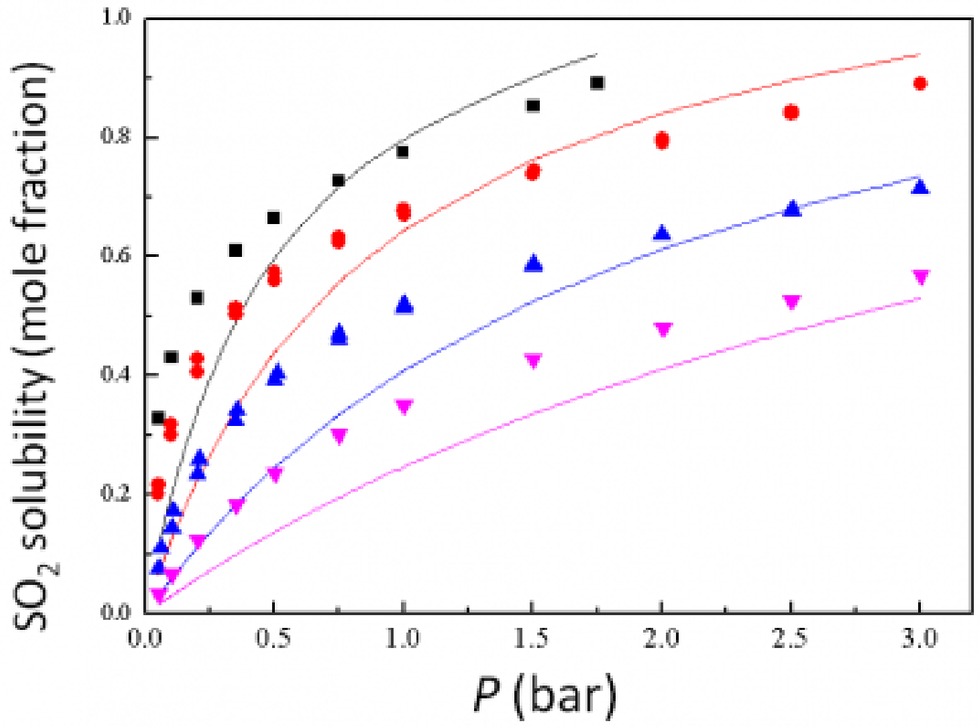
Quantum Chemistry & QSPR for quick property predictions

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

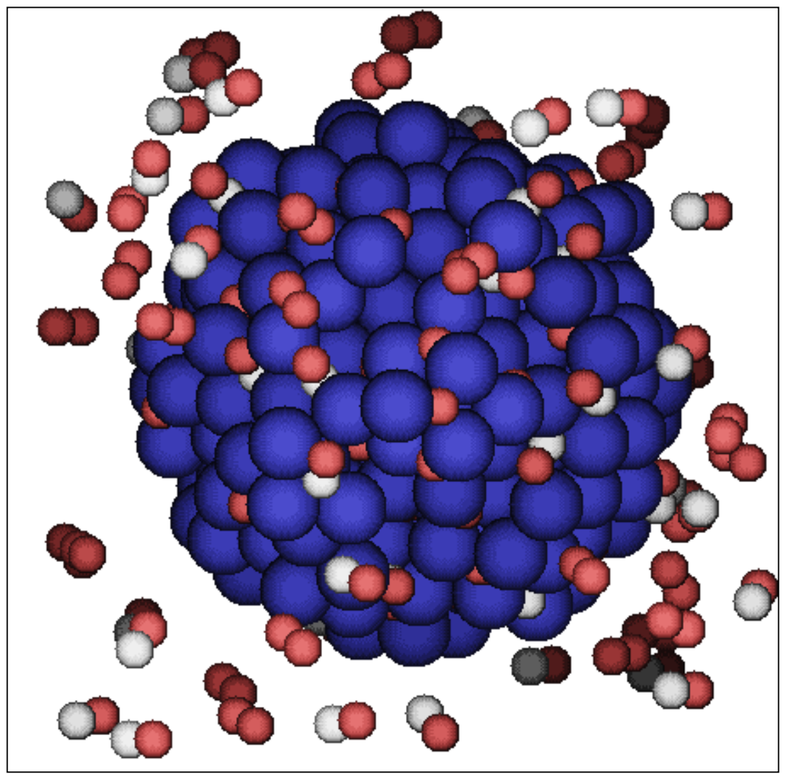
- Solvation & excess energies, pKa
- Solubilities, LLE, VLE, boiling points
- Optimize mixtures: solubility, LLE
- Polymers: Flory-Huggins X

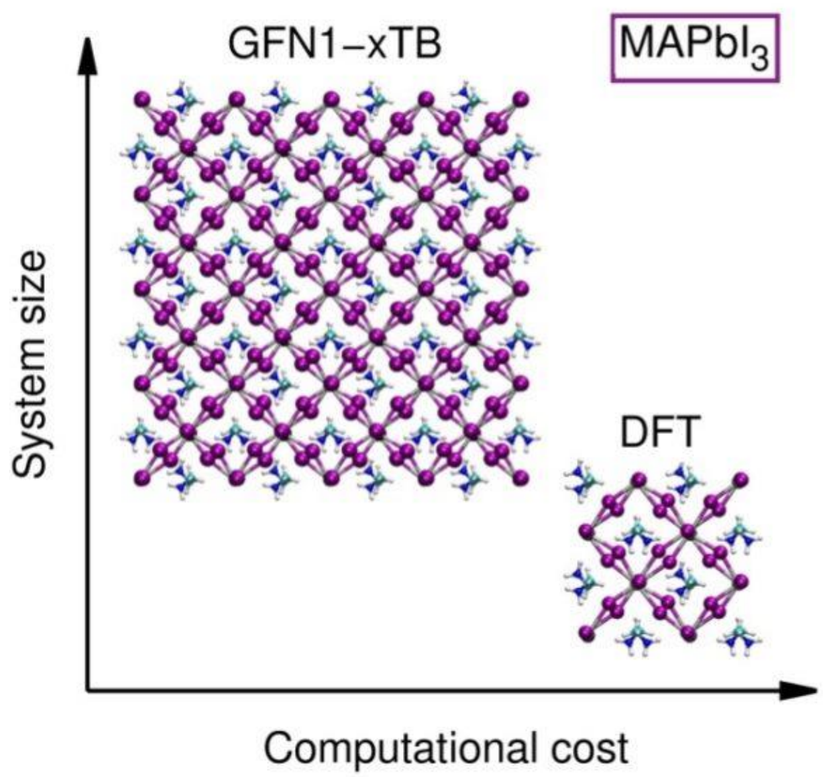


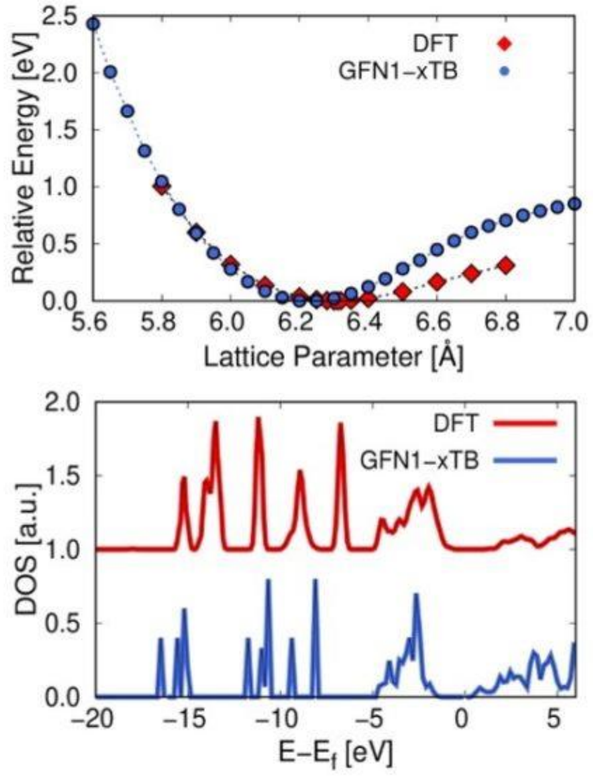




Parametrizing fast methods with ParAMS
DFTB, ReaxFF (ML)

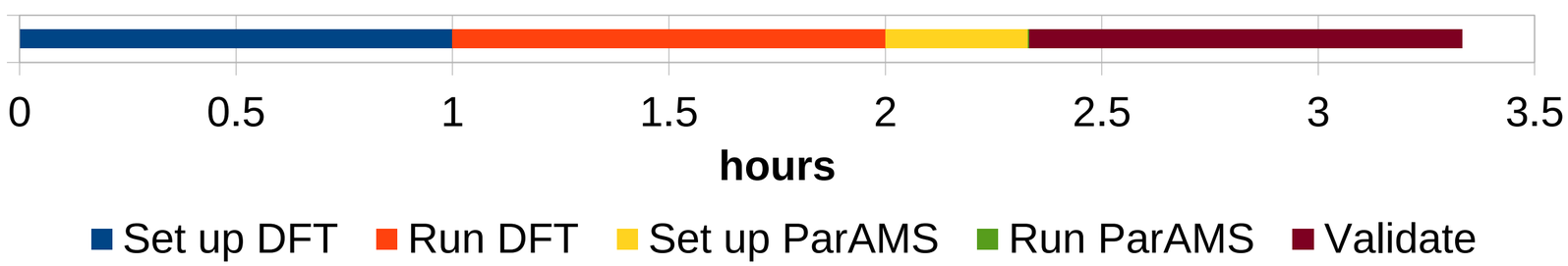


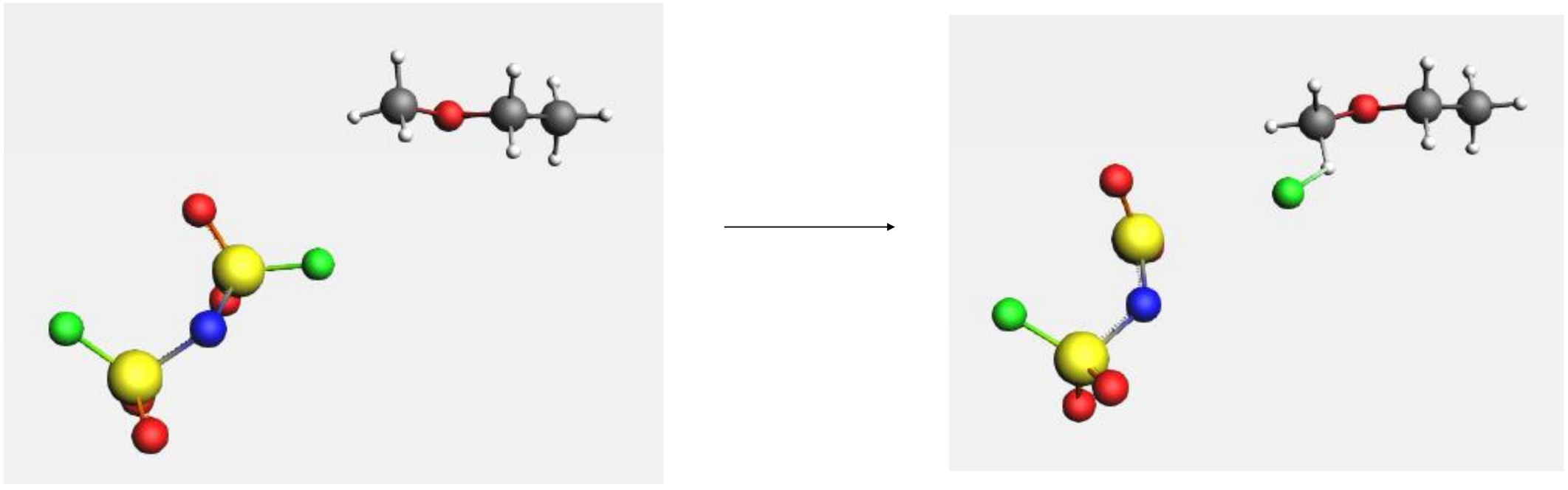




ReaxFF and DFTB problems

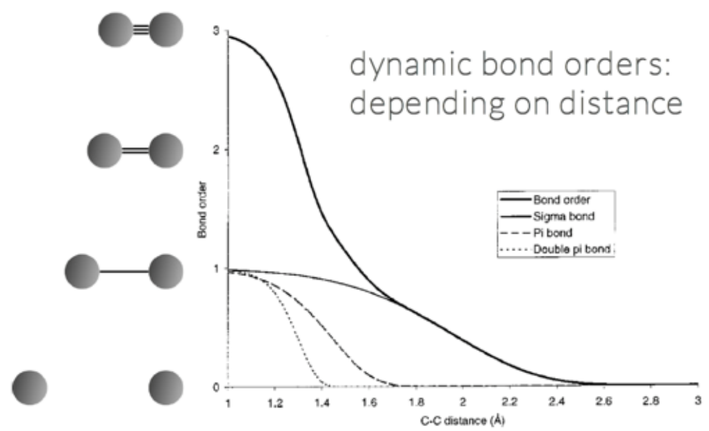
- ReaxFF force field may not exist for your application
- Not always accurate enough for “unseen” structures or molecules
- Example AMS industry customer: lithium bis(fluorosulfonyl)imide in organic solvent
- Published ReaxFF force field predicts that a fluorine atom dissociates from the anion
- Fix: 3.5h





General ReaxFF rules

- No discontinuities in energy or forces
- No pre-defined reaction sites or types
- Only 1 atom type per element



$(E_{bond} \rightarrow 0)$ A.C.T. van Duin *et al*,*J. Phys. Chem. A* **2001**, 105, 9396-9409.

$$E_{system} = E_{bond} + E_{lp} + E_{over} + E_{under} + E_{val} + E_{pen} + E_{coa} + E_{C_2} + E_{tors} + E_{conj} + E_{H-bond} + E_{vdWaals} + E_{Coulomb}$$

$$BO'_{ij}(r_{ij}) = \exp\left[p_{bo,1} \cdot \left(\frac{r_{ij}}{r_o}\right)^{p_{bo,2}}\right] + \exp\left[p_{bo,3} \cdot \left(\frac{r^{\pi}_{ij}}{r_{o,\pi}}\right)^{p_{bo,4}}\right] + \exp\left[p_{bo,5} \cdot \left(\frac{r^{\pi\pi}_{ij}}{r_{o,\pi\pi}}\right)^{p_{bo,6}}\right]$$

In: distance between atoms, r_{ij}

Out: 1, 2, 1.42, etc...

Parameters = 16

$p_{bo,1}, p_{bo,2}, p_{bo,3}, p_{bo,4}, p_{bo,5}, p_{bo,6}, r_o, r_{o,\pi}, r_{o,\pi\pi}$
$val_1, val_2, \lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5$

Correction terms f_1, f_2, f_3: $\mathbf{BO_{ij}(r_{ij})} = BO'_{ij}(r_{ij}) \cdot f_1(BO'_{ij}) \cdot f_2(BO'_{ij}) \cdot f_3(BO'_{ij})$

Review NPJ Comp. Materials (2016):
The ReaxFF reactive force field: development, applications and future directions

The Optimization Challenge

Which parameters do I optimize?

Are my parameter ranges appropriate?

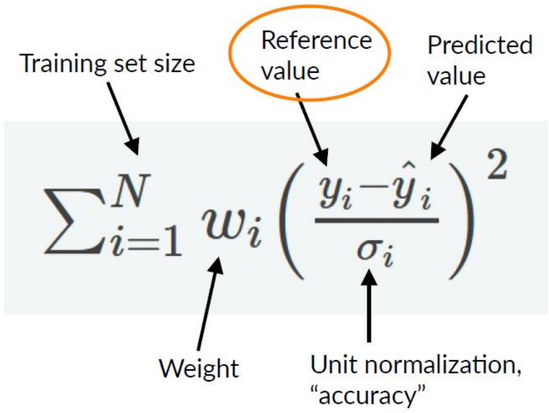
Is my training set balanced?

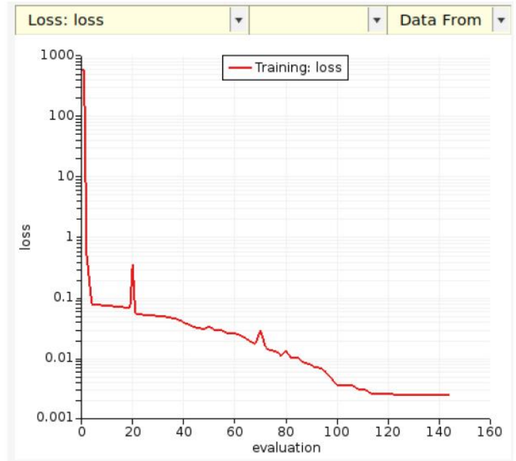
Are any training set items problematic?

```
49     -7.0147   3.4991   1.0564   4.0000   2.9680   0.0000   0.0000   0.0000
50 H    0.6646   1.0000   1.0080   1.6030   0.0600   0.7625  -0.1000   1.0000
51      9.3951   5.3036   1.0000   0.0000 121.1250   3.8196   9.8832   1.0000
52     -0.1000   0.0000  -0.1339   1.3343   1.3154   2.2824   1.0698   0.0000
53    -11.6319   3.0626   1.0338   1.0000   2.8793   0.0000   0.0000   0.0000
54 O    1.2699   2.0000  15.9990   1.9741   0.0880   1.0804   1.0624   6.0000
55     10.2186   7.7719   4.0000  27.3264 116.0768   8.5000   7.8386   2.0000
56      0.9446   8.6170  -1.2371  17.0845   3.7082   0.5350   0.9745   0.0000
57     -3.1456   2.6656   1.0493   4.0000   2.9225   0.0000   0.0000   0.0000
58 S    1.6725   2.0000  32.0600   1.8920   0.4079   1.0336  -0.1000   6.0000
59      9.7560   4.9222   4.0000  39.3552 112.1416   6.5000   8.2545   2.0000
60     -0.1000   9.7177  -2.3700  15.8739  18.0516  10.5526   0.9745   0.0000
61     -5.7373   2.7288   1.0338   4.0000   2.8177   0.0000   0.0000   0.0000
62 10    ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6
63                        pbe2;pbo3;pbo4;n.u.;pbo1;pbo2;ovcorr
64  1  1 145.4070 103.0681  73.7841   0.2176  -0.7816   1.0000  28.4167   0.3217
65         0.1111  -0.1940   8.6733   1.0000  -0.0994   5.9724   1.0000   0.0000
66  1  2 167.1752   0.0000   0.0000  -0.4421   0.0000   1.0000   6.0000   0.5969
67        17.4194   1.0000   0.0000   1.0000  -0.0099   8.5445   0.0000   0.0000
68  1  3 171.0470  67.2480 130.3792   0.3600  -0.1696   1.0000  12.0338   0.3796
69         0.3647  -0.2660   7.4396   1.0000  -0.1661   5.0637   0.0000   0.0000
70  1  4 123.3159   0.0000   0.0000   1.0464   0.0000   1.0000   6.0000   0.3436
71         6.1557   1.0000   0.0000   1.0000  -0.1907   4.6655   1.0000   0.0000
72  2  2 188.1606   0.0000   0.0000  -0.3140   0.0000   1.0000   6.0000   0.6816
73         8.6247   1.0000   0.0000   1.0000  -0.0183   5.7082   0.0000   0.0000
74  2  3 216.6018   0.0000   0.0000  -0.4201   0.0000   1.0000   6.0000   0.9143
75         4.7737   1.0000   0.0000   1.0000  -0.0591   5.9451   0.0000   0.0000
76  2  4 143.5209   0.0000   0.0000   0.9244   0.0000   1.0000   6.0000   0.4891
77         3.7612   1.0000   0.0000   1.0000  -0.1511   5.3134   1.0000   0.0000
78  3  3  90.2465 160.9645  40.0000   0.9950  -0.2435   1.0000  28.1614   0.9704
79         0.8145  -0.1850   7.5281   1.0000  -0.1283   6.2396   1.0000   0.0000
80  3  4   0.0000   0.0000   0.0000   0.5563   0.0000   1.0000   6.0000   0.6000
81         0.4259  -0.4577  12.7569   1.0000  -0.1100   7.1145   1.0000   0.0000
82  4  4 116.9963   0.0000   0.0000   0.2723   0.0000   1.0000   6.0000   0.6268
83         7.2513   1.0000   0.0000   1.0000  -0.1969   6.5238   1.0000   0.0000
84  6    ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
85  1  2   0.0455   1.7218  10.4236   1.0379  -1.0000  -1.0000
86  1  3   0.1186   1.9820   9.5927   1.2936   1.1203   1.0805
87  1  4   0.5076   1.9364  10.1175   1.4125  -1.0000  -1.0000
88  2  3   0.0469   1.9185  10.3707   0.9406  -1.0000  -1.0000
89  2  4   0.2412   1.5000   9.1407   1.3138  -1.0000  -1.0000
90  3  4   0.1359   2.0203  10.1000   1.6050   1.3050  -1.0000
91 31    ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2
92  1  1  1  70.0265  13.6338   2.1884   0.0000   0.1676  26.3587   1.0400
93  1  1  2  69.7786  10.3544   8.4326   0.0000   0.1153   0.0000   1.0400
94  1  1  3  72.9588  16.7105   3.5244   0.0000   1.1127   0.0000   1.1880
95  1  1  4  81.7078  19.9130   7.1552   0.1463   2.4464   0.0000   1.7029
96  1  2  1   0.0000   3.4110   7.7350   0.0000   0.0000   0.0000   1.0400
97  1  3  1  79.1091  45.0000   0.7067   0.0000   0.6142   0.0000   1.0783
98  1  3  2  78.1533  44.7226   1.3136   0.0000   0.1218   0.0000   1.0500
99  1  3  3  83.7151  42.6867   0.9699   0.0000   0.6142   0.0000   1.0783
100  1  3  4  85.3644  36.9951   2.0903   0.1463   0.0559   0.0000   1.0400
101  1  4  1  78.7122  32.2800   6.4410   0.1463   3.1550   0.0000   1.8075
102  1  4  2  86.1791  36.9951   2.0903   0.0000   0.0000   0.0000   1.0400
103  1  4  3  85.3644  36.9951   2.0903   0.1463   0.0559   0.0000   1.0400
104  1  4  4  70.2150  21.0147   2.5908   0.1463   1.9899   0.0000   1.8466
105  2  1  2  74.6020  11.8629   2.9294   0.0000   0.1367   0.0000   1.0400
106  2  1  3  66.6150  13.6403   3.8212   0.0000   0.0755   0.0000   1.0500
107  2  1  4  74.9397  25.0560   1.8787   0.0000   0.0000   0.0000   1.0400
108  2  3  2  79.2954  26.3838   2.2044   0.0000   0.1218   0.0000   1.0500
109  2  3  3  84.1057   9.6413   7.5000   0.0000   0.1218   0.0000   1.0500
110  2  3  4  84.1057   9.6413   7.5000   0.0000   0.1218   0.0000   1.0500
111  2  4  2  66.7704  22.1733   3.6203   0.0000   2.3997   0.0000   1.0400
```

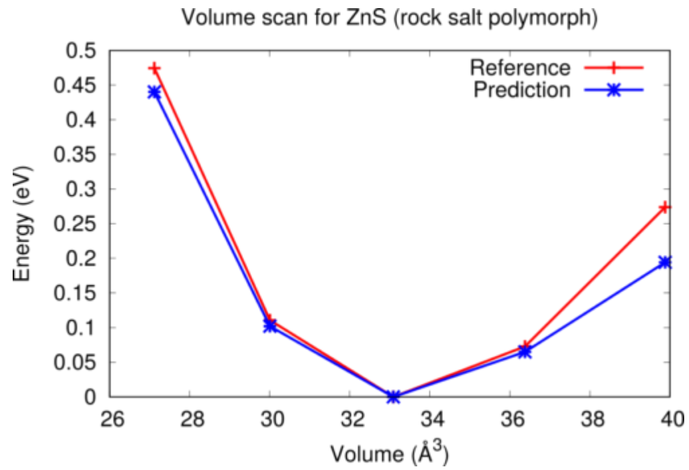
ParAMS: GUI + scripts for Parametrization
GloMPO: Global parallel optimizations

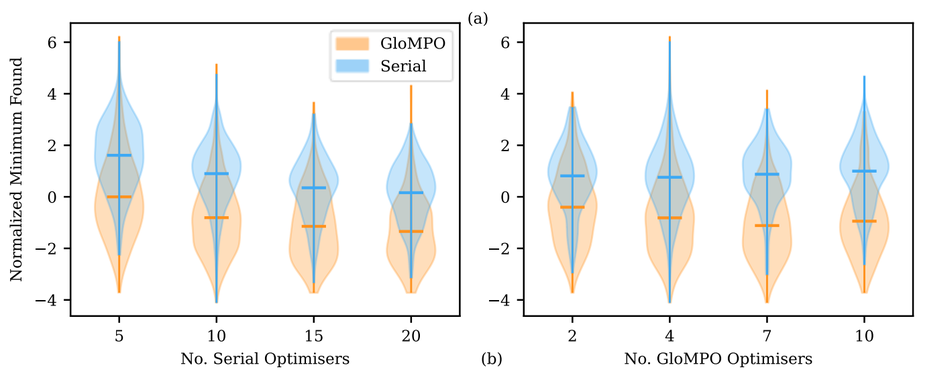
- Build training sets with AMS
  - ADF, BAND, (+VASP, QE, Gaussian)
- Define references & loss function
- Choose & optimize parameters
  - Lennard-Jones
  - ReaxFF
  - DFTB
  - AMS2024: ML Potentials (active learning)
- Validate (& iterate)





New parameters for every evaluation



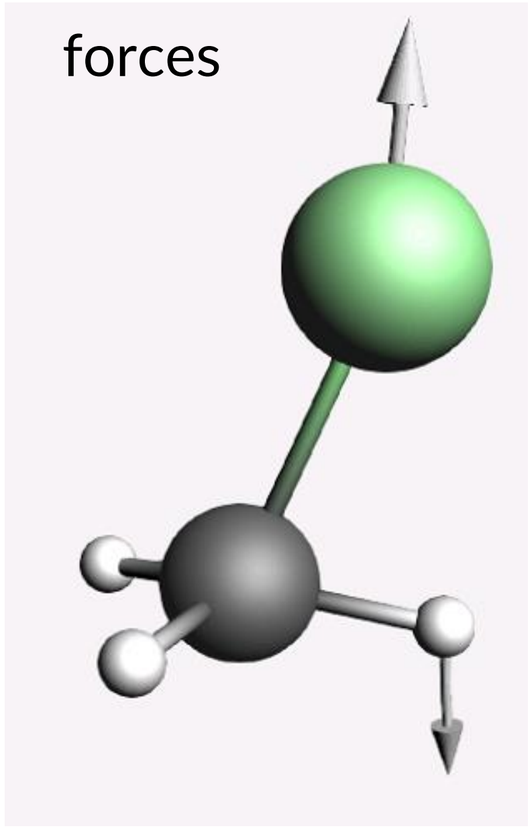


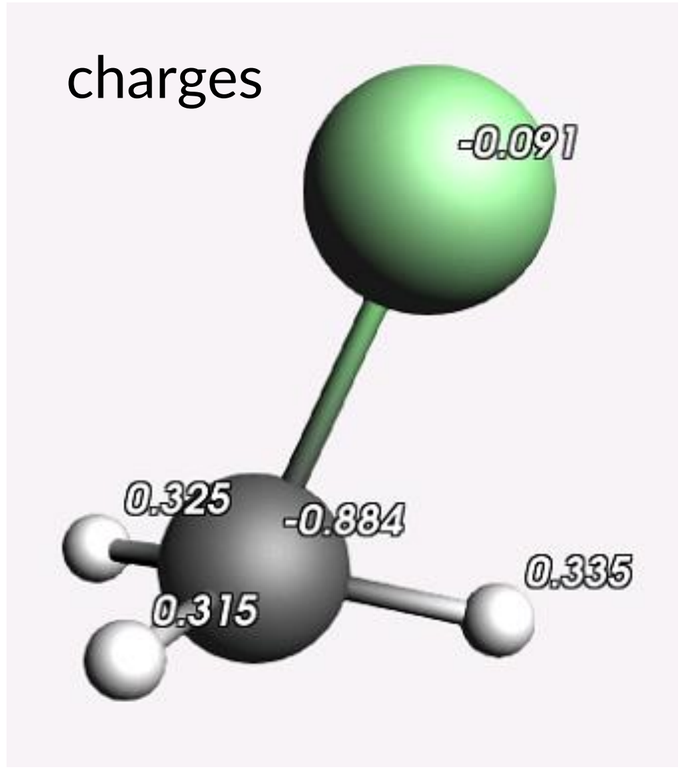
- Komissarov, L.; Rüger, R.; Hellström, M.; Verstraelen, T. ParAMS: Parameter Optimization for Atomistic and Molecular Simulations *J. Chem. Inf. Model.* **2021**, *61*, 8, 3737-3743
- Freitas Gustavo, M., Verstraelen, T. GloMPO (Globally Managed Parallel Optimization): a tool for expensive, black-box optimizations, application to ReaxFF reparameterizations. *J. Cheminform.* **2022**, *14*, 7.

ParAMS: Types of reference values

- “Anything” that can be extracted from a **job** can be used as a reference value

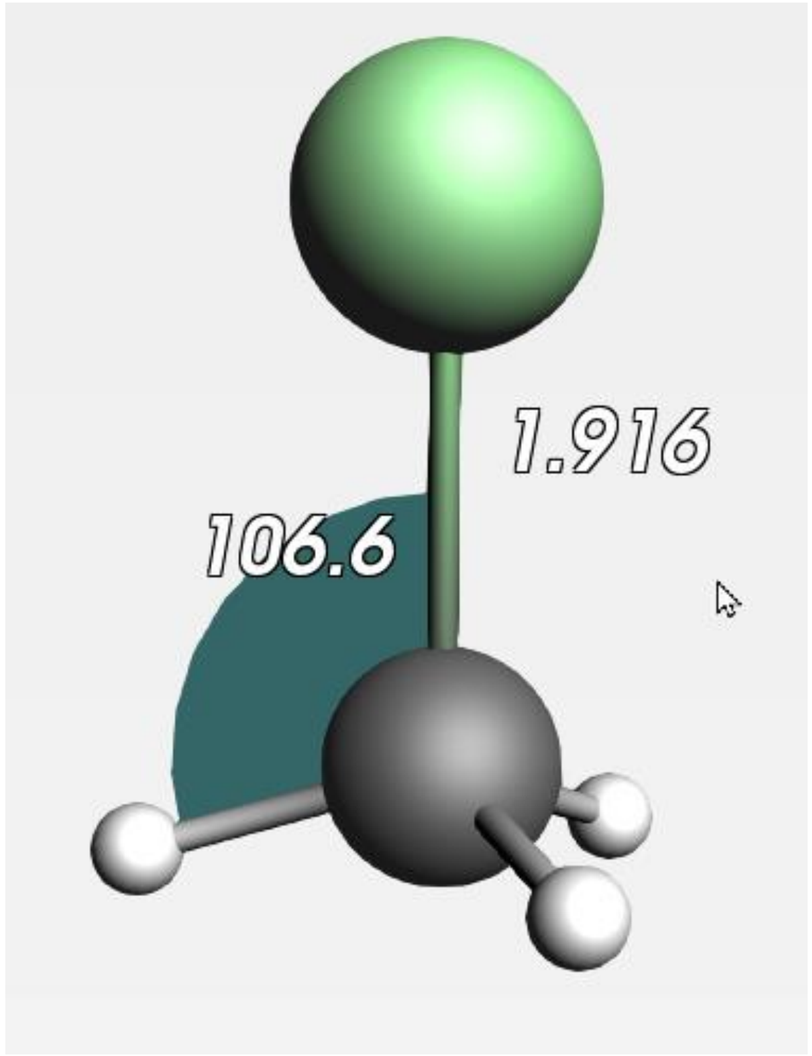
- Forces, atomic charges





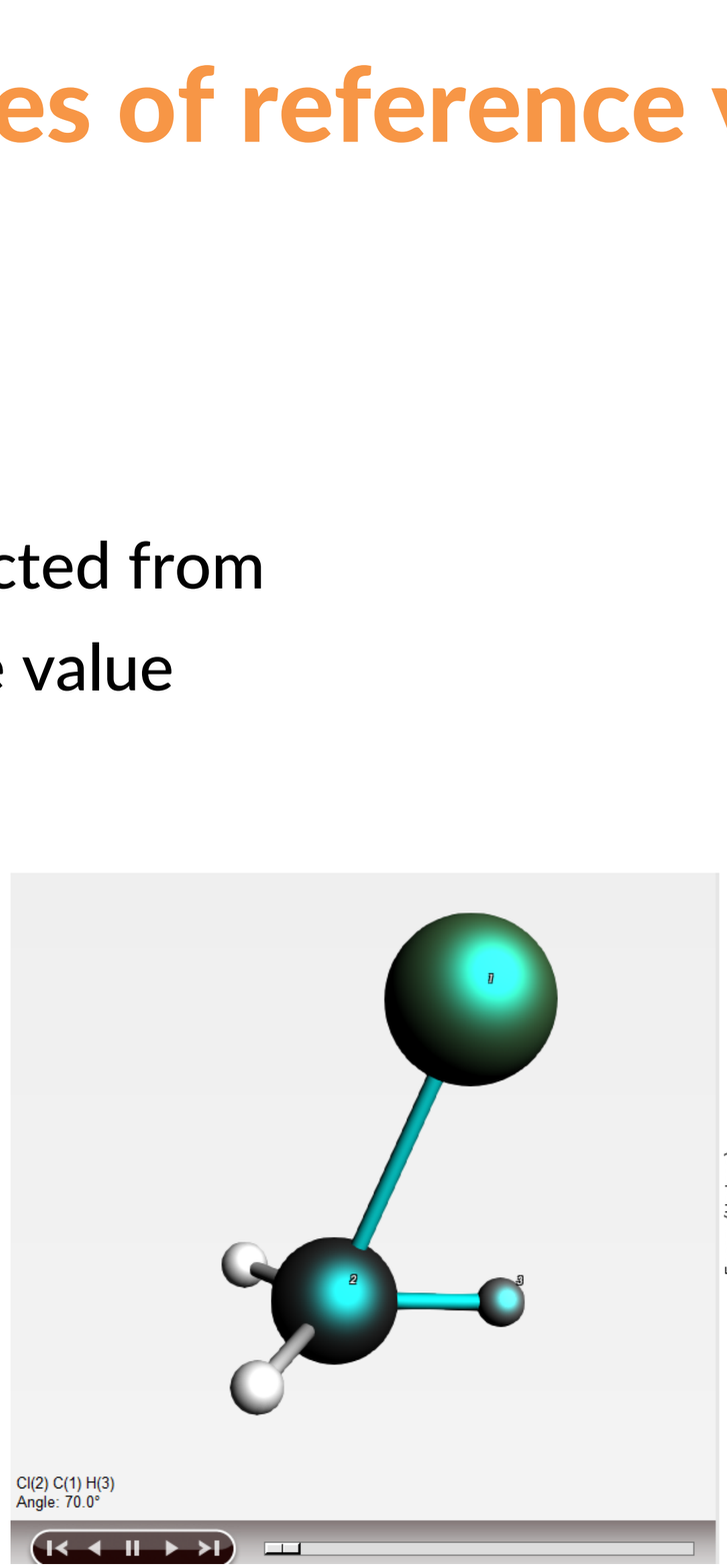
ParAMS: Types of reference values

- “Anything” that can be extracted from a **job** can be used as a reference value
- (optimized) Bond distances, angles



ParAMS: Types of reference values

- "Anything" that can be extracted from a **job** can be used as a reference value
- PES Scans: Energy vs. bond length, angle, or cell volume



ParAMS: Types of reference values

- Values from **multiple jobs**:

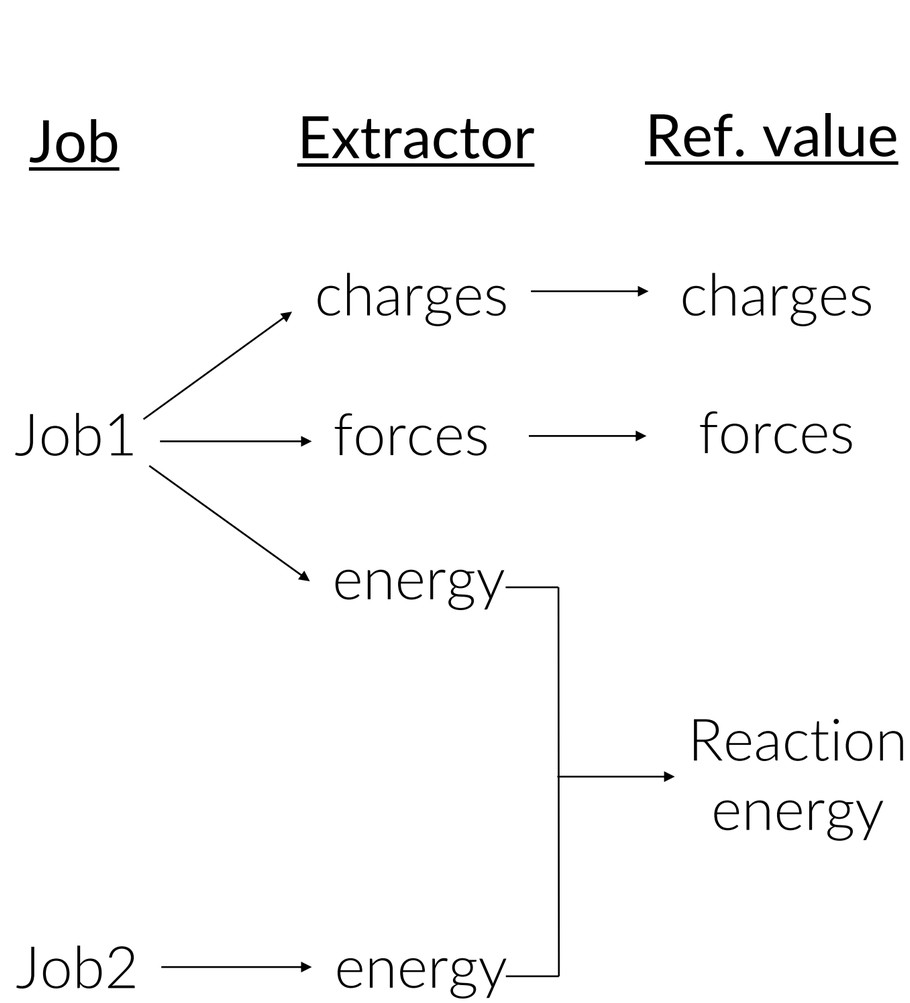
Reaction energies (adsorption energy, surface energy, formation energy, …)

$$C_3H_6(g) + (9/2)\ O_2(g) \rightarrow 3\ CO_2(g) + 3\ H_2O(g)$$

$$\Delta H_r^0 = -491.8\ \text{kcal/mol}$$

ParAMS: Types of reference values

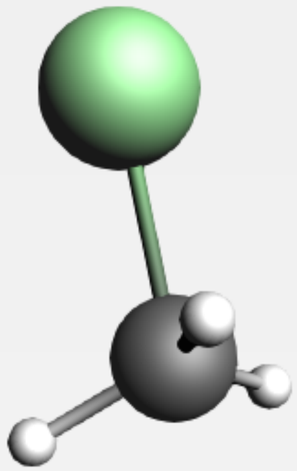
- "Anything" that can be extracted from **jobs** can be used as a reference value
- Forces, atomic charges
- Optimized bond lengths or angles
- PES Scans: Energy vs. bond length, angle, or cell volume
- Reaction energies (adsorption energy, surface energy, formation energy, ...)



Example reference values: Charges and forces of chloromethane

ParAMS 2022.101

SCM File Edit Jobs Parameters Training Set View Help



Job chloromethane-forces

All | Jobs | Training Set | Validation Set | Engines

Type	Detail	JobID	W	Value / Engines	
Engine	Engine lennardjones EndEngine			ParAMS	
Job	Single Point + gradients	chloromethane-forces		adf;;xc;;gga;PBE;	
Charges	chloromethane-forces	chloromethane-forces	1.0	[-0.8835, 0.3345] (5	au
Engine	Engine adf xc gga PBE End EndEngine			adf;;xc;;gga;PBE;	
Forces	chloromethane-forces	chloromethane-forces	1.0	[-0.1095, 0.0735] (5	Hartree/Bc

Errors Only 5 items

Parameters | Settings | Info | Graphs | Results

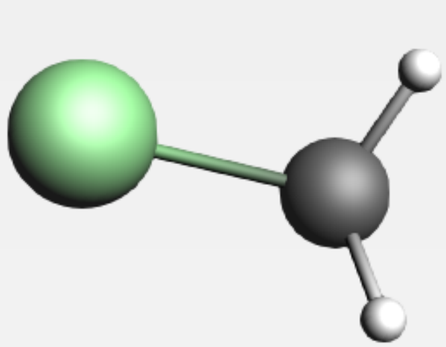
Weight: +1.000000000

Value:

-0.016768241	+0.018544396	-0.018888589
+0.043055409	-0.109488031	-0.015582138
-0.022345467	+0.073456592	+0.026842484
-0.002046089	+0.011289727	+0.017385490
-0.001895612	+0.006197316	-0.009757247

Example reference values: Optimized bond lengths and angles

- For bond lengths and angles, add **geometry optimization** jobs!

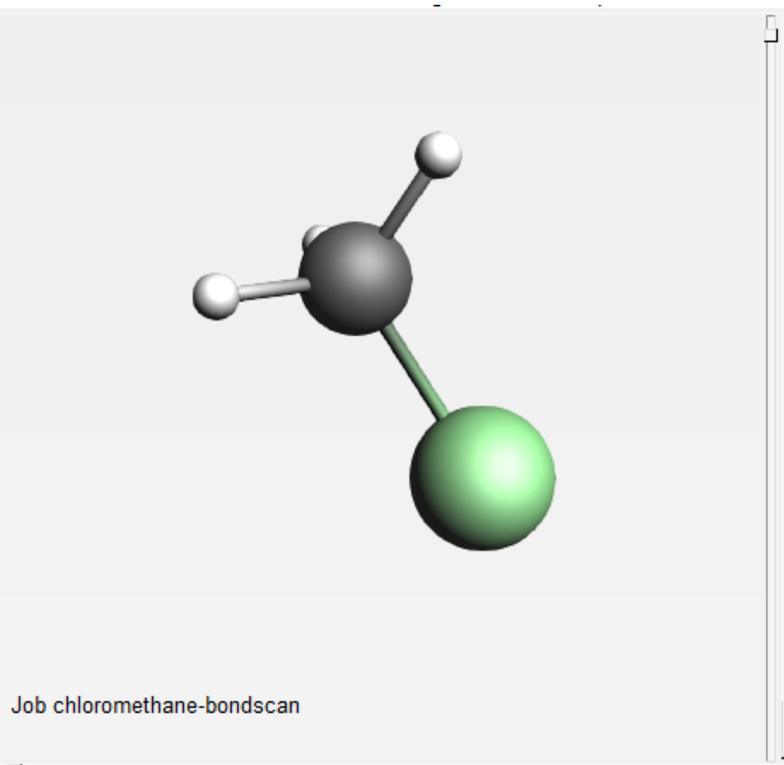


All | Jobs | Training Set | Validation Set | Engines

Type	Detail	JobID	W	Value / Engines	
Engine	Engine lennardjones EndEngine			ParAMS	
Job	Geometry Optimization + gradients + ...	chloromethane-geometry		adf;;xc;;gga;PBE;	
Engine	Engine adf xc gga PBE End EndEngine			adf;;xc;;gga;PBE;	
Geo: distanc	chloromethane-geometryoptimization, 0, 1 (C-Cl)	chloromethane-geometry	1.0	+1.91567508	Å
Geo: distanc	chloromethane-geometryoptimization, 0, 2 (C-H)	chloromethane-geometry	1.0	+1.09398928	Å
Geo: angle	chloromethane-geometryoptimization, 1, 0, 2 (Cl-C-H)	chloromethane-geometry	1.0	+106.60000000	°
Geo: angle	chloromethane-geometryoptimization, 2, 0, 3 (H-C-H)	chloromethane-geometry	1.0	+112.40000000	°

Example reference values: Bond scan, angle scan, lattice scan

- For PES scans, add **PES Scan** jobs!



Job chloromethane-bondscan

All | Jobs | Training Set | Validation Set | Engines

Type	Detail	JobID	W	Value / Engines	
Engine	Engine lennardjones EndEngine			ParAMS	
Job	PES Scan + gradients + ...	chloromethane-bondscar		adf;;xc;;gga;PBE;	
PES	chloromethane-bondscan, relative_to=3	chloromethane-bondscar	1.0	[0.0000, 9.6074] (7)	kcal/mol
Engine	Engine adf xc gga PBE End EndEngine			adf;;xc;;gga;PBE;	

Errors Only 4 items

Parameters | Settings | Info | Graphs | Results

Weight: +1.000000000

Value: +9.607422193 +4.075588043 +1.082804509 +0.000000000 +0.348957323
+1.763552064 +3.960264837

Example reference values: Reaction energy

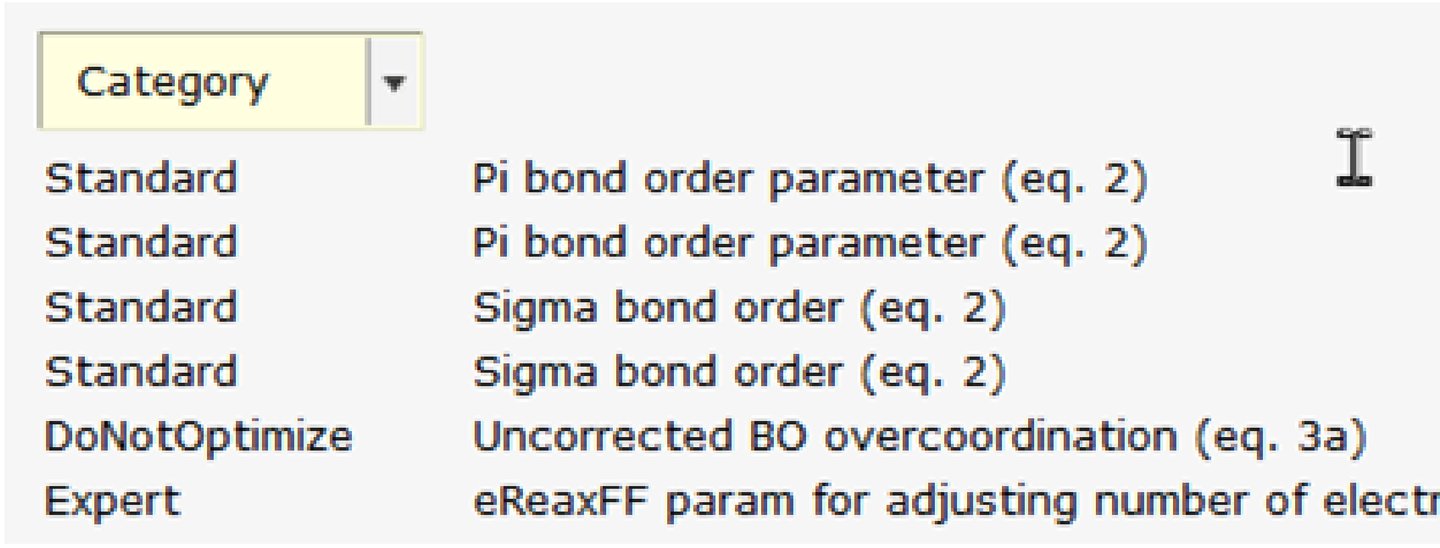
- Propene combustion: $C_3H_6(g) + (9/2)\ O_2(g) \rightarrow 3\ CO_2(g) + 3\ H_2O(g)$
- Automatically balanced stoichiometric coefficients!

All | Jobs | Training Set | Validation Set | Engines

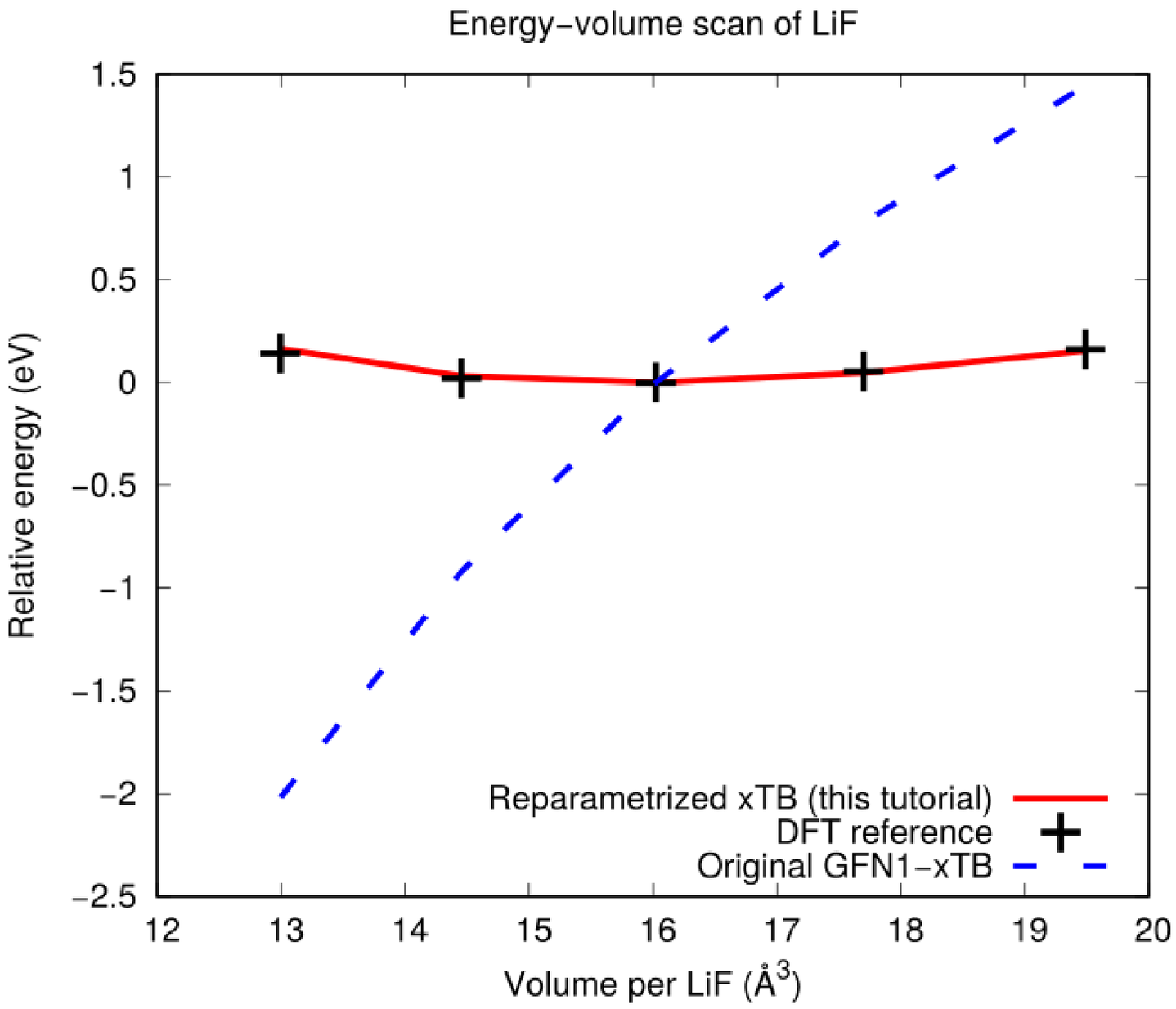
Type	Detail	JobID	W	Value / Engines	
Engine	Engine lennardjones EndEngine			ParAMS	
Job	Geometry Optimization + ...	water		adf;;xc;;gga;PBE;	
Engine	Engine adf xc gga PBE End EndEngine			adf;;xc;;gga;PBE;	
Job	Geometry Optimization + ...	propene		adf;;xc;;gga;PBE;	
Job	Geometry Optimization + ...	co2		adf;;xc;;gga;PBE;	
Job	Geometry Optimization + ...	o2		adf;;spinpolarization;2;unr	
Engine	Engine adf spinpolarization 2 unrestricted yes xc gga PBE			adf;;spinpolarization;2;unr	
Energy	+3.0*co2+3.0*water-1.0*propene-4.5*o2	propene ...	1.0	-358.85844881	kcal/mol

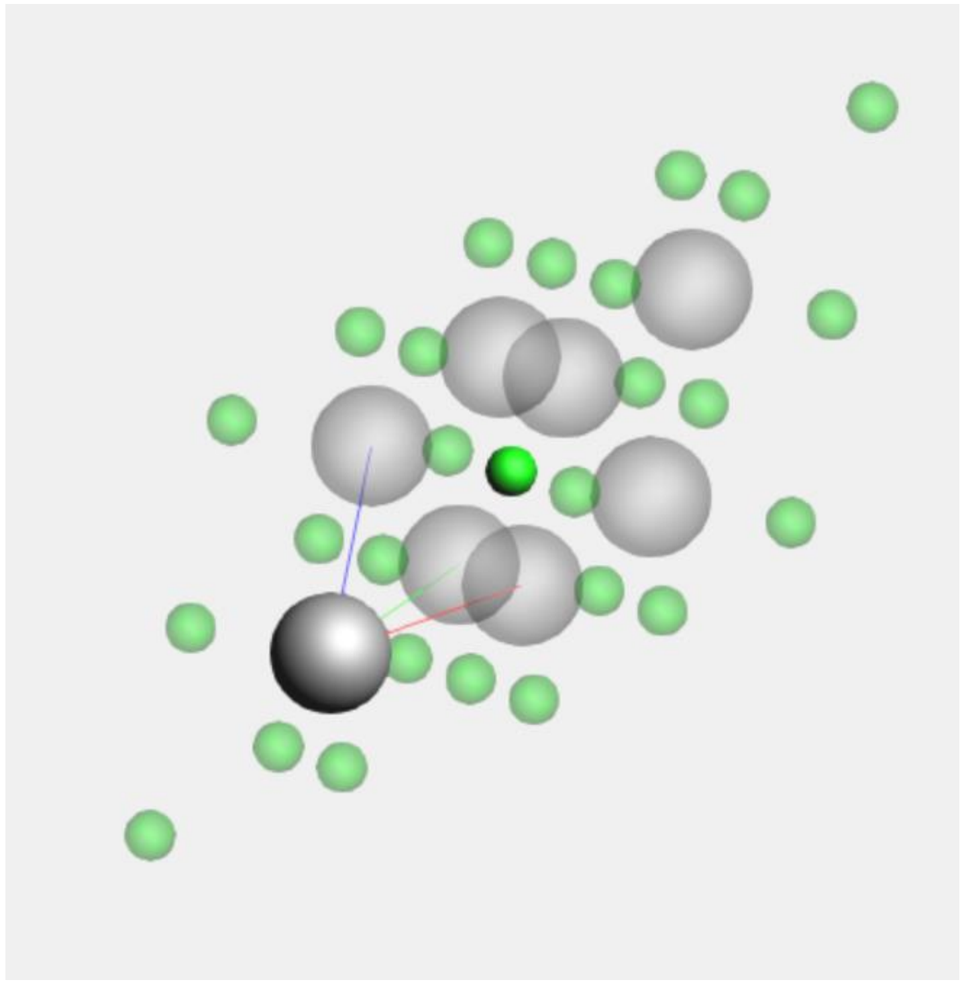
ParAMS settings

- Which parameters to optimize?
- Choose as **few** as possible
- First try parameters in the "**standard**" category
- If a parameter value is close to min/max, change the range and continue
- Which optimization algorithm?
- We recommend **CMA-ES** for most optimization problems
- Webinar about this algorithm: https://youtu.be/Icv7kWUaoTI



Tutorial: reparametrize xTB for LiF



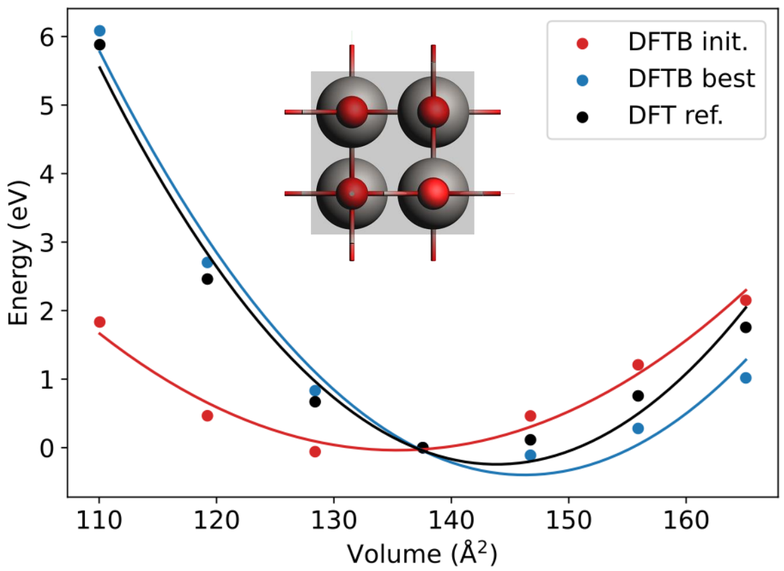


Reparametrize repulsive xTB parameters against DFT EOS + exp H_f

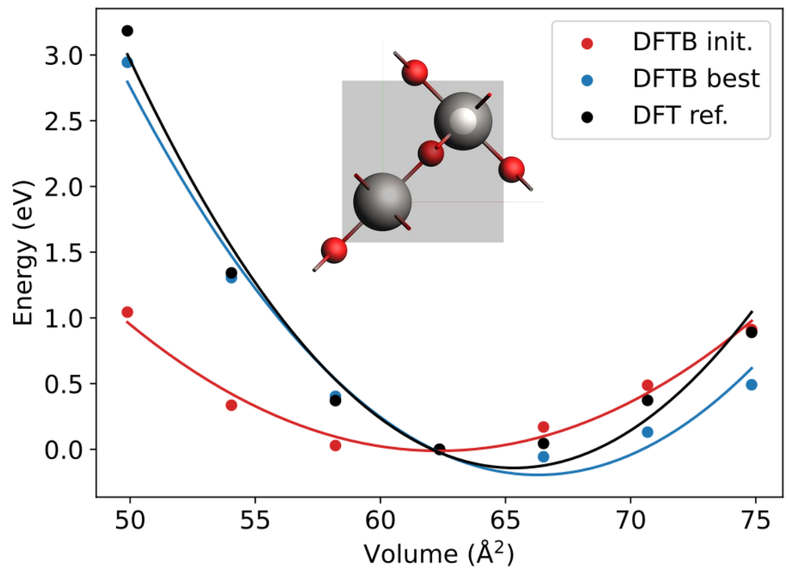
https://www.scm.com/doc/params/examples/xtb_lif/xtb_lif.html

Example: reparametrize xTB for TiO_2

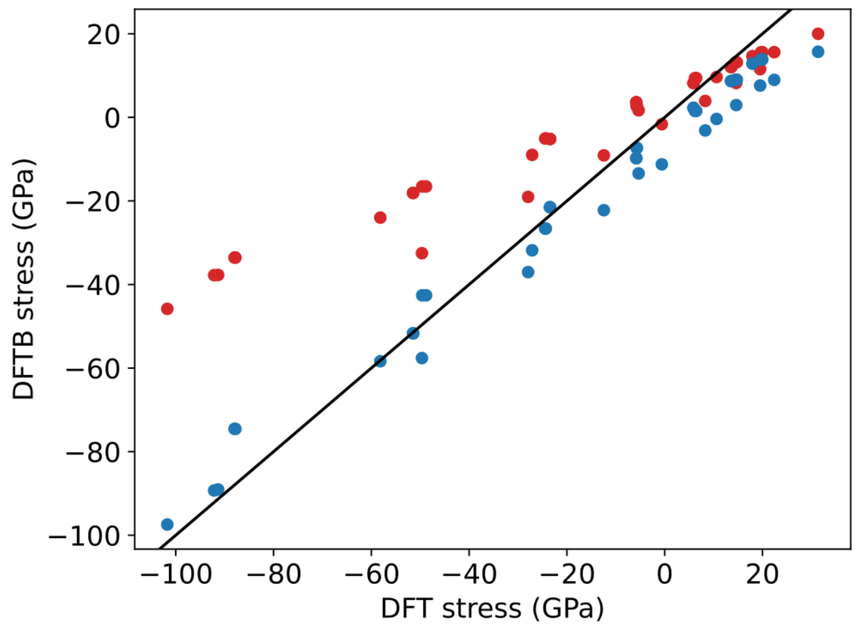
Equation of states (Anatase)



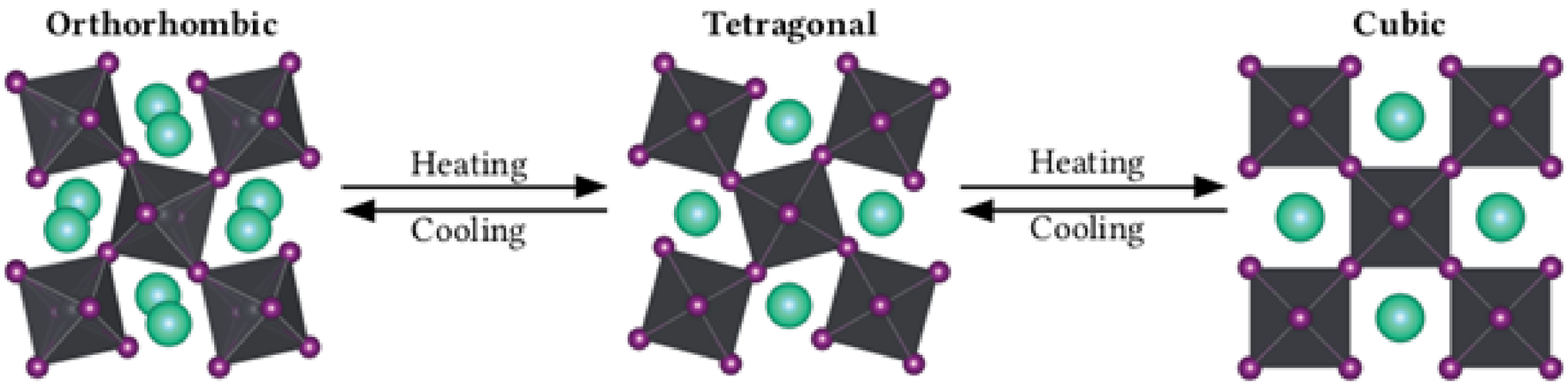
Equation of states (Rutile)

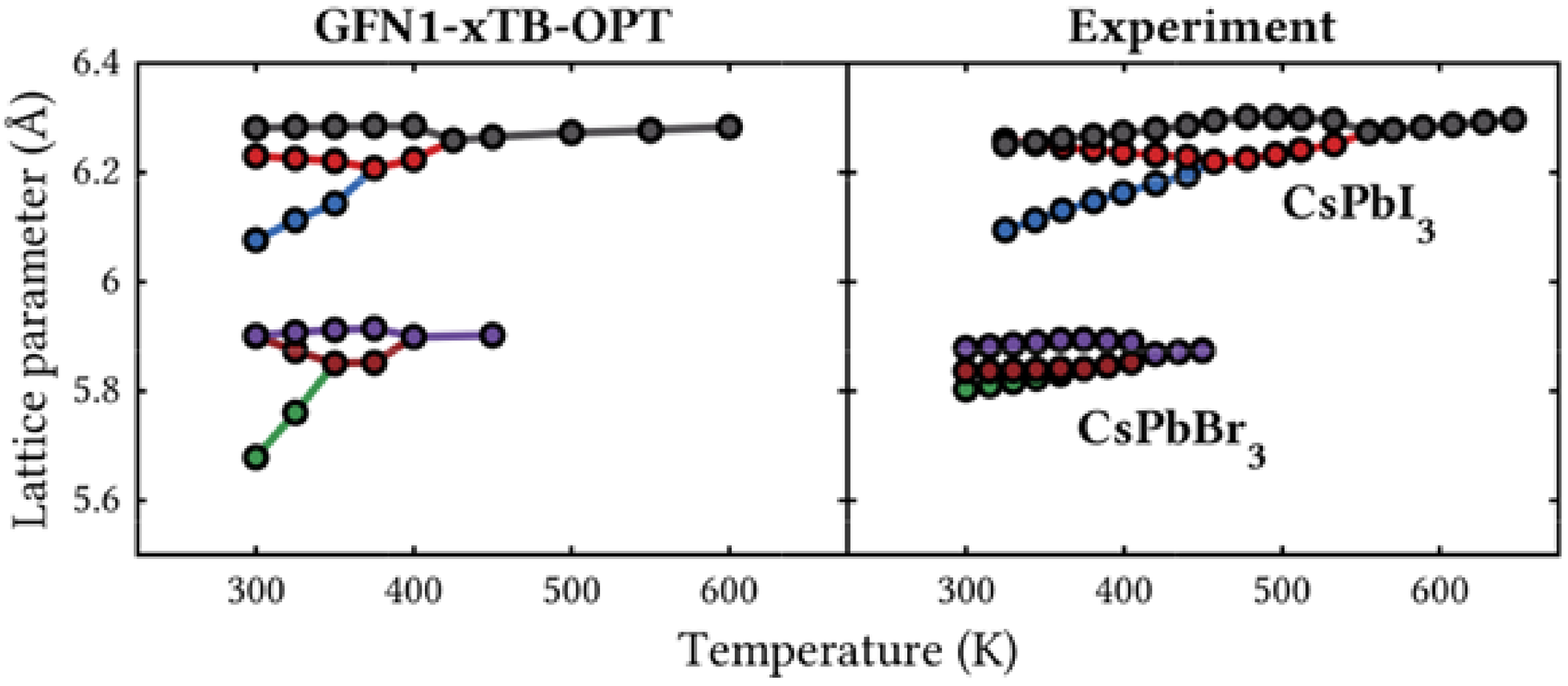


Diagonal stress tensor



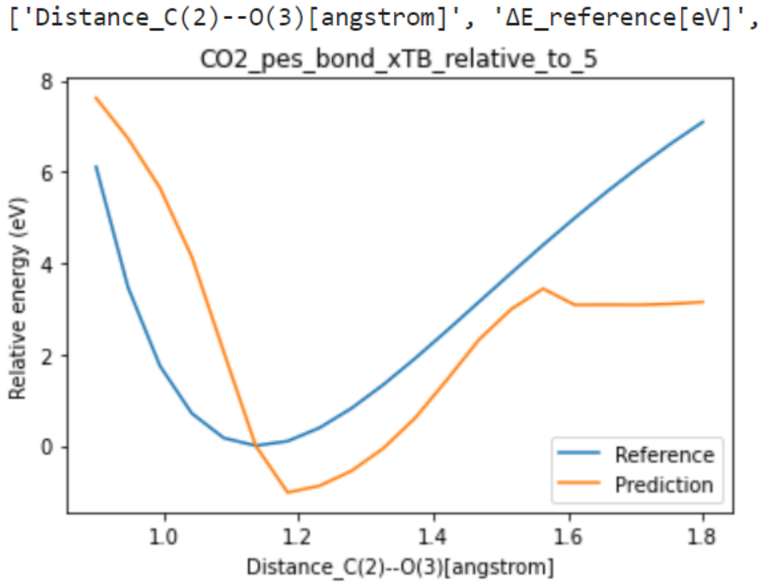
Example: reparametrize xTB for perovskites



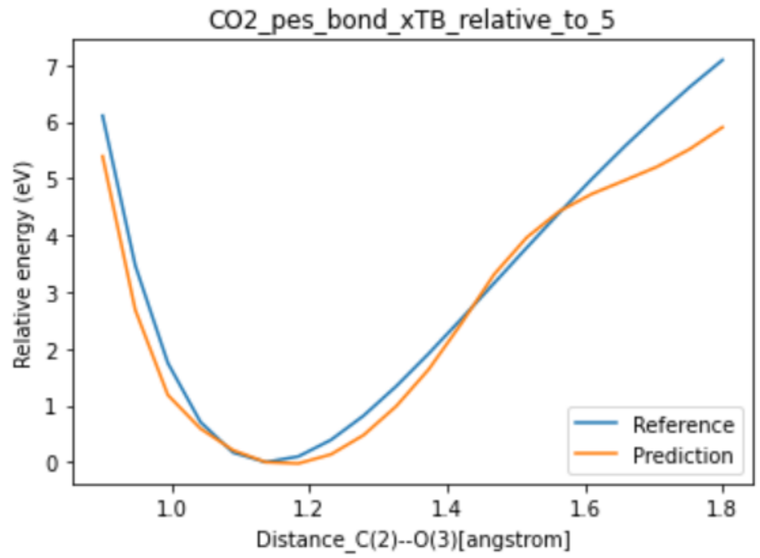


S. Raaijmakers, M. Pols, J. M. Vicent-Luna, S. Tao, ***Refined GFN1-xTB Parameters for Engineering Phase-Stable CsPbX3 Perovskites***, J. Phys. Chem. C, **126**, 9587-9596 (2022)

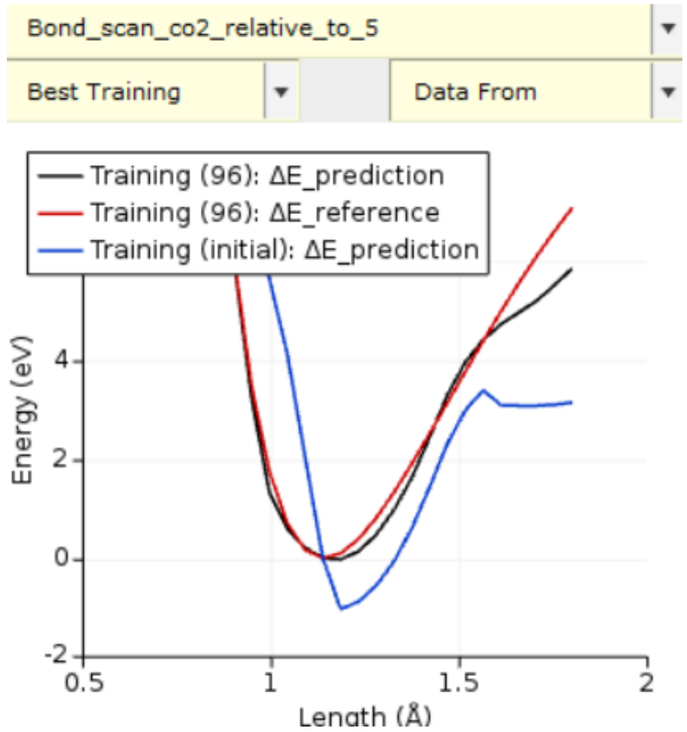
Demo: fix CO_2 bond scan



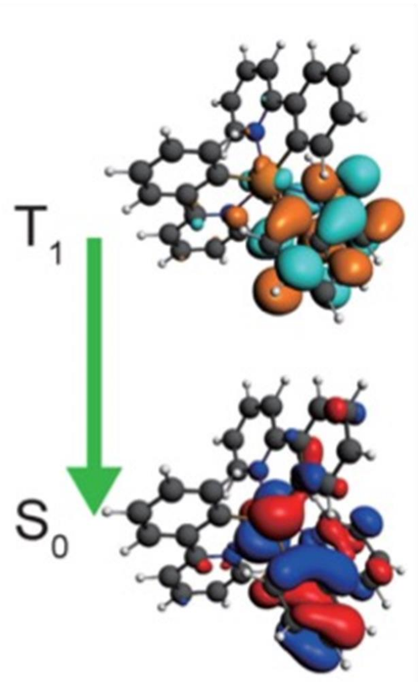

```
s = Settings()
parameter_interface = ReaxFFParameters(settings=s,ffieldfile='AgZnO.ff')
parameter_interface.yaml_store(os.path.join(params_folder,'parameter_interface.yaml'))

parameter_interface.header['head'] = "Reparametrization of AgZnO.ff"
for p in parameter_interface:
    if p.name in ['C.O:D_e^pipi','C.O:r_0^pipi']:
        p.is_active = True
parameter_interface.yaml_store(os.path.join(params_folder,'parameter_interface.yaml'))
```

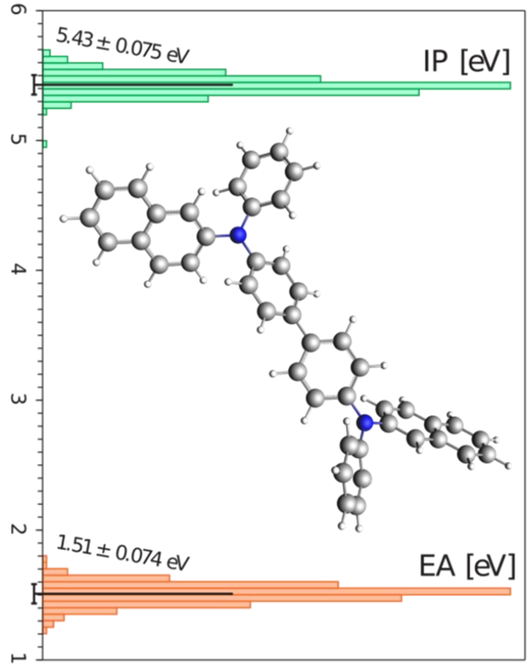


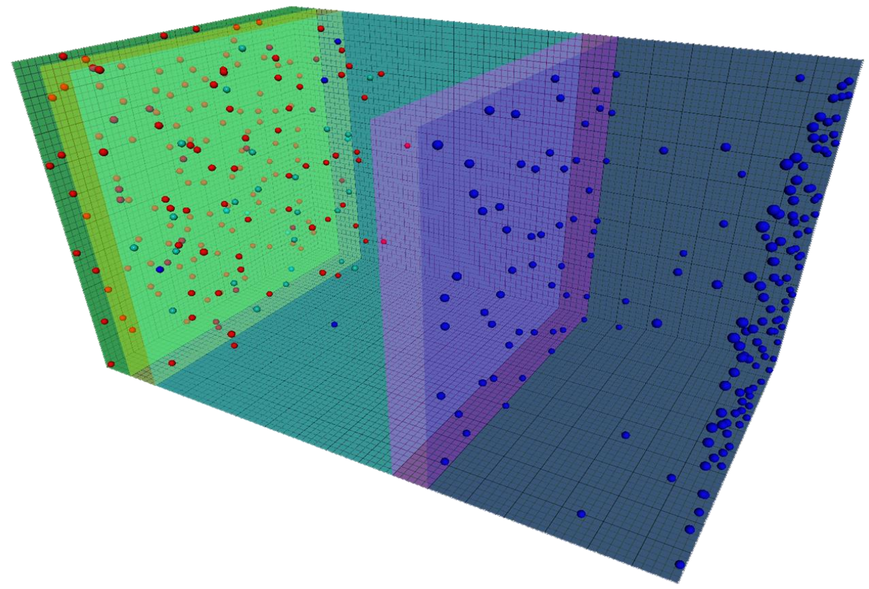
[JuPyter Notebook](): CO2-reparam.ipynb
GUI files in CO2-reparam directory

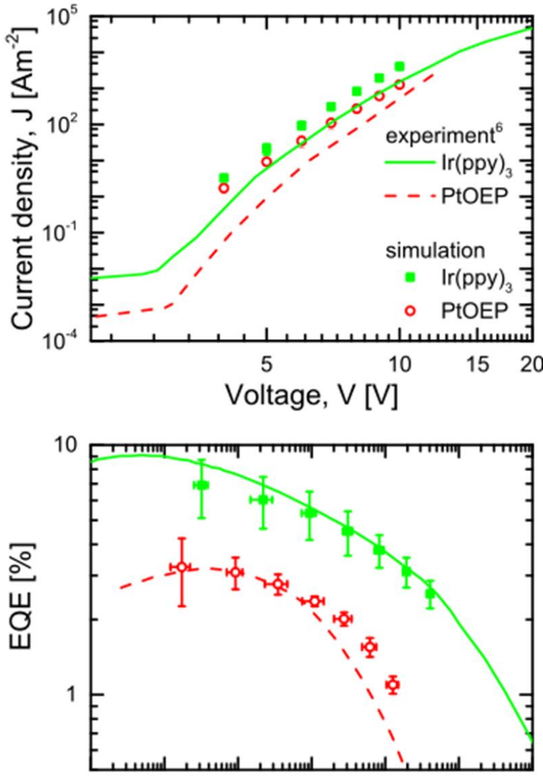


(Multi-scale) modeling OLED materials

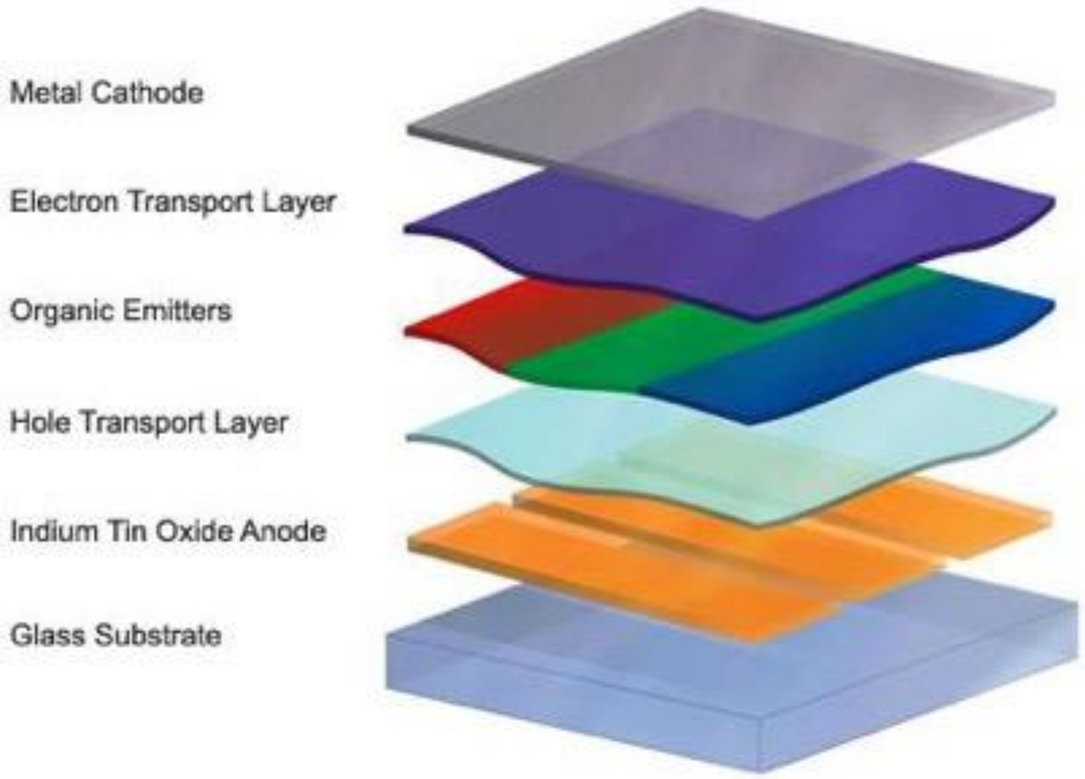








Integrated OLED multi-level modeling



- Maximize luminescence
- Optimize color
- Minimize destructive processes
- Optimize charge & exciton transport

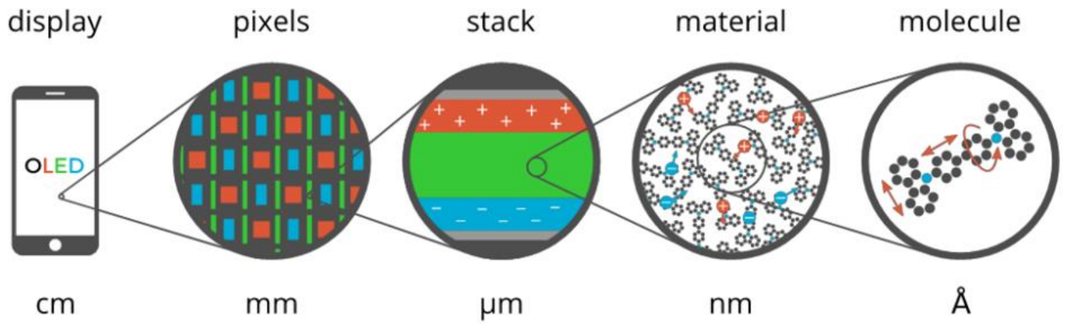
OPV: same properties

Atom & electrons determine single material properties

Predict, understand & improve with **atomistic modeling**

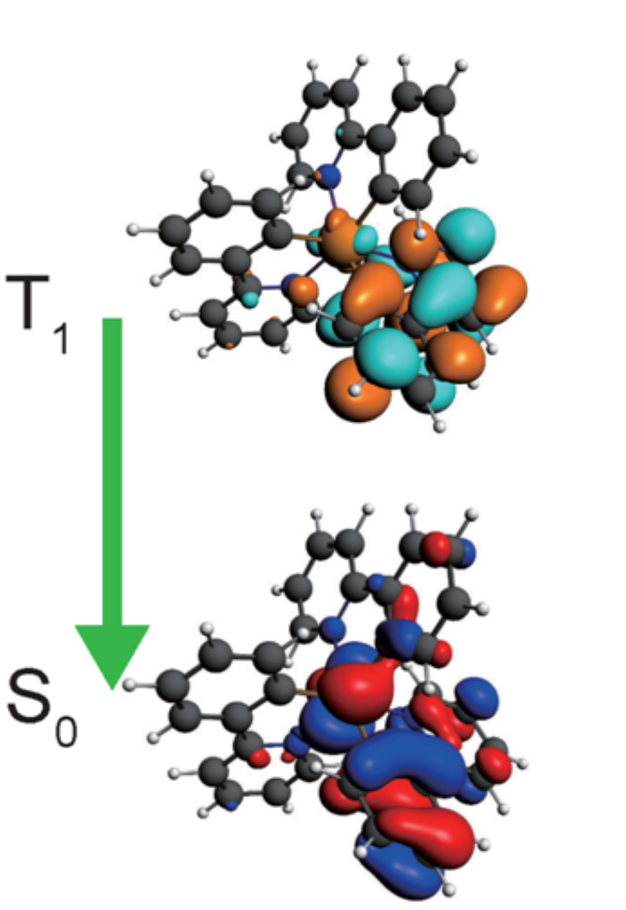
Interactions between materials determine device-level behavior

Predict, understand & improve with **meso- & macroscale modeling (with Simbeyond)**

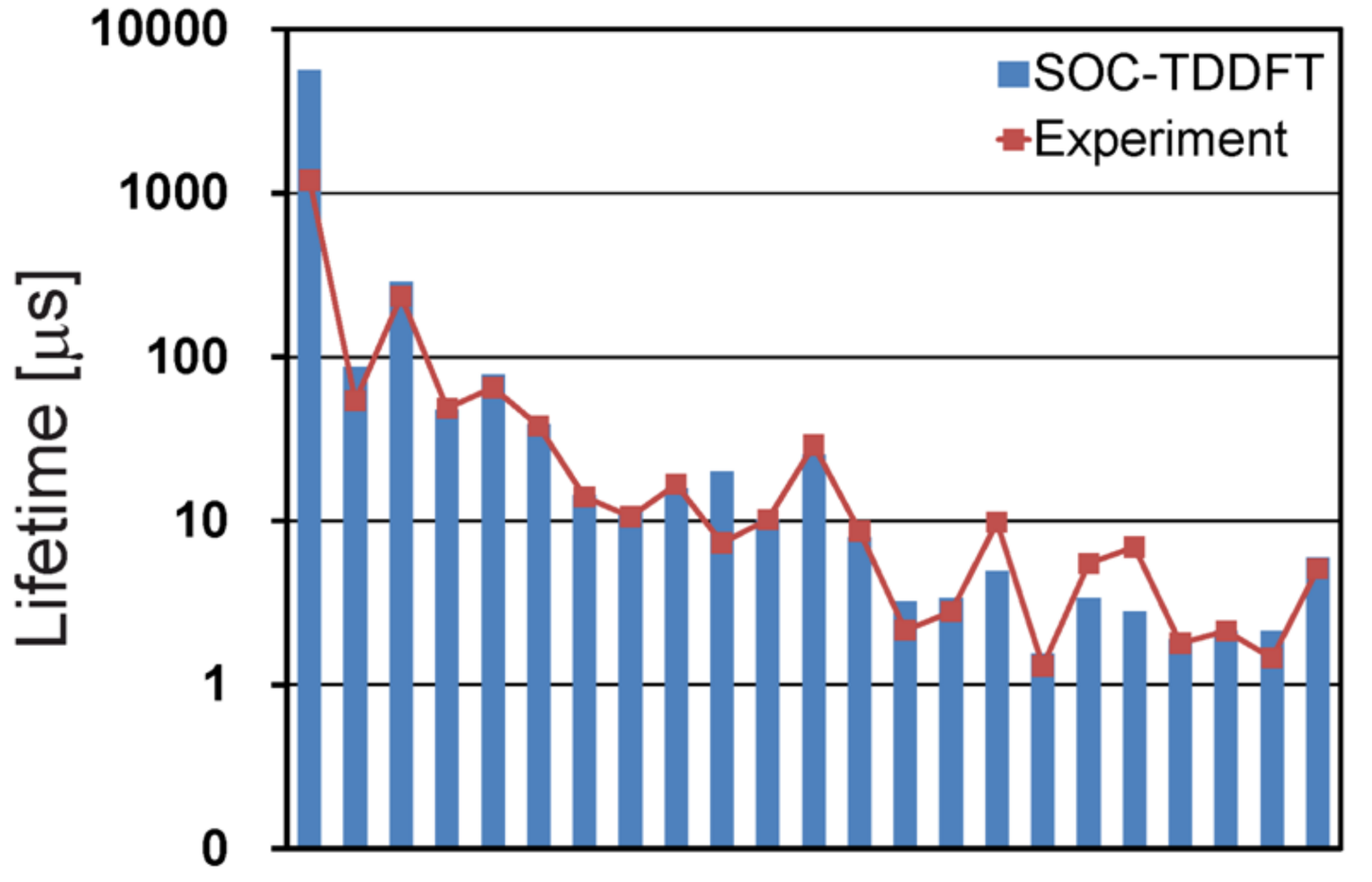


Optimize OLED emitter lifetimes

ADF 2005: Spin-orbit TDDFT => phosphorescence lifetimes



Phosphorescence

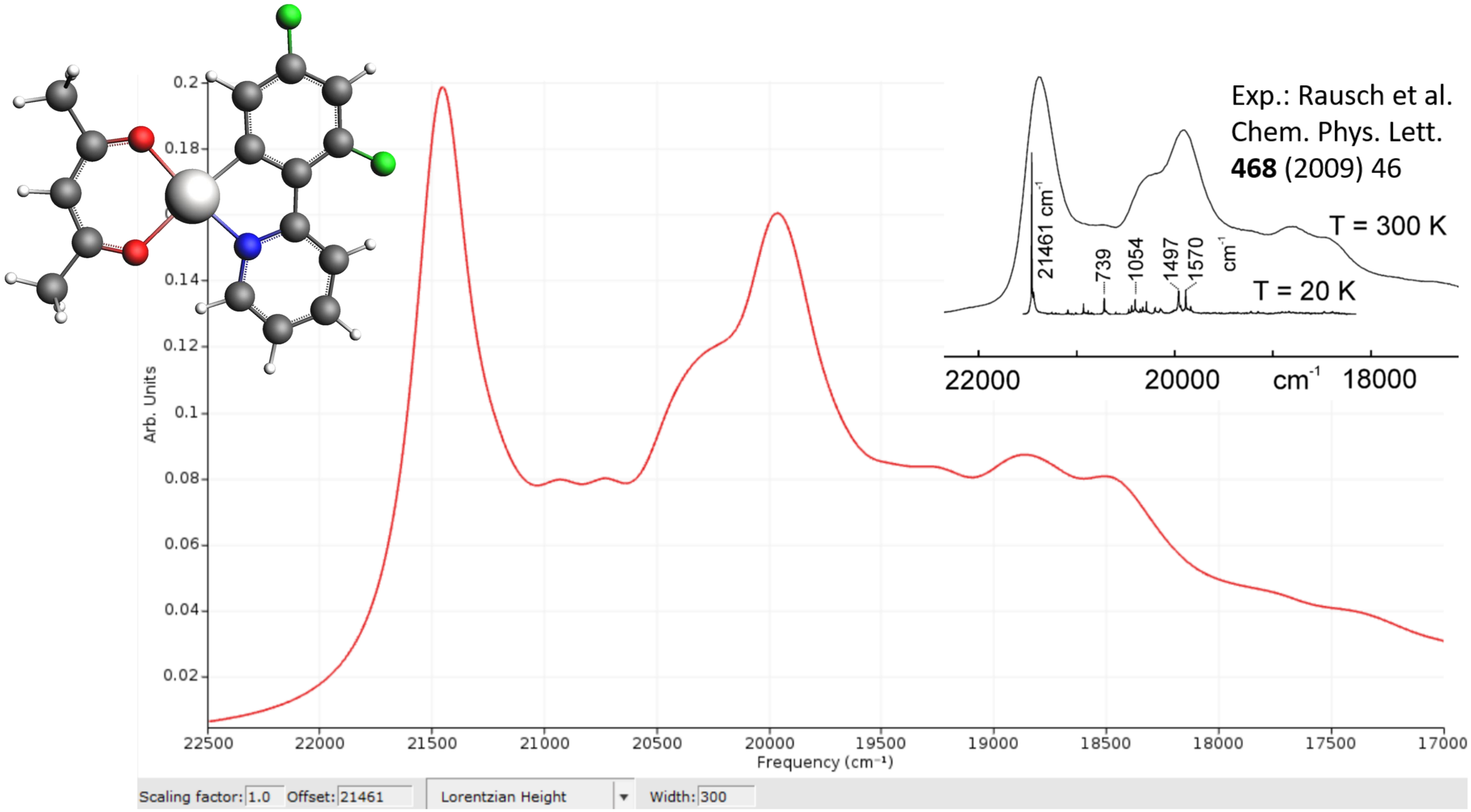


Ru, Rh, Pd, Re, Os, Ir, Pt complexes

PCCP 16, 14523 (2014)

- **BASF**: efficient blue emitter (Adv. Mater. 2010), patent 2016 (=> UDC)
- **DuPont**: protocol for screening lifetimes (JPCC 2013)

Optimize OLED emitter color / emission width

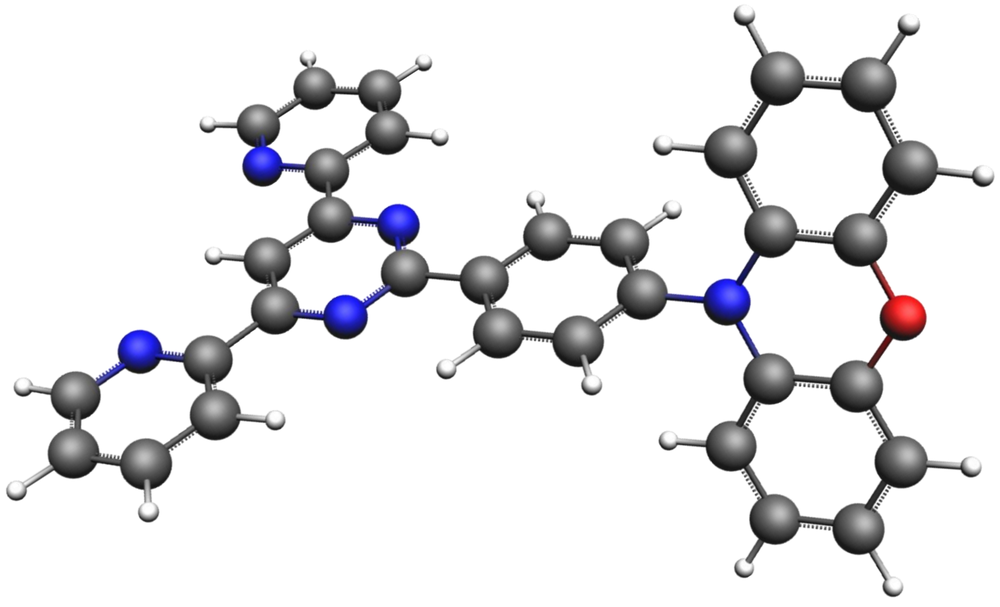


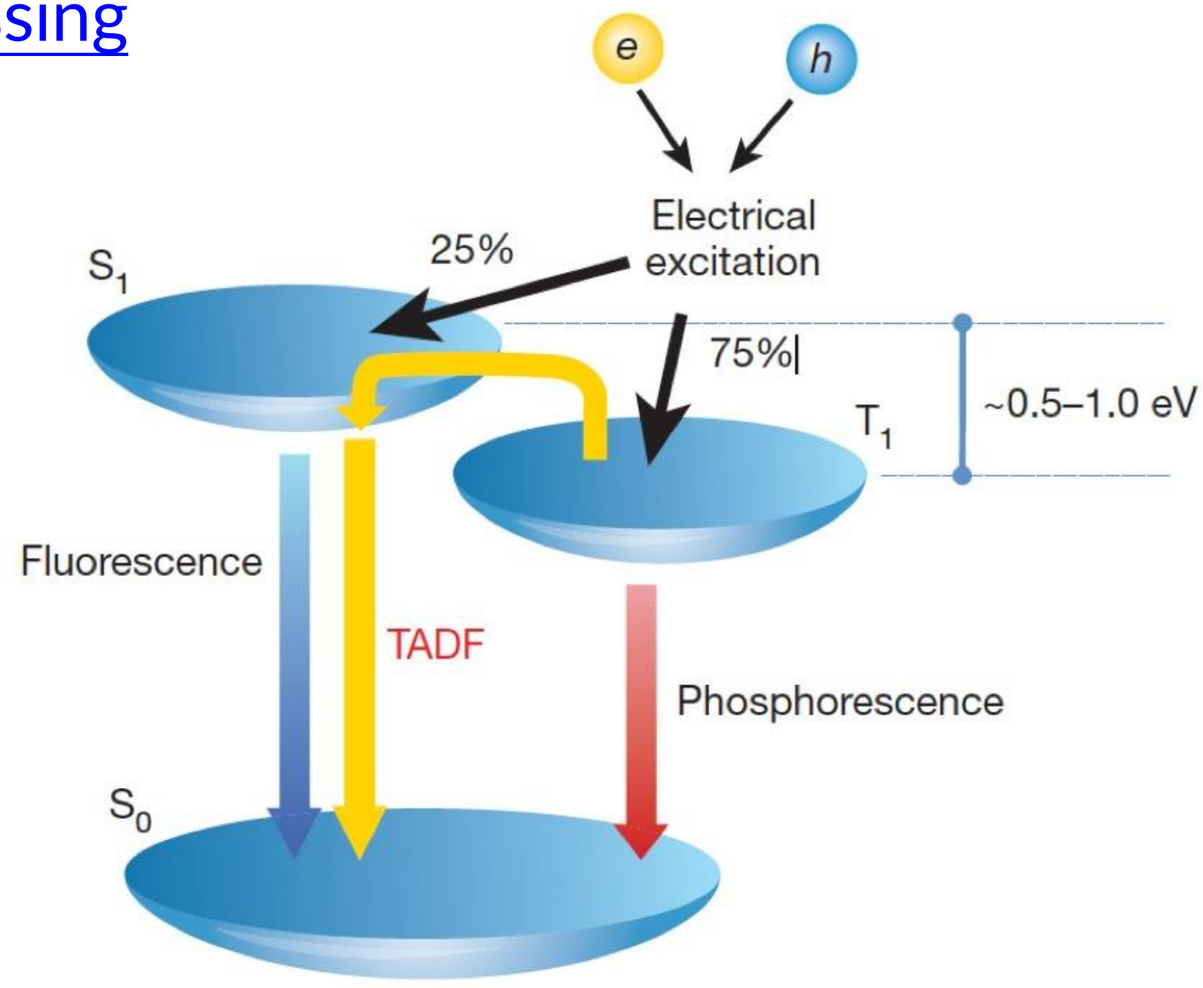
- Excellent agreement vibrational progression FCF T_1-S_0
- 0-0 well reproduced by Delta SCF calculation (22,000 cm^{-1})

Optimize TADF emission rate

Spin-orbit TDDFT => Intersystem crossing

- Min. S_1-T_1 gap & Max. SOC
- Min. emission width
- Max. k_{phos} & k_{TADF}





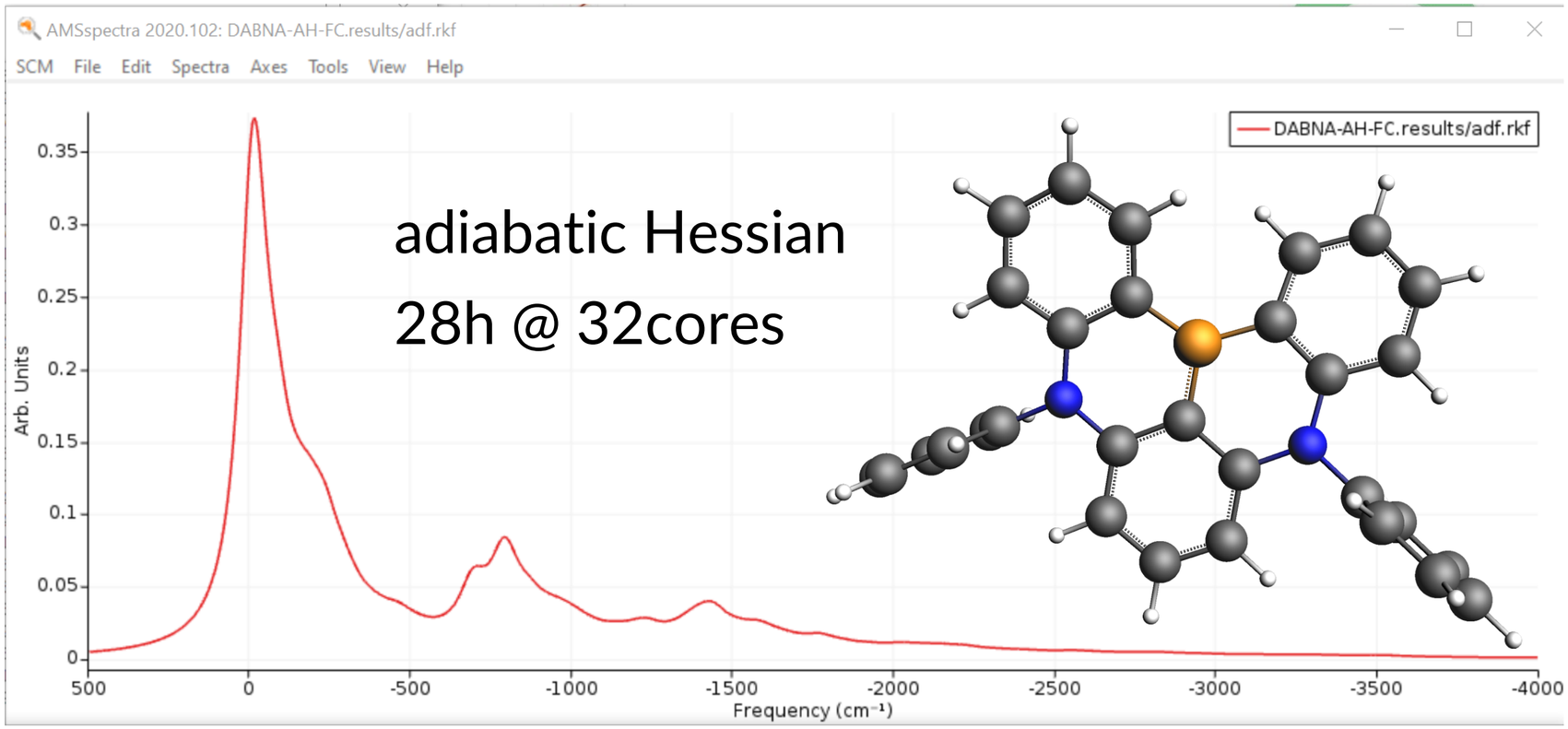
- Z.-M. Su et al Dyes & Pigments 2017, Bredas et al. J. Am. Chem. Soc. 2017
- **OSRAM**: patent 2018, **Cynora**: patent 2019
- blue TADF emitter: Nanomat. 2019; Organic Electronics 2020

Emission width TADF emitters: faster calculations

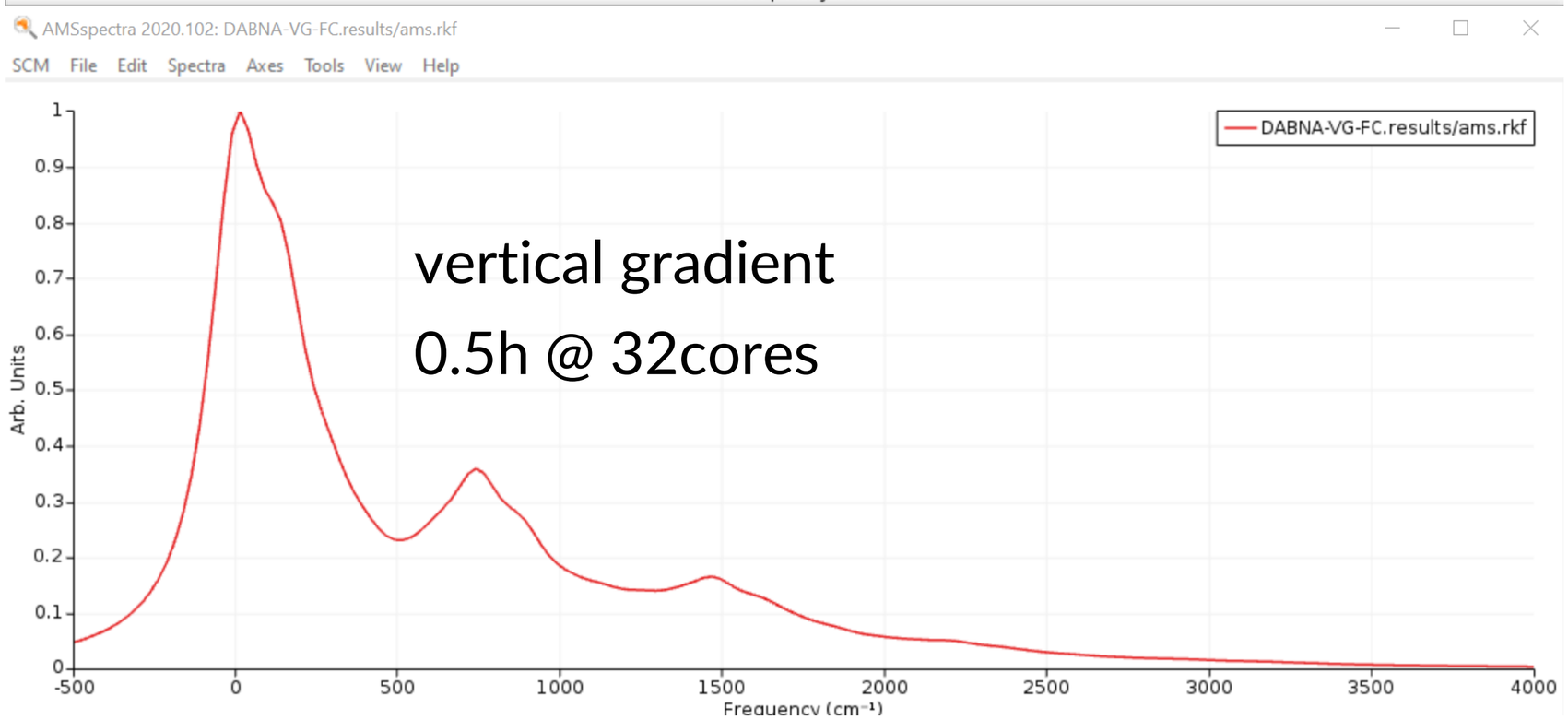
quicker screening

vibronic spectrum
DABNA & related

TADF emitters

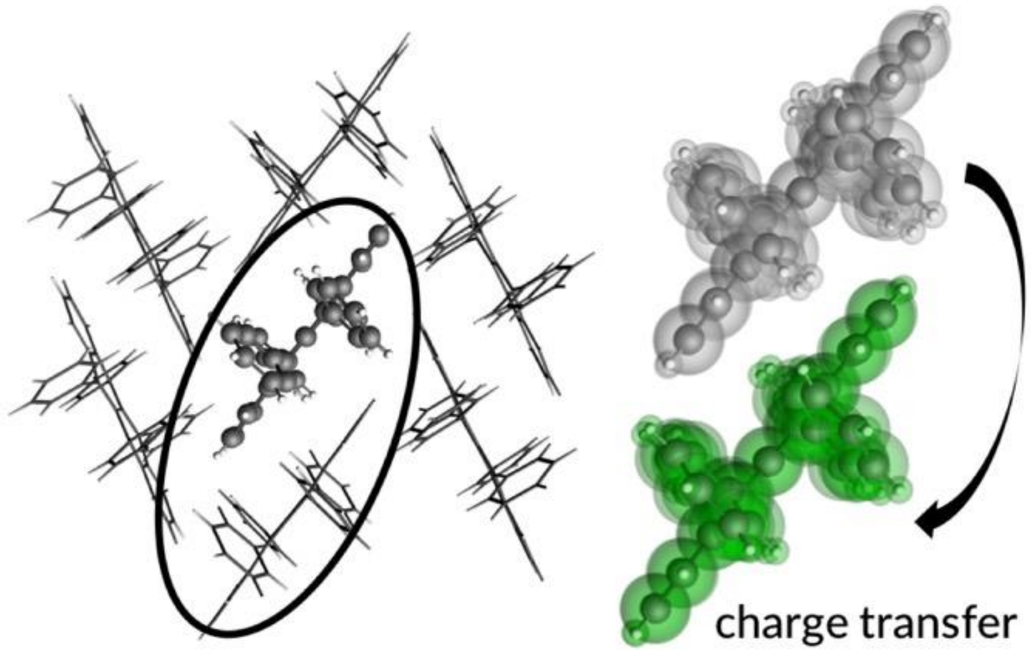


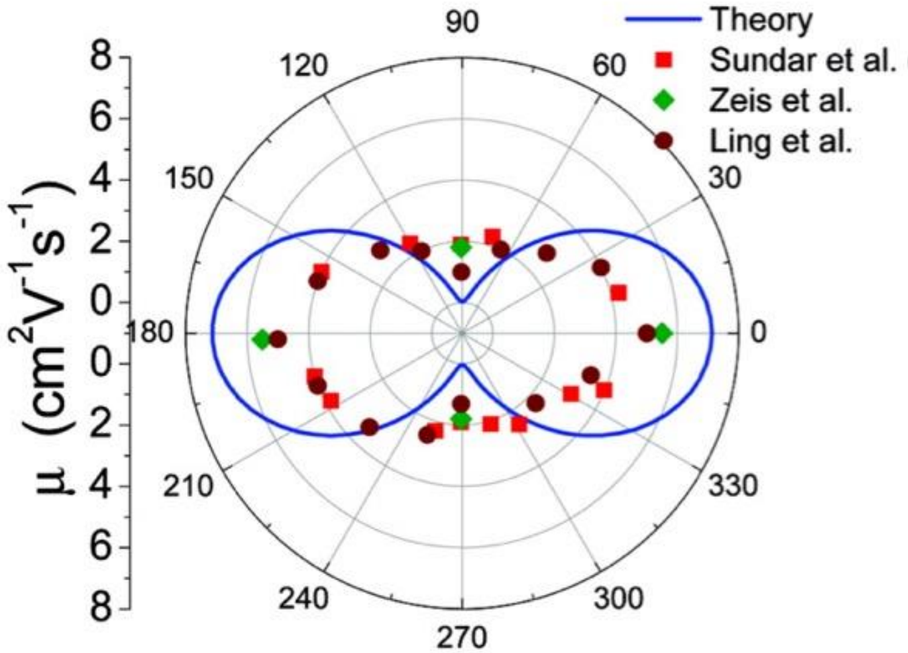
Protocol + modify ->
python workflow->
cluster/cloud



Optimize charge mobility (OLED, OFET)

- 2003: easy to get transfer integrals from ADF (fragment-based)
- 2007: organic semiconductors (**BASF**): hole and electron mobility



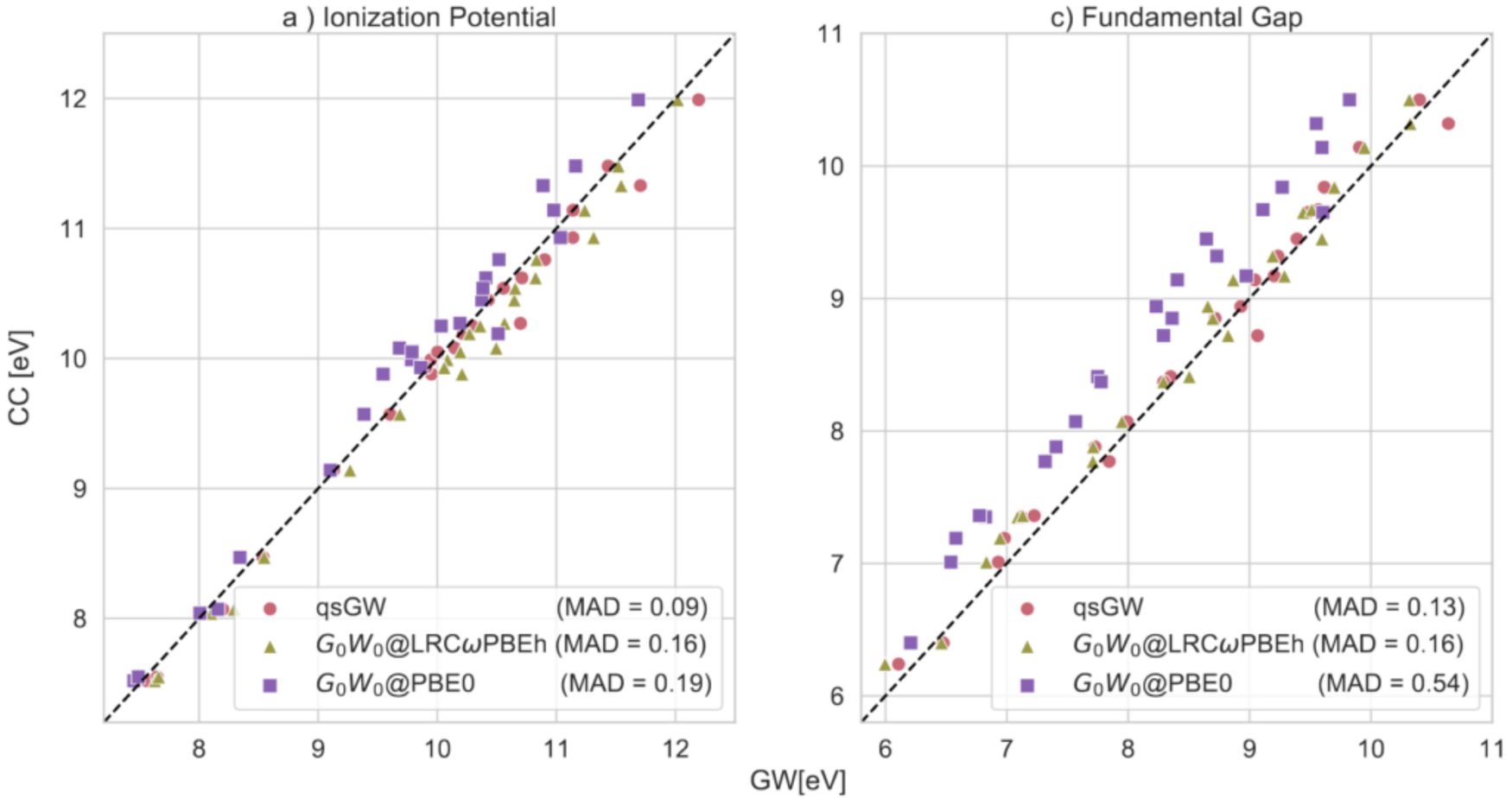


- Solubility / miscibility: COSMO-RS

From adiabatic states (FDE)

- Environment polarization
- Charge generation
- Charge recombination
- Exciton transfer

Ionization Potentials & Electron Affinities: qsGW



Webinar

Recommended:

- qsGW
- TZ2P or larger

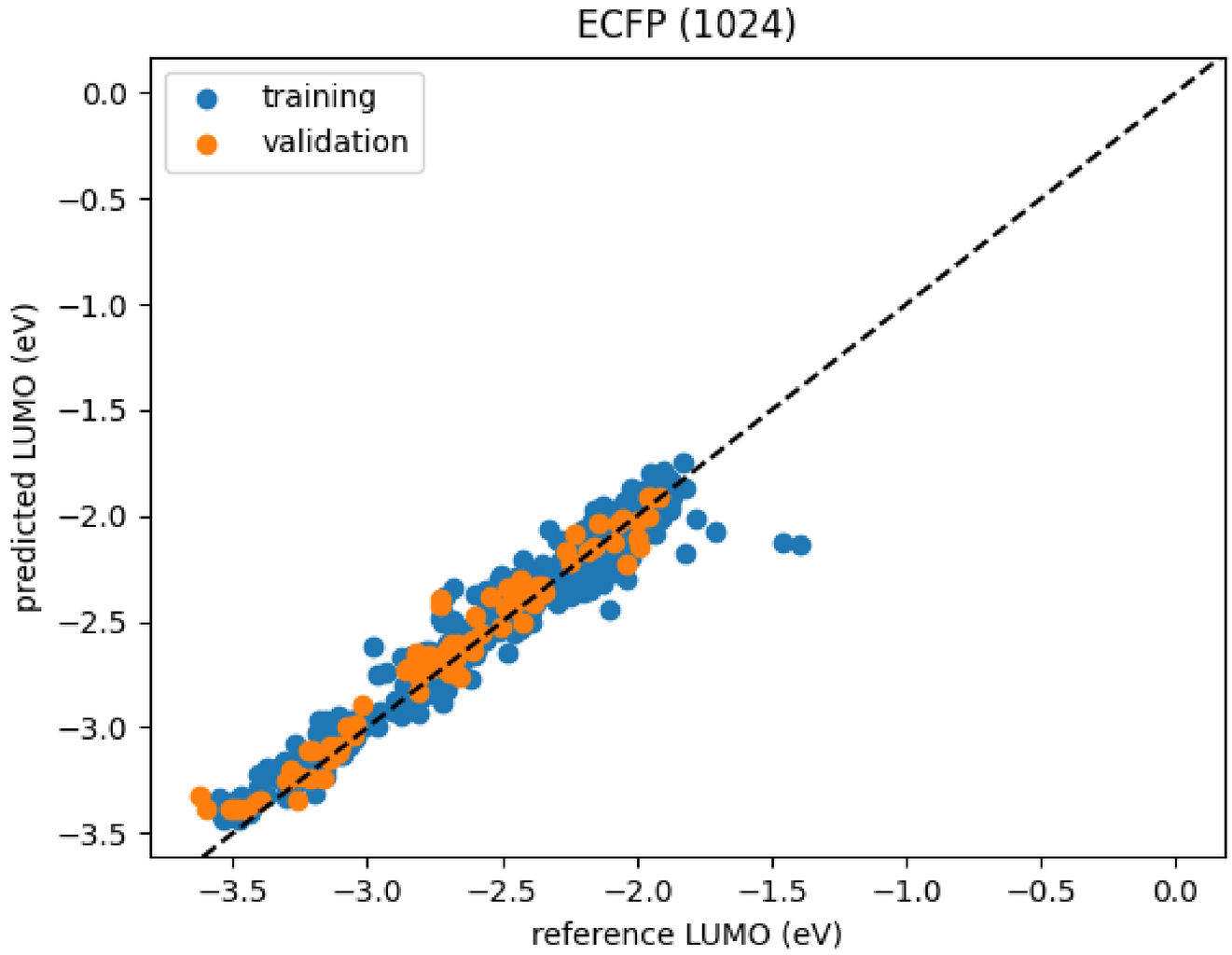
IP = -HOMO
EA = -LUMO

- Quasiparticle self-consistent GW: can use a GGA
- Spin-orbit coupling **and** excitations with BSE possible (qsGW-BSE)
- In progress: qsGW embedding, alternative: COSMO corr. with DFT

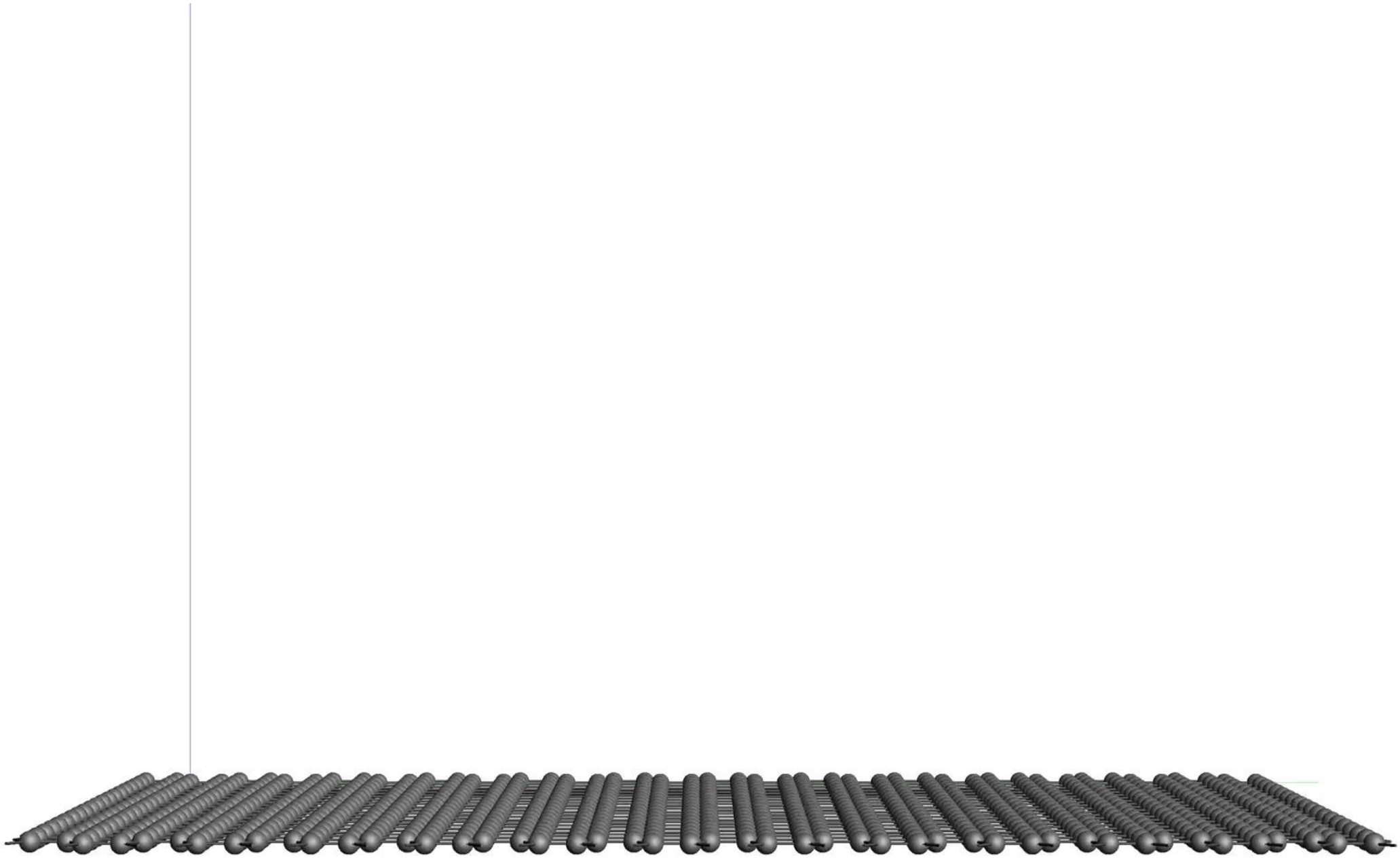
A. Förster, L. Visscher, Low-Order Scaling Quasiparticle Self-Consistent GW for Molecules, Frontiers in Chemistry, 2021, 9: 736591; A. Förster, L. Visscher, Quasiparticle Self-Consistent GW-Bethe-Salpeter equation calculations for large chromophoric systems, J. Chem. Theory Comput. 2022, 18, 11, 6779–6793

Accurate predictions, IP, EA, S1, T1

- Gas phase HOMO/LUMO can be well trained with NN
- Environment effects important!
- Fast GW + BSE (webinar)
- Bottleneck: deposition



Deposition: sequential = slow

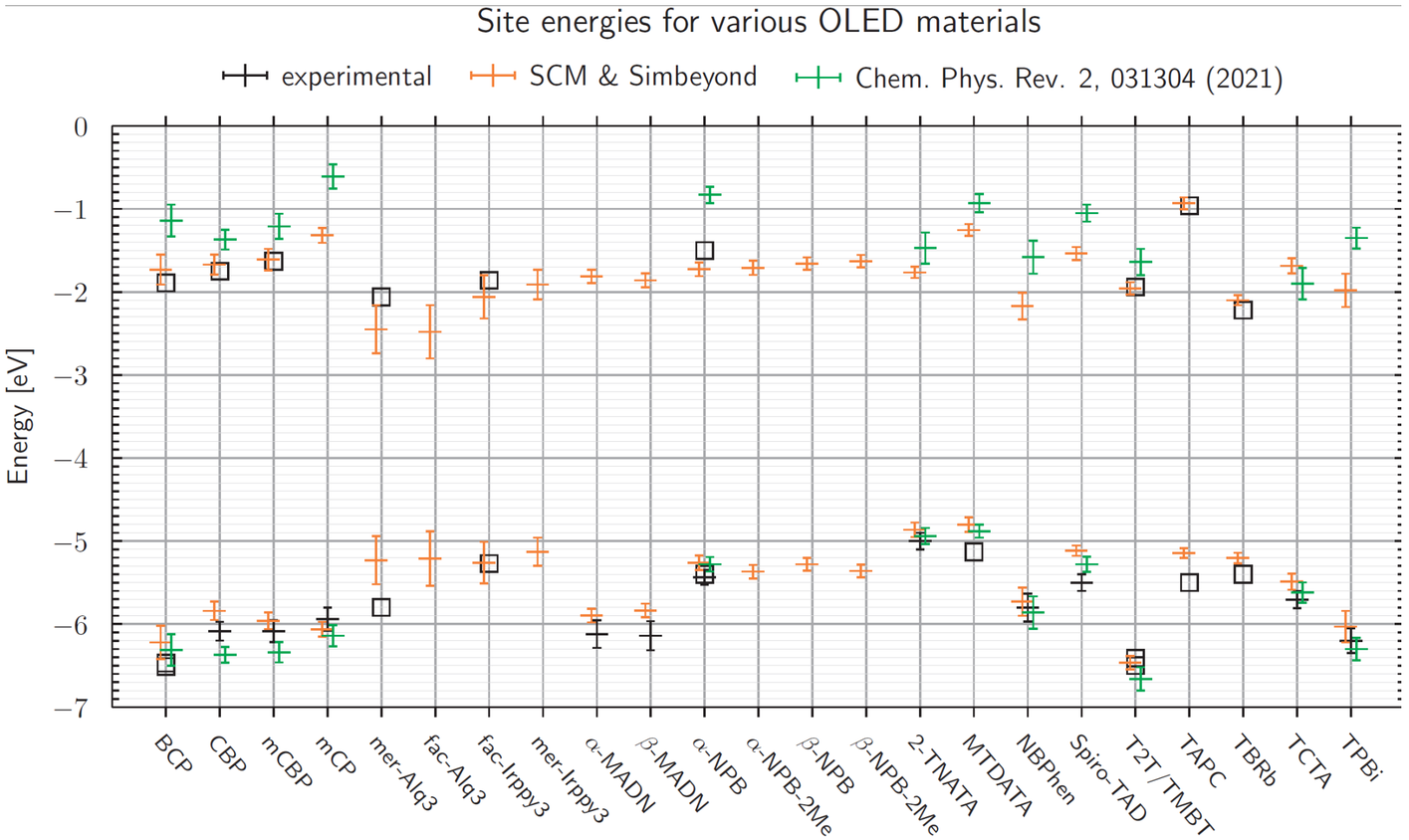


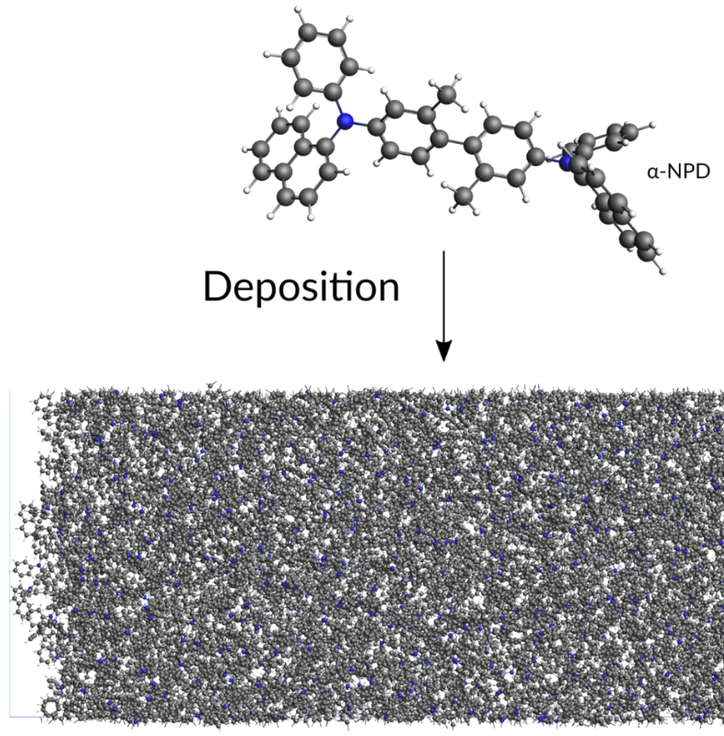
Ionization Potentials & Electron Affinities: workflow

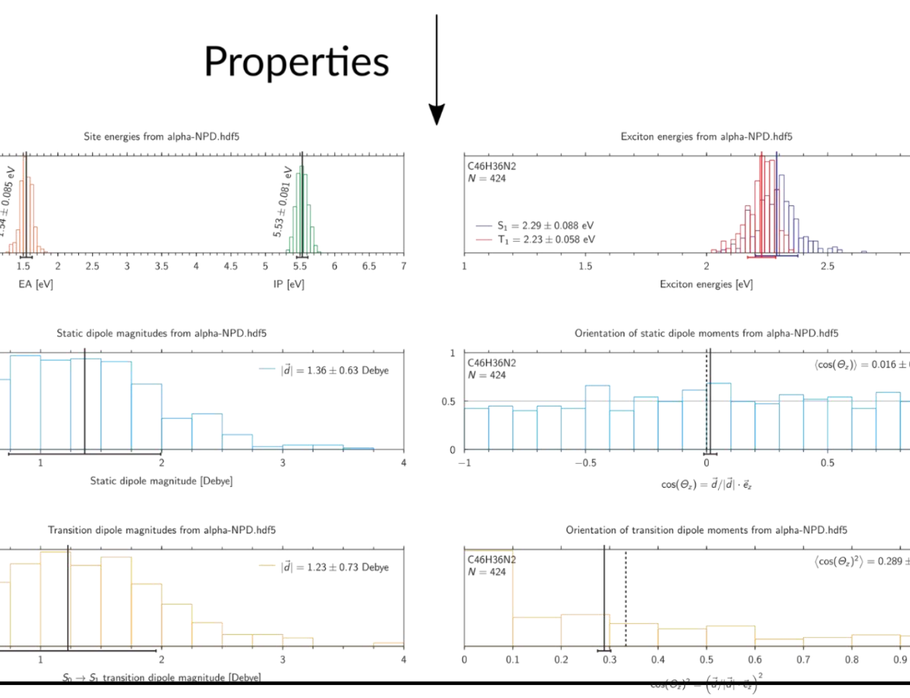
1) deposit (UFF4MOF-II) Video
fbMC, with graphite support that is later removed

2) Opt neutral, cation, anion + environment (xTB/UFF4MOF-II)

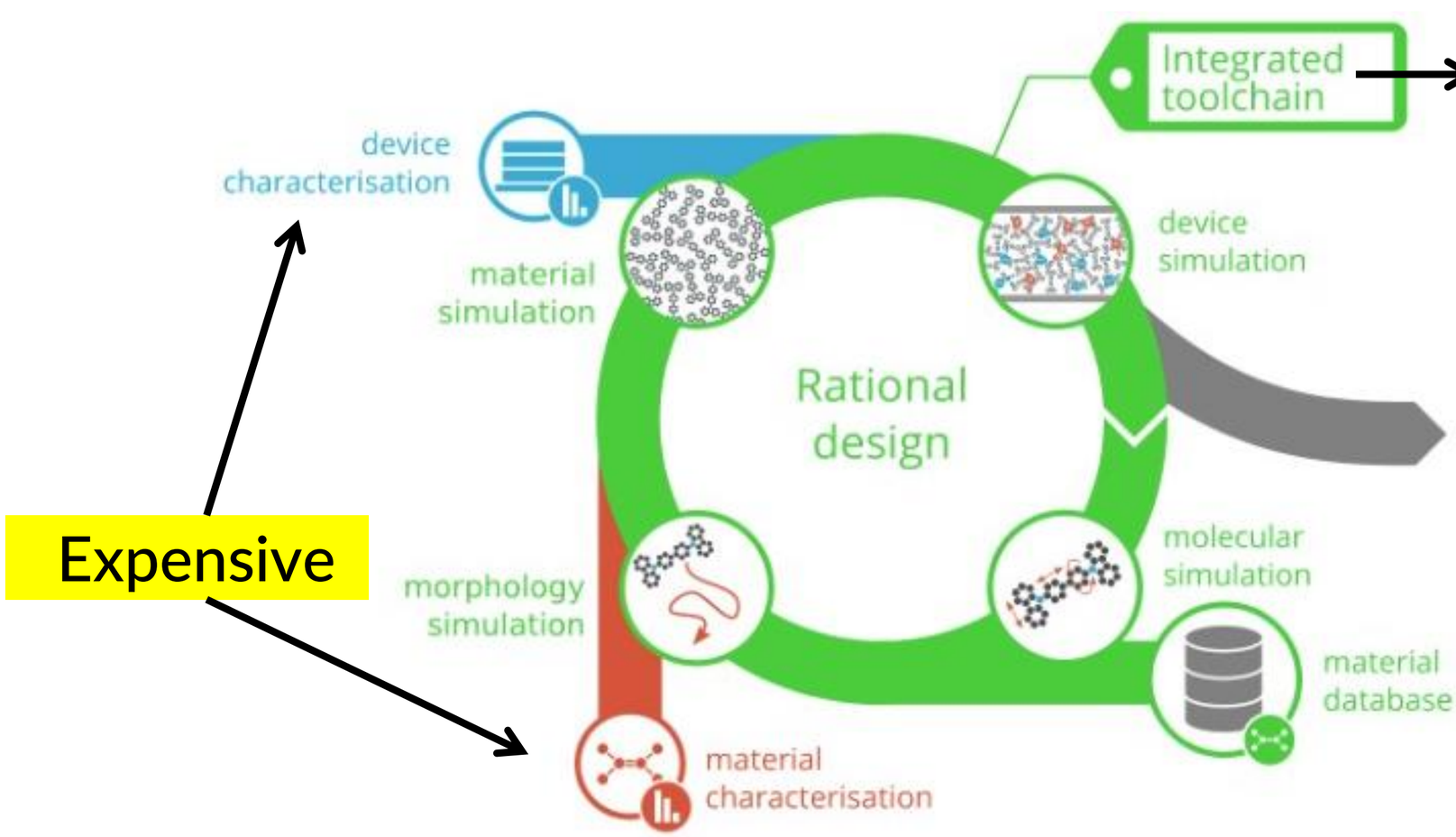
3) Calculate properties
- IP, EA: DFT+embedding
- Transfer integrals
- Exciton properties



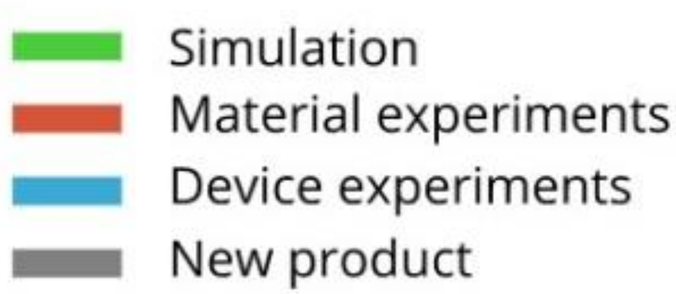




OLEDs: Optimize many materials & properties



Predict promising materials + stacks

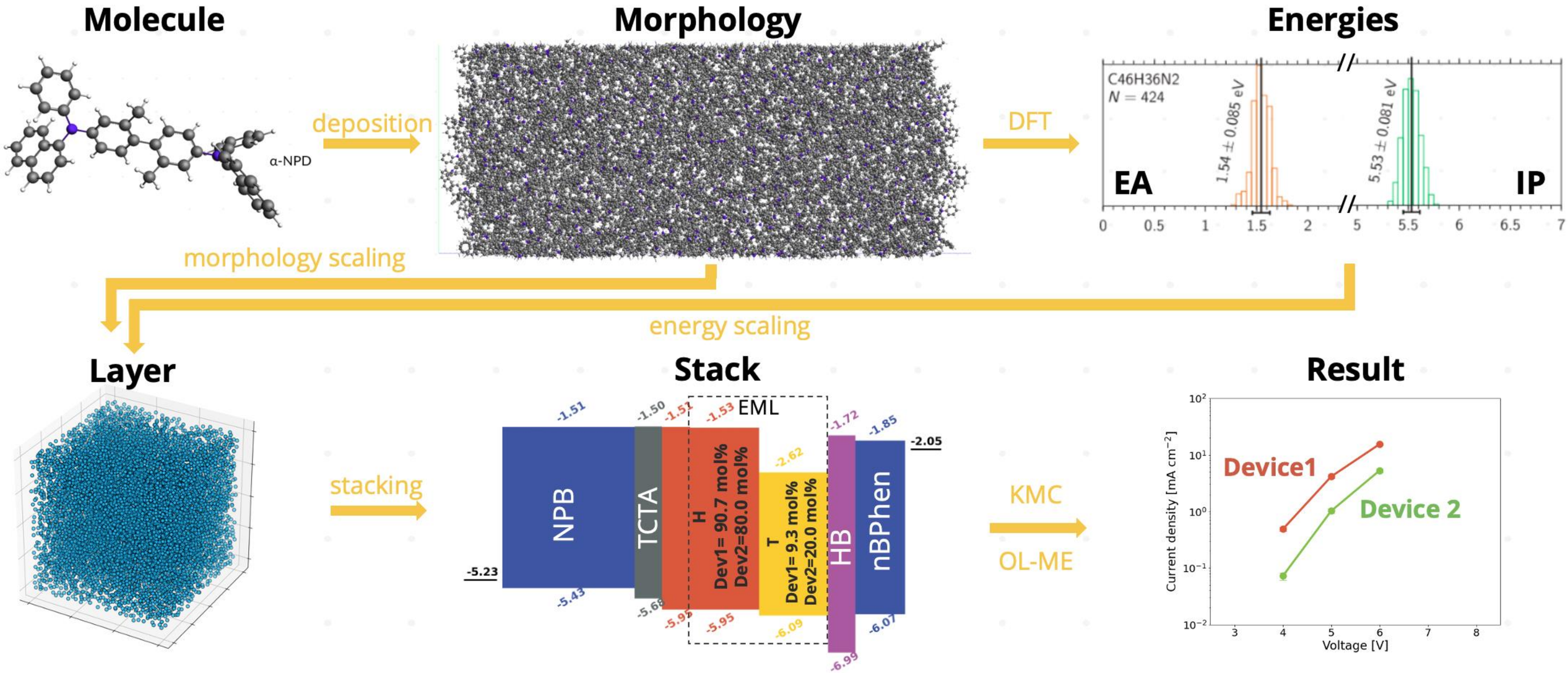


SIMBEYOND

- Molecular level:
  - Electron affinity(EA)/LUMO
  - Ionization potential(IP)/HOMO
  - Decay rates
  - Exciton energies
  - Transfer integrals

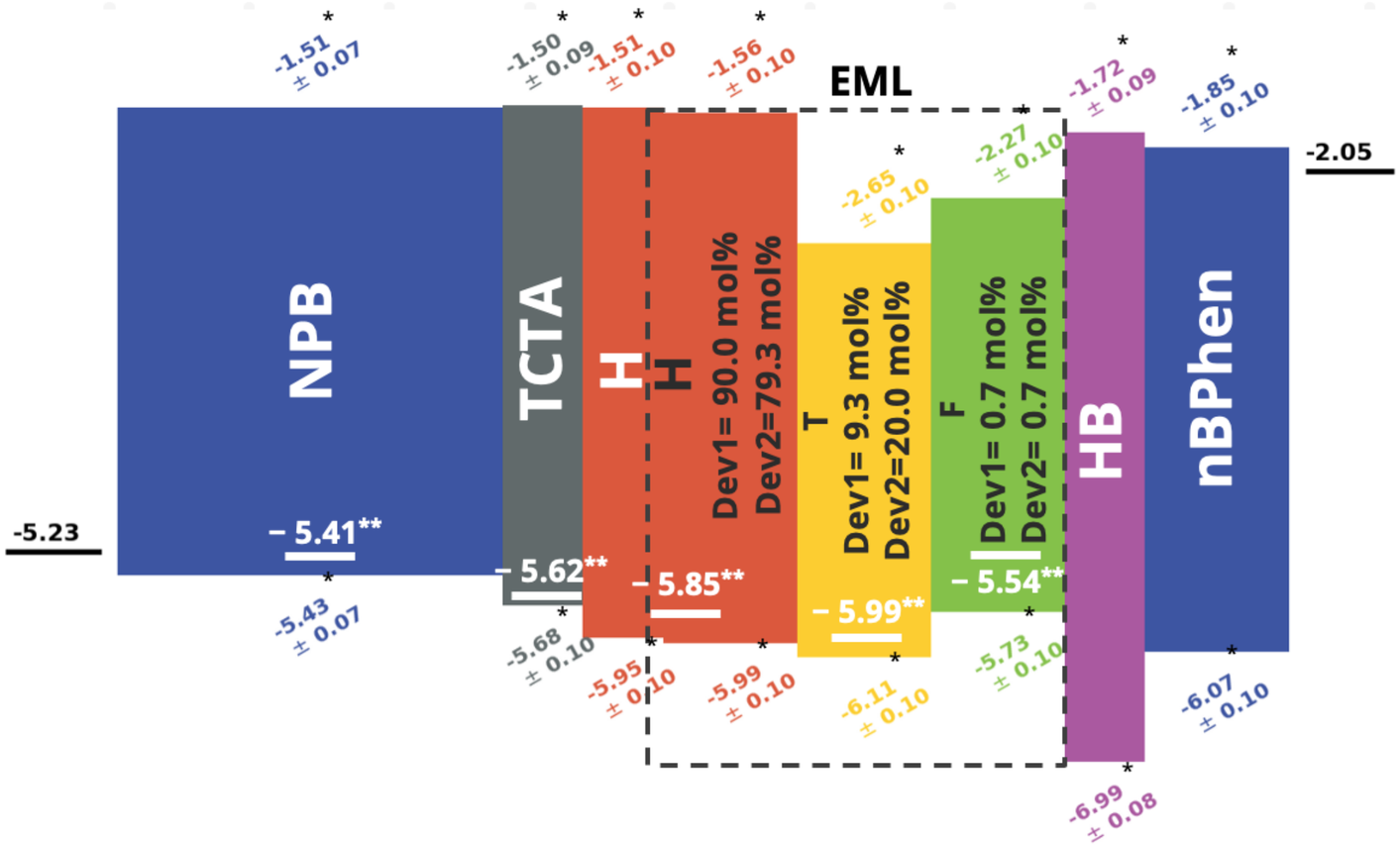
- Device level: kMC, OL-ME
- + scaling (x10)
  - Material combinations
  - Layer thickness
  - Material concentrations

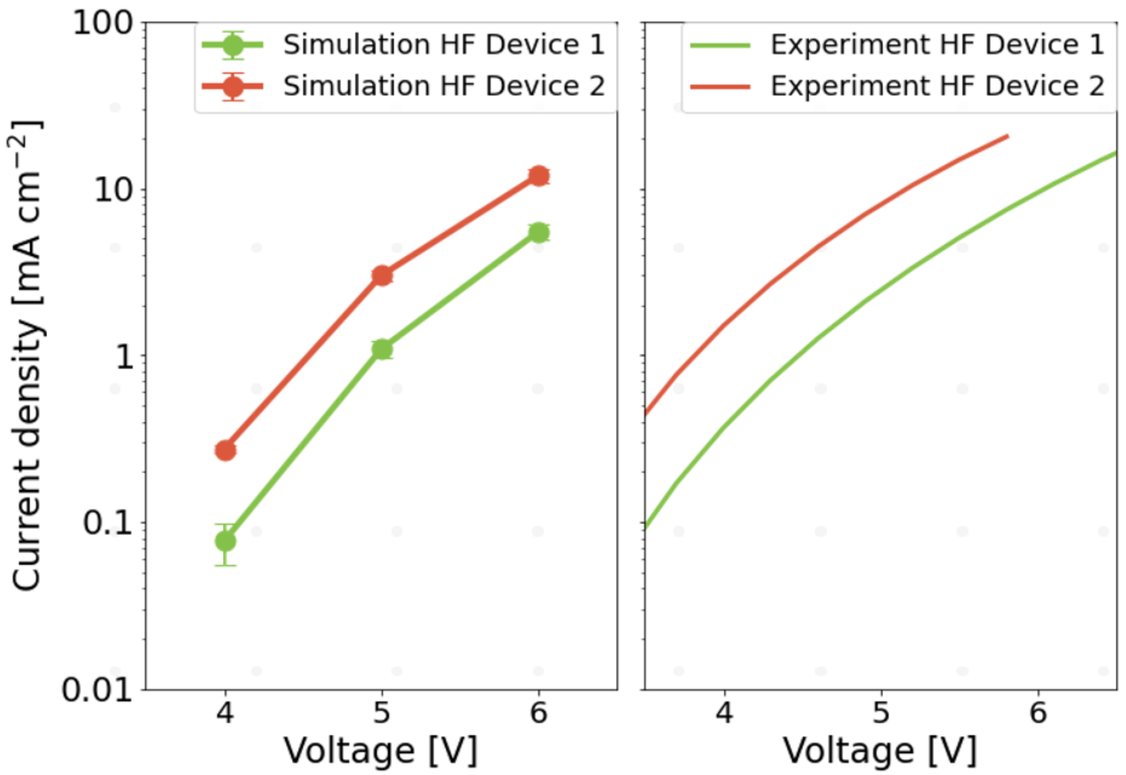
Multi-scale OLED workflow



[Webinar]

Pilot project: hyperfluorescent devices

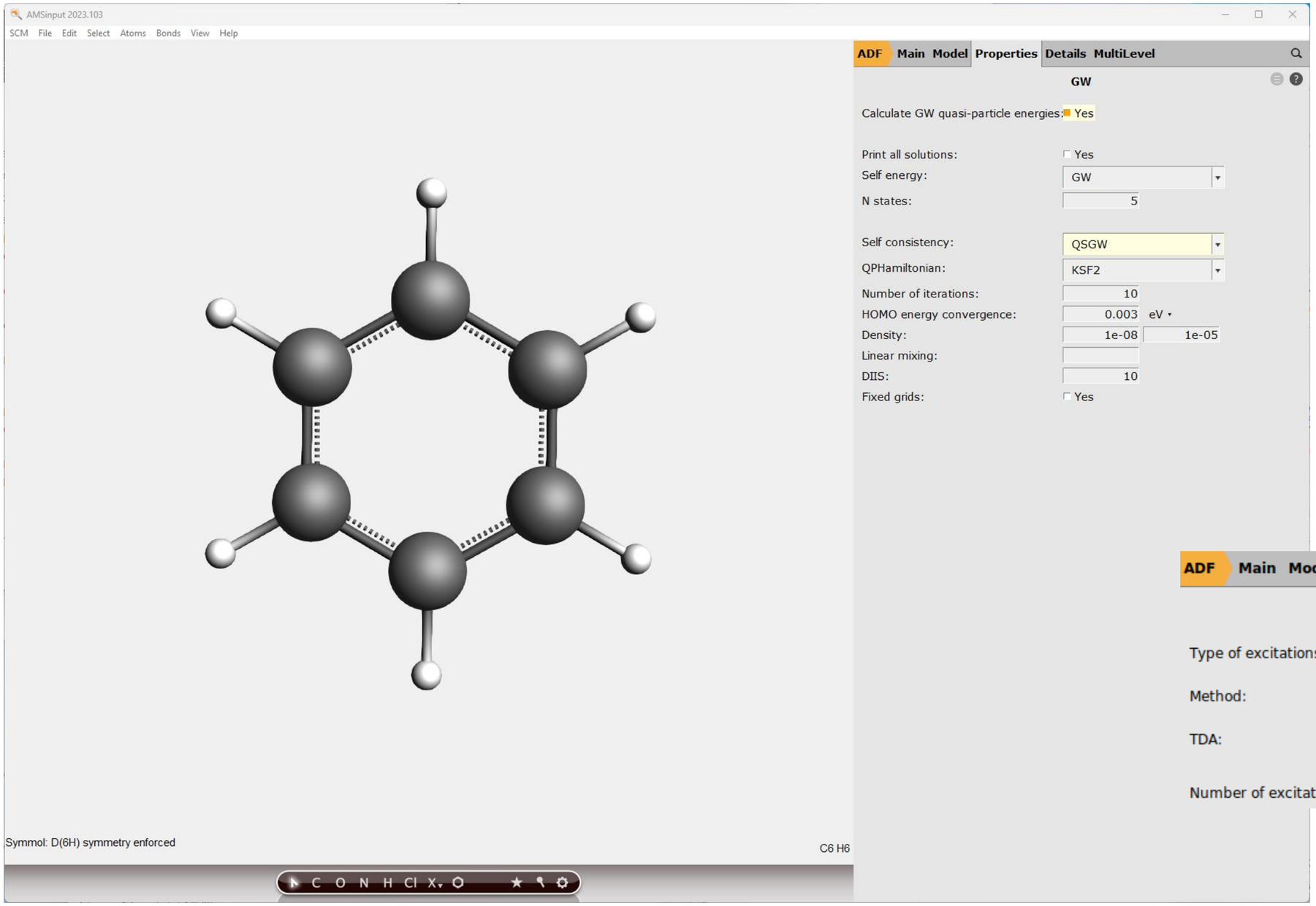


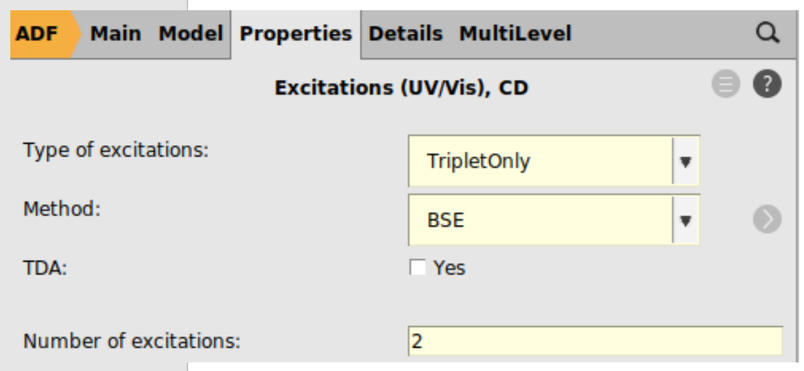


. Experimental** and computed* IP in OK agreement
. Experimental J(V) trends well captured by simulations
. Speed vs accuracy

* Calculated values from multiscale toolchain
**Experimental values Cynora

Demo: qsGW+BSE (tutorial)

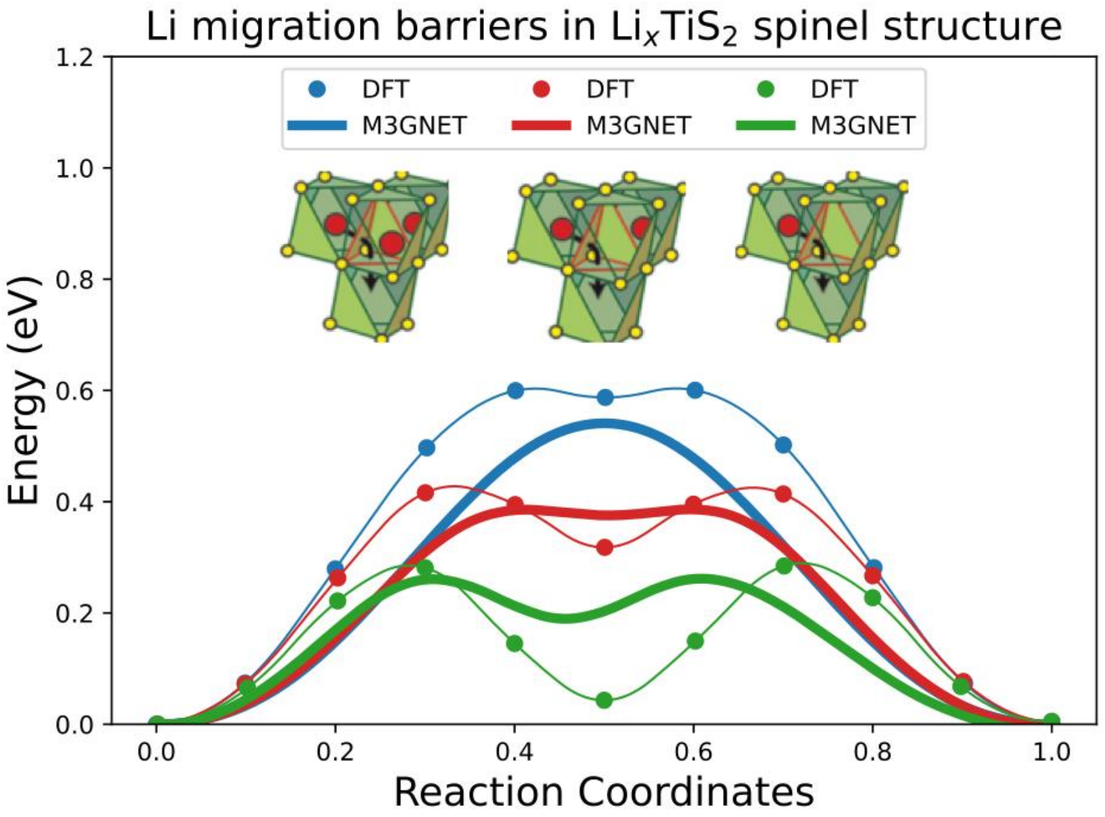


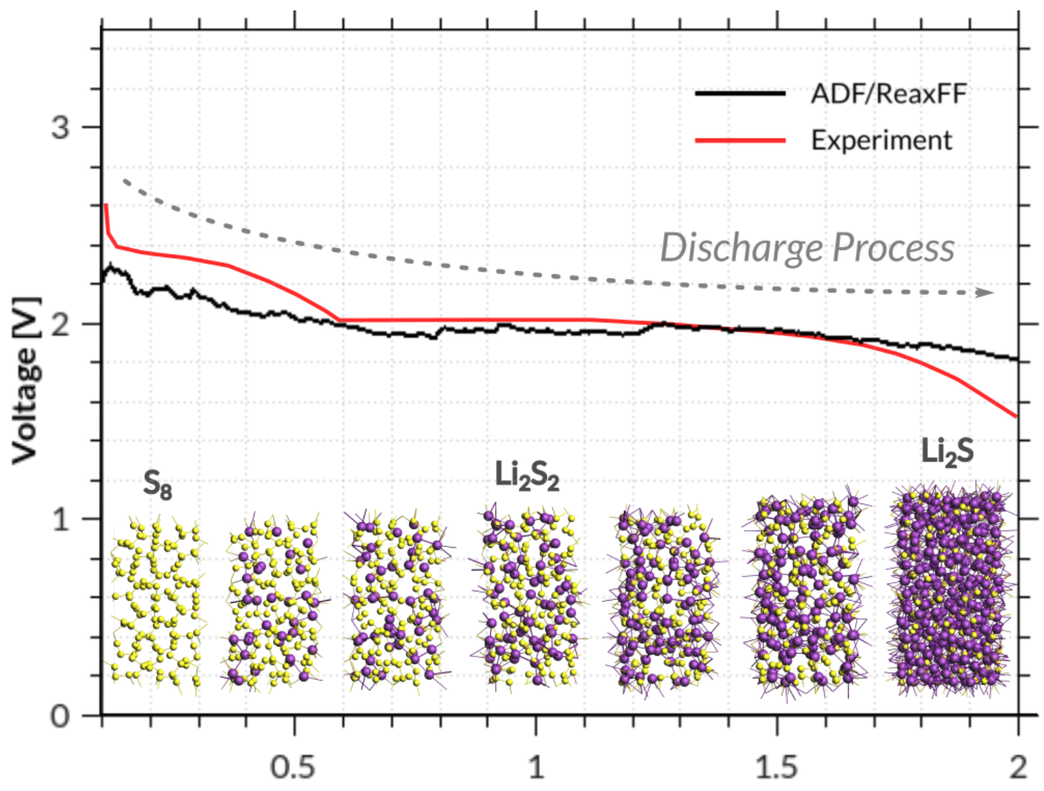


All SINGLET-TRIPLET excitation energies

no.	E/a.u.	E/eV	f	tau/s	Symmetry
1:	0.13628	3.70847	0.000		B1.u
2:	0.18139	4.93582	0.000		B2.u

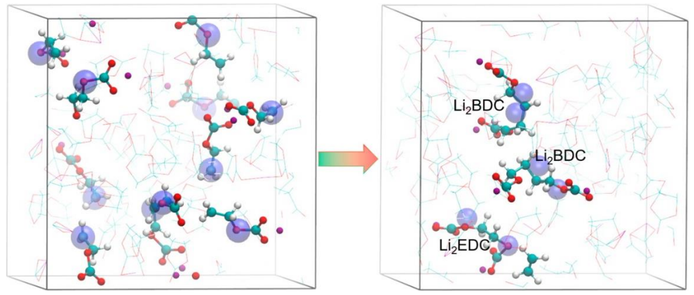
Modeling battery materials



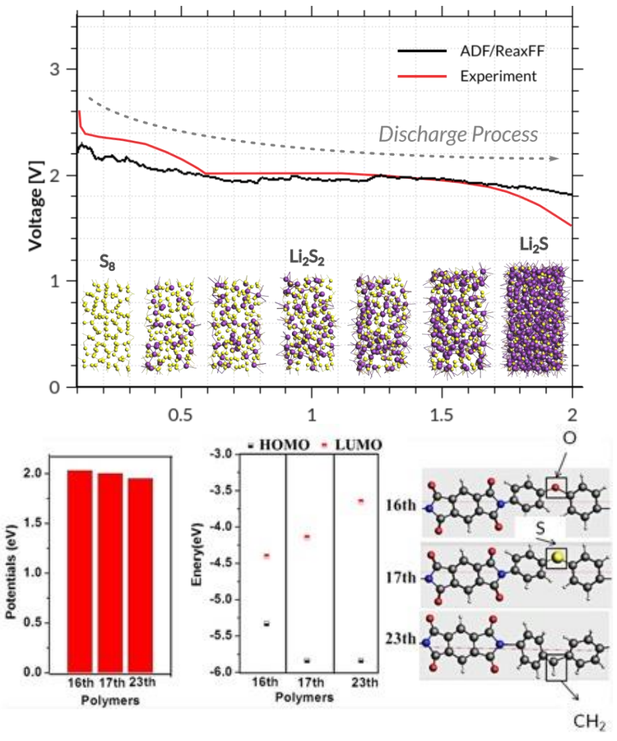


Properties for battery materials

- Charge mobility, diffusion, viscosity
  - ReaxFF, APPLE&P, DFTB-MD
  - NEGF: I-V curves, mobility across interface

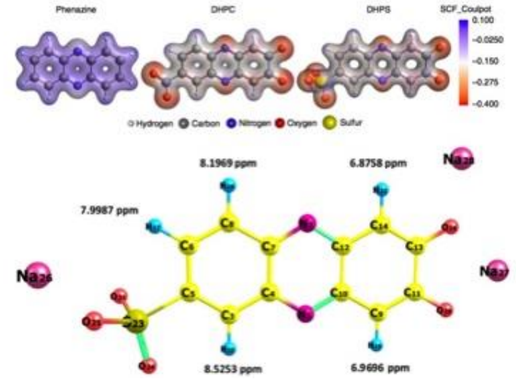


- Electrolyte solubility & electrochemistry
  - Accurate redox potentials (ADF+COSMO-RS), ionization potentials
  - Solubility: COSMO-RS
  - (e)ReaxFF: electrolyte degradation
  - ReaxFF, DFTB, BAND, polymer properties (band gaps)
  - BAND: include solvation, E field



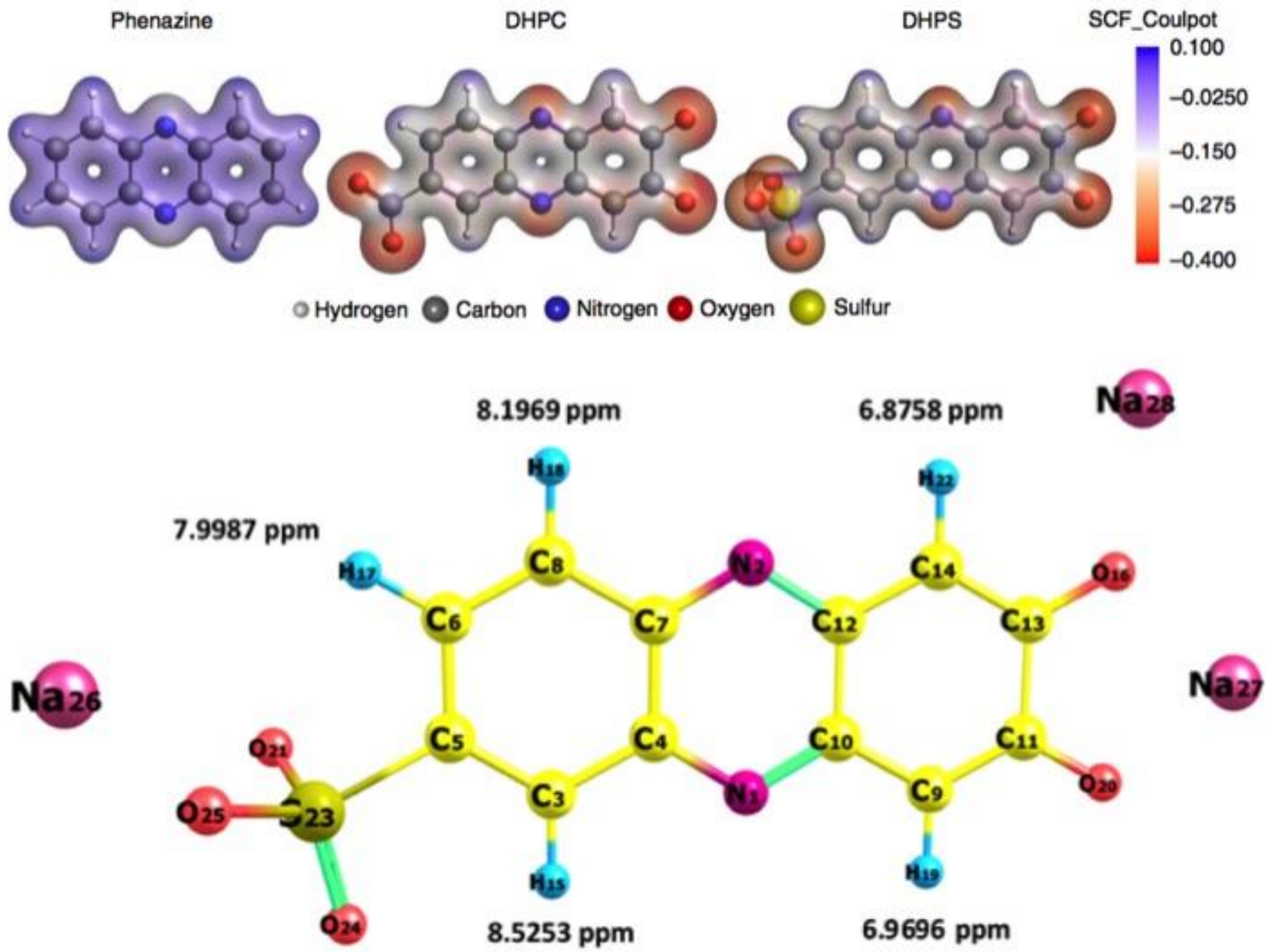
- (Dis)charge processes
  - GCMC with ReaxFF, or DFT(B)

- Understand battery ‘operando’
  - ADF - Spectroscopy: NMR, NEXAFS



Solvation energies, redox potentials, NMR spectra

Developing non-flammable electrolytes:
DFT + Continuum Solvation (COSMO) aids experiments

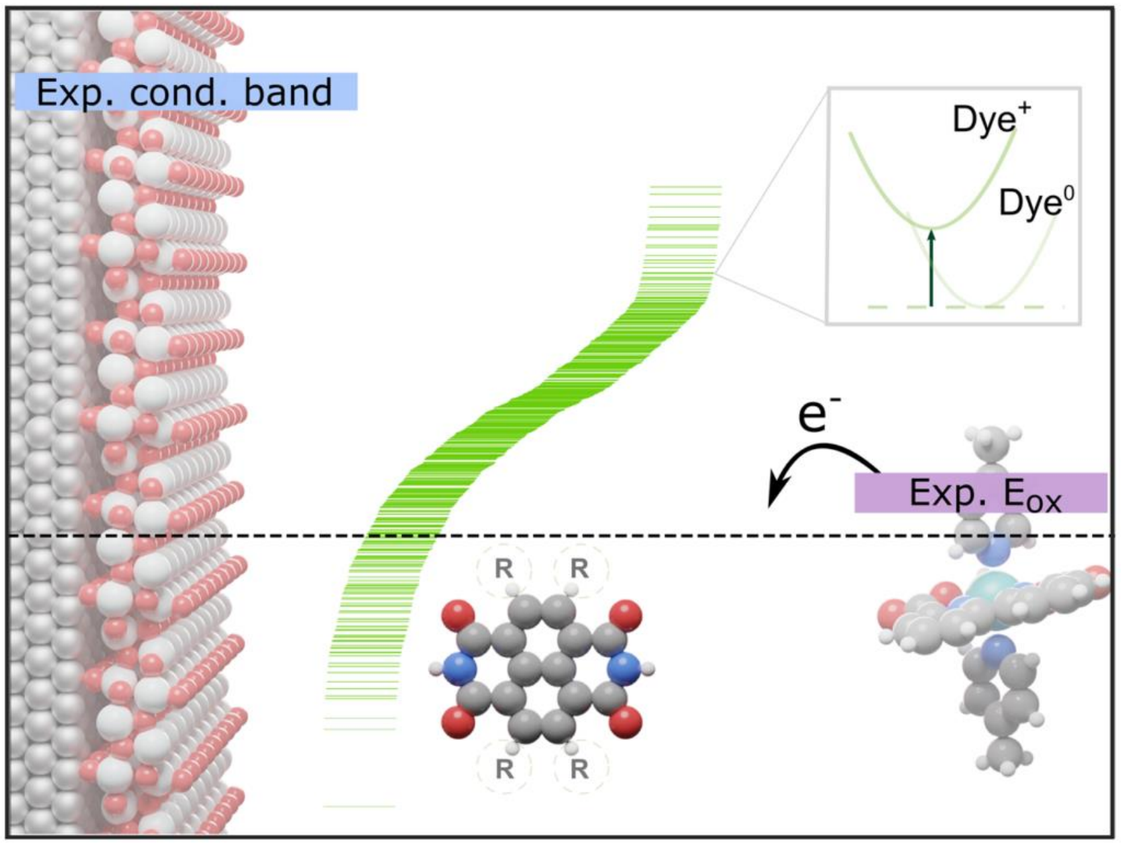


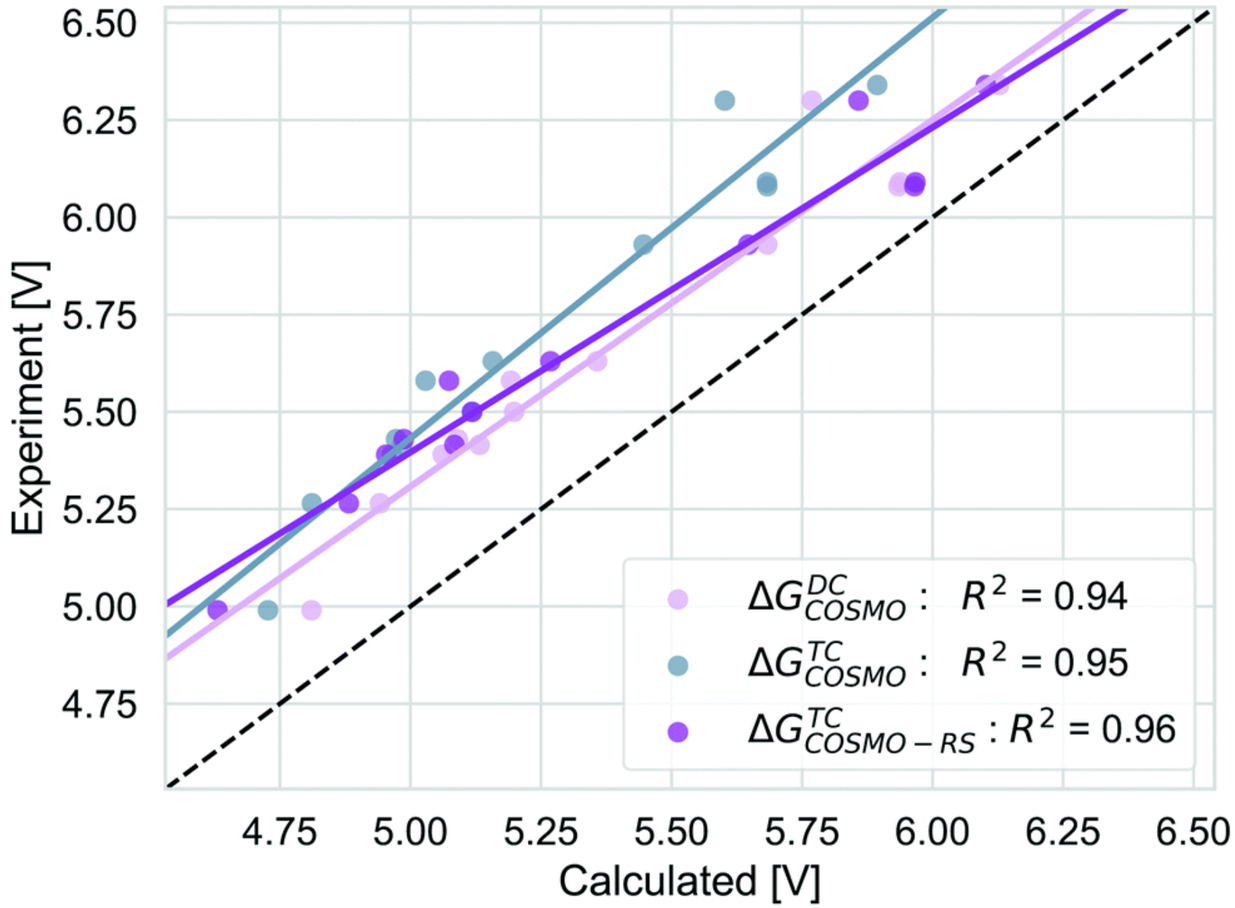
A biomimetic high-capacity phenazine-based anolyte for aqueous organic redox flow batteries, Nature Energy 3, 508-514 (2018)
Non-flammable electrolytes with high salt-to-solvent ratios for Li-ion and Li-metal batteries, Nature Energy 3, 674–681 (2018)

Solvation energies, redox potentials, NMR spectra

(python) workflow screening redox potentials: $E^0 = - \Delta G (A + e^- \rightarrow A^-)/F$ (reduction)

DFTB + solvation (first pass) -> ADF + solvation (more accurate)
Use directly with COSMO, or through thermodynamic cycle with COSMO-RS

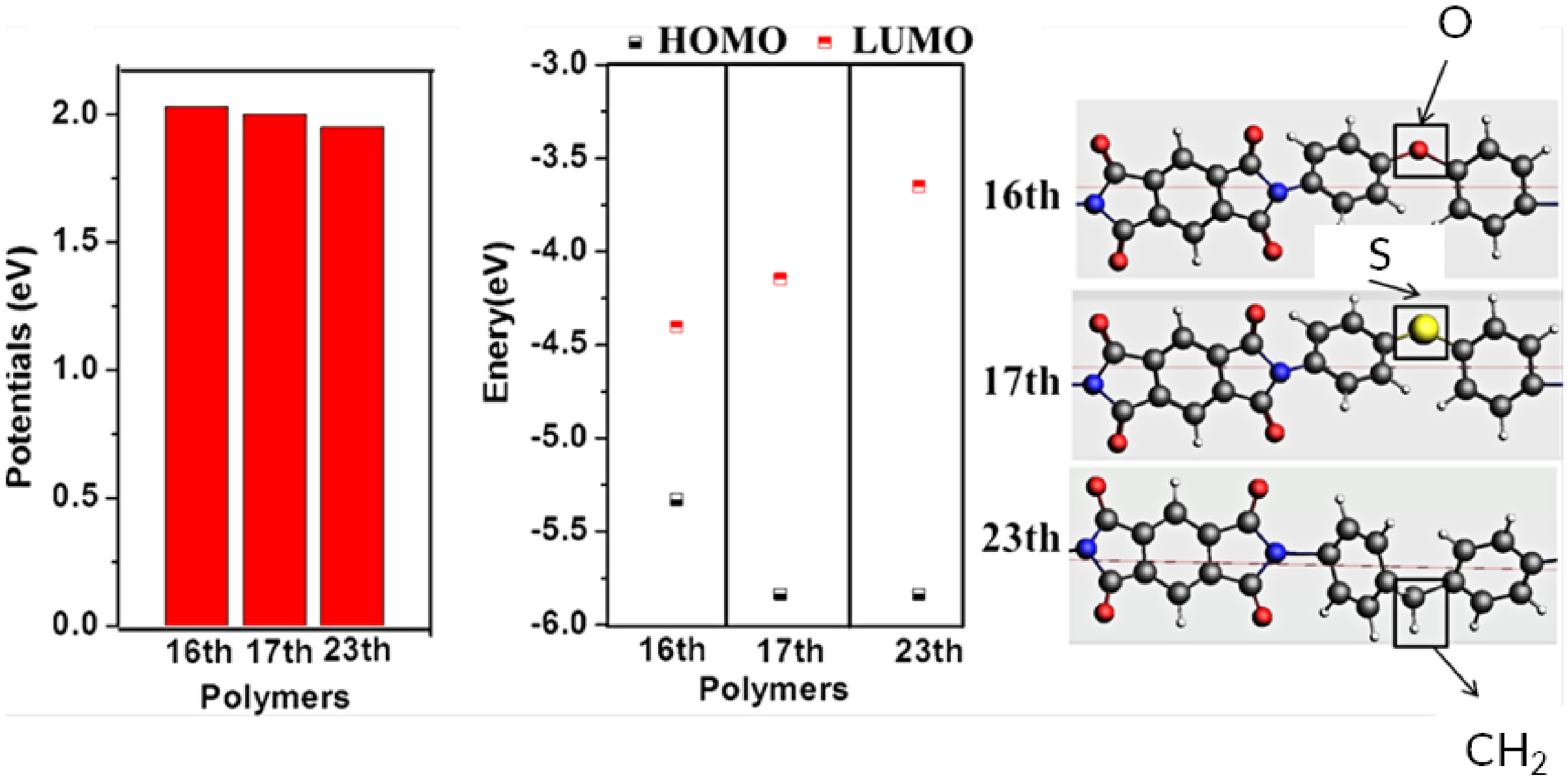




J. Belić, A. Förster, J. P. Menzel, F. Buda, and L. Visscher, ***Automated assessment of redox potentials for dyes in dye-sensitized photoelectrochemical cells***, Phys. Chem. Chem. Phys. **24,** 197-210 (2022)

Screening polymers for Lithium Ion Batteries

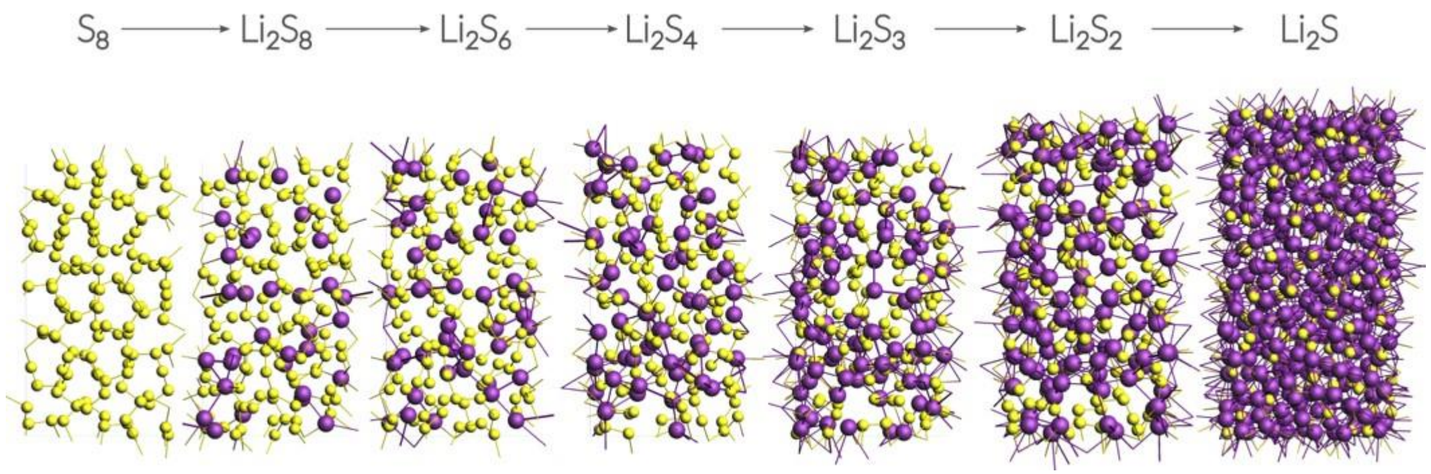
Screening band gaps and lithiation energies with 1D periodic DFT + COSMO



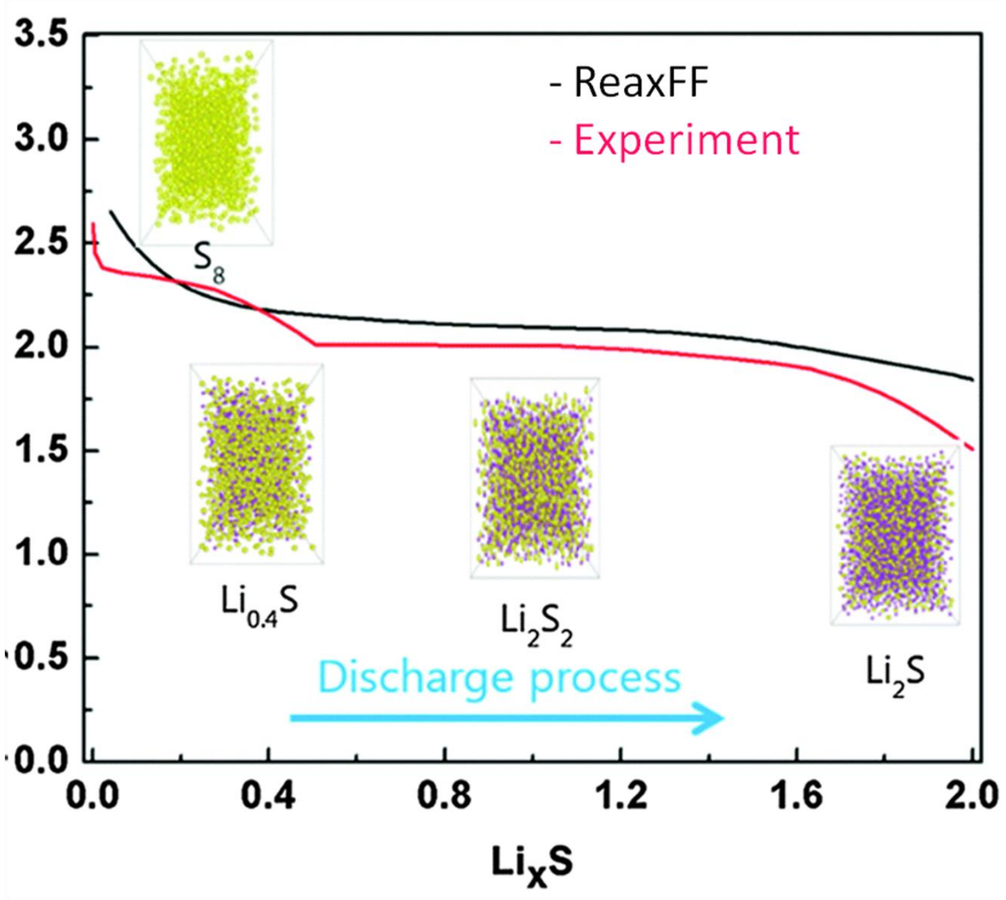
H. Lu, J. Yu, G. Chen, and S. Sun, Theoretical screening of novel electrode materials for lithium–ion batteries from industrial polymers, Ionics (2019)

Discharge process Li-S batteries

- Cathode expansion
- Voltage reduction
- Diffusion induced stress



Tutorials: Battery discharge (GCMC) & Li ion diffusion

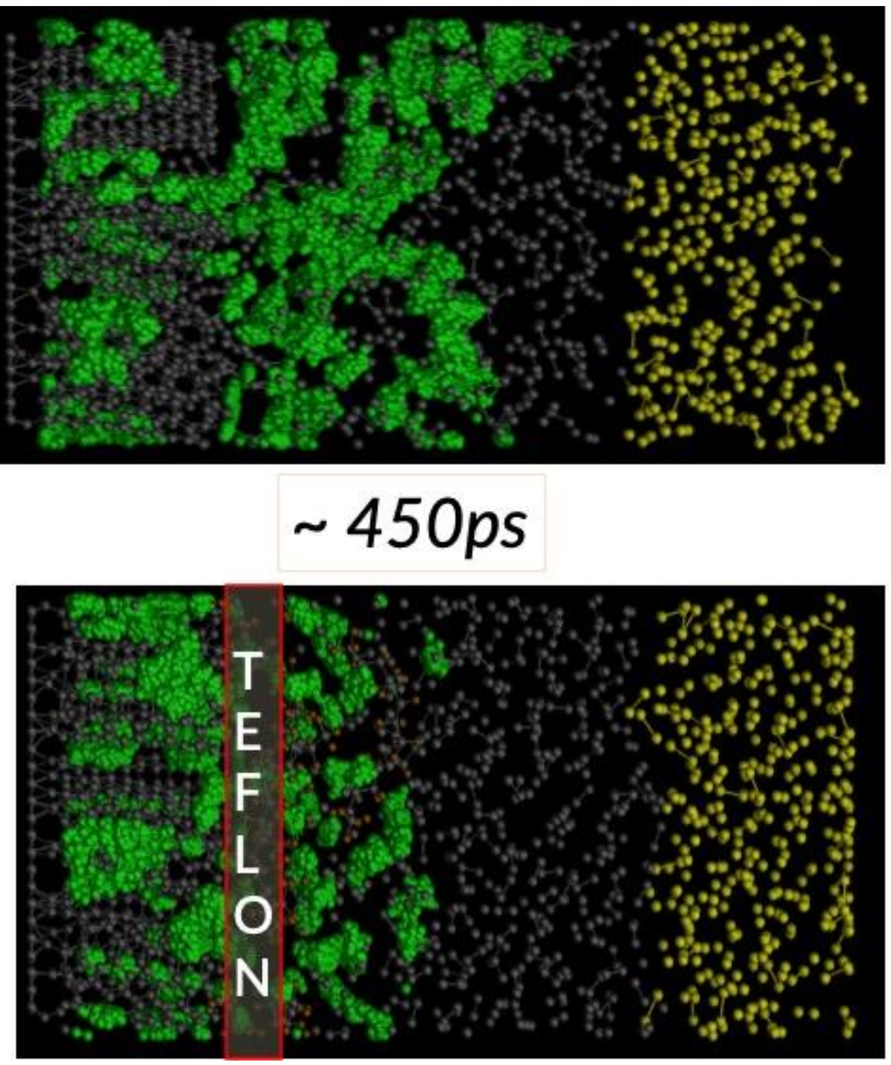


Battery discharge video

M. M. Islam, A. Ostadhossein, O. Borodin, A. T. Yeates, W. W. Tipton, R. G. Hennig, N. Kumar, and A. C. T. van Duin, *ReaxFF molecular dynamics simulations on lithiated sulfur cathode materials*, Phys. Chem. Chem. Phys. **17**, 3383-3393 (2015)

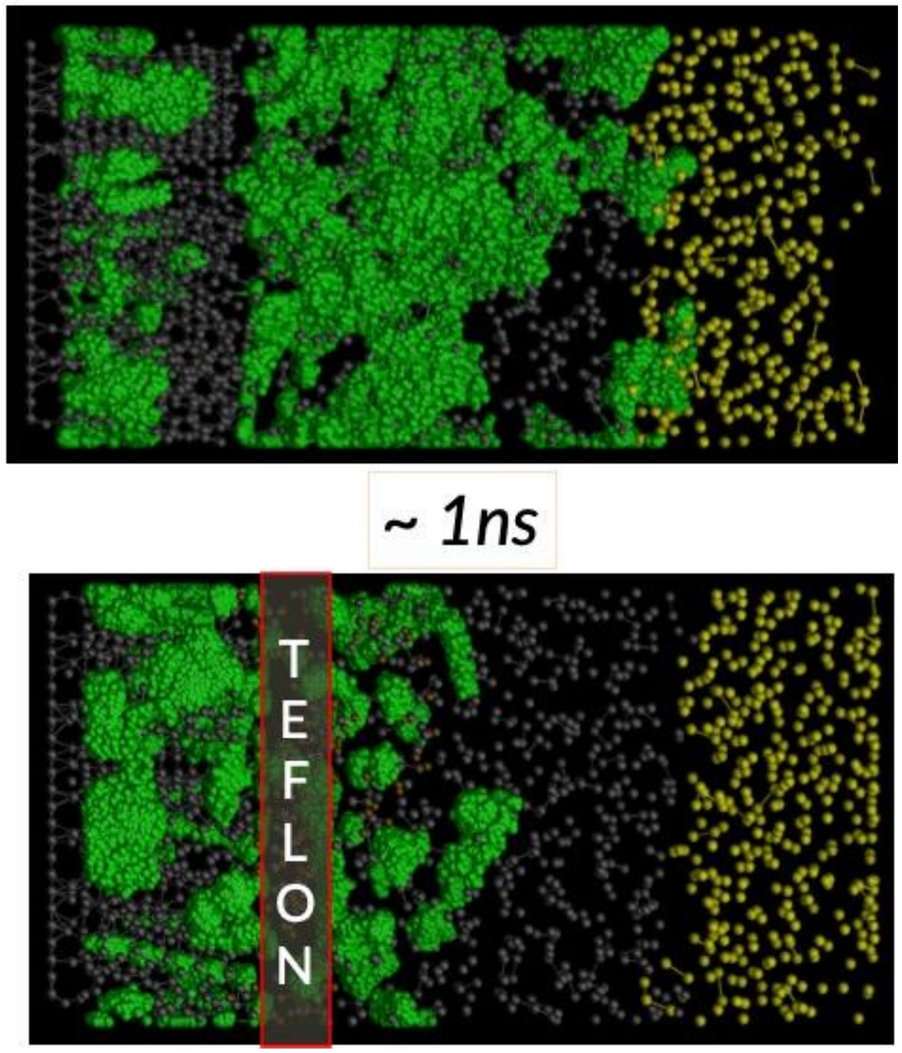
Teflon protects electrolyte in Li battery

Teflon layer on anode-electrolyte interface significantly reduces lithium reactivity and diffusion through the electrolyte phase



NVT, 300K

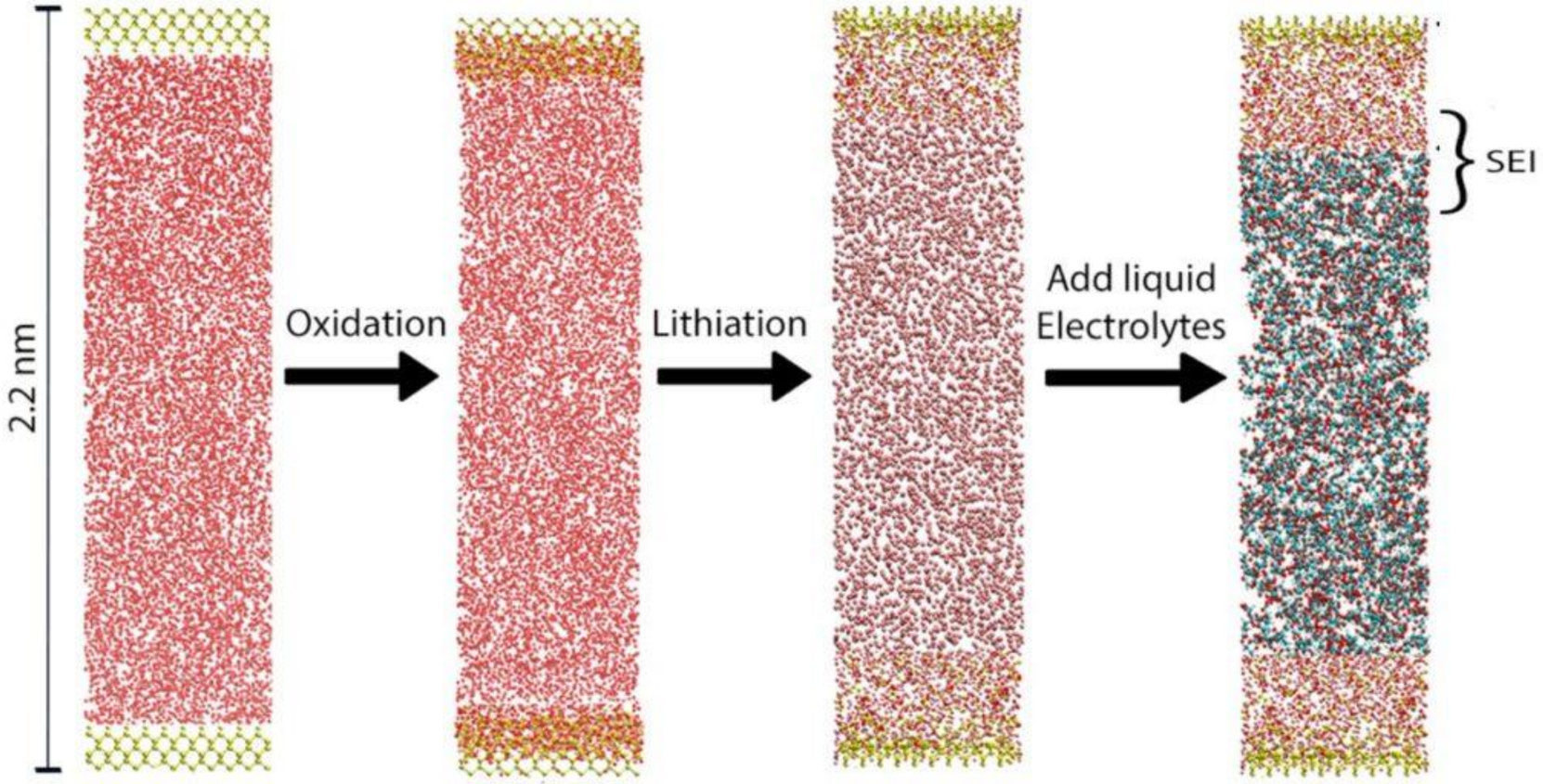
Li discharge



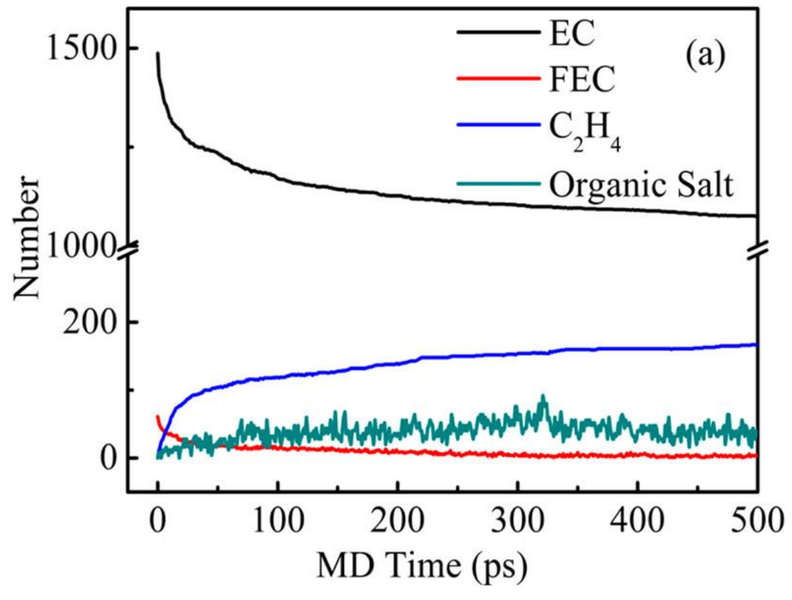
J. Electrochem. Soc. **161**, E3009-E3014 (2014).

Solid electrolyte interface formation Lithium Ion Batteries

ReaxFF protocol to study the initial formation stages of SEI formation

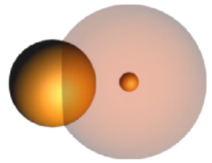


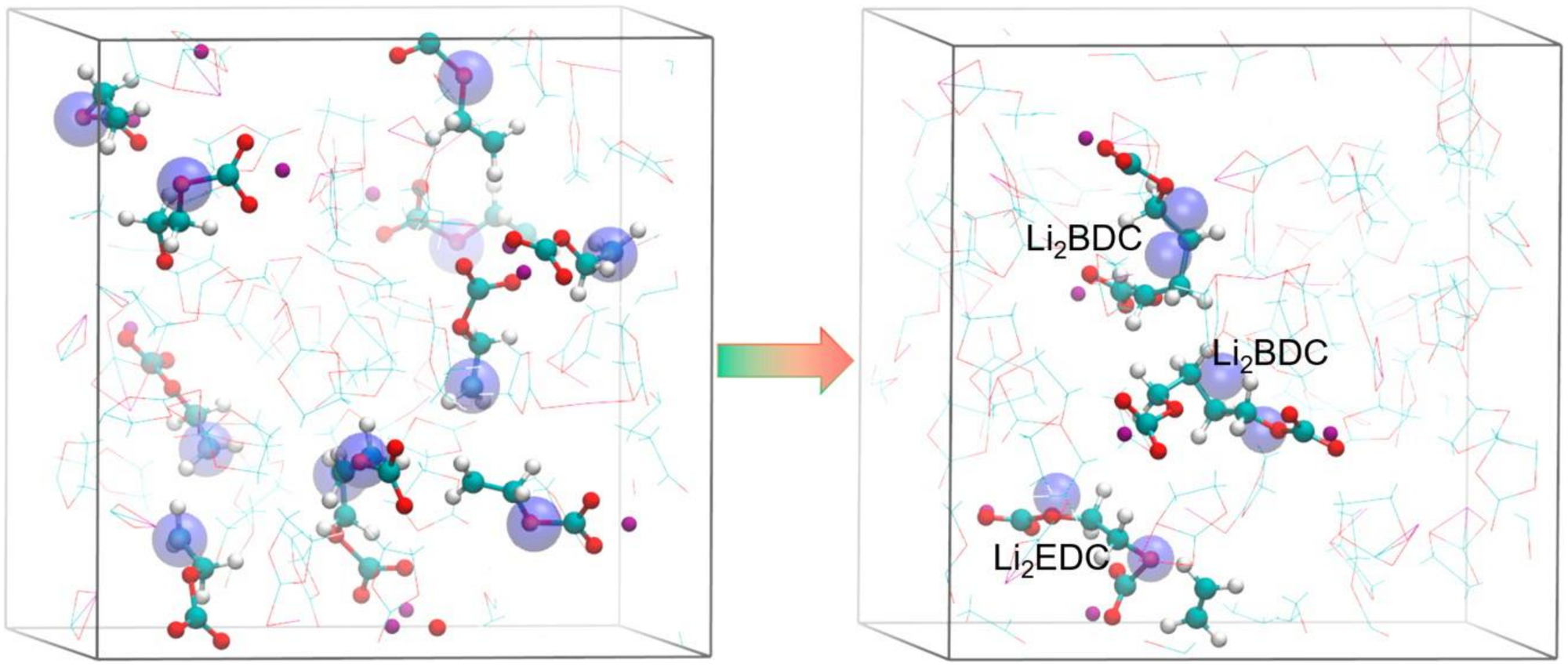
Wang J, Liun Y, Tu Y, Wang Q, Reductive Decomposition of Solvents and Additives toward Solid-Electrolyte Interphase Formation in Lithium-Ion Battery, J. Phys. Chem. (2020).



eReaxFF – explicit electrons

Reductive decomposition of ethylene carbonate in Li ion batteries

Setup: Li-atom →  (Li^+/e^- -pair)

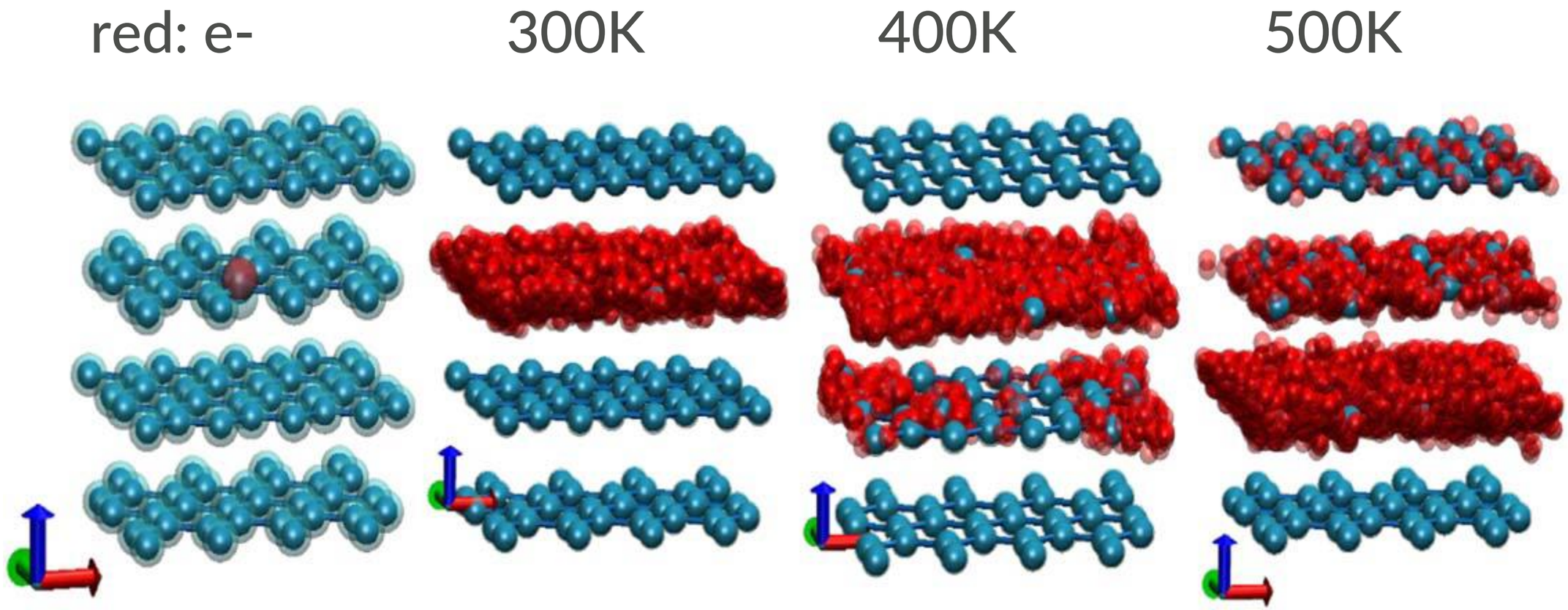


[eReaxFF video]

M. M. Islam and A. C. T. van Duin, J. Phys. Chem. C 2016, 120 (48), 27128-27134.

eReaxFF – Li on graphitic anodes

eReaxFF to study electron mobility & Li ion reduction, including (video)
- explicit electrons
- electric fields

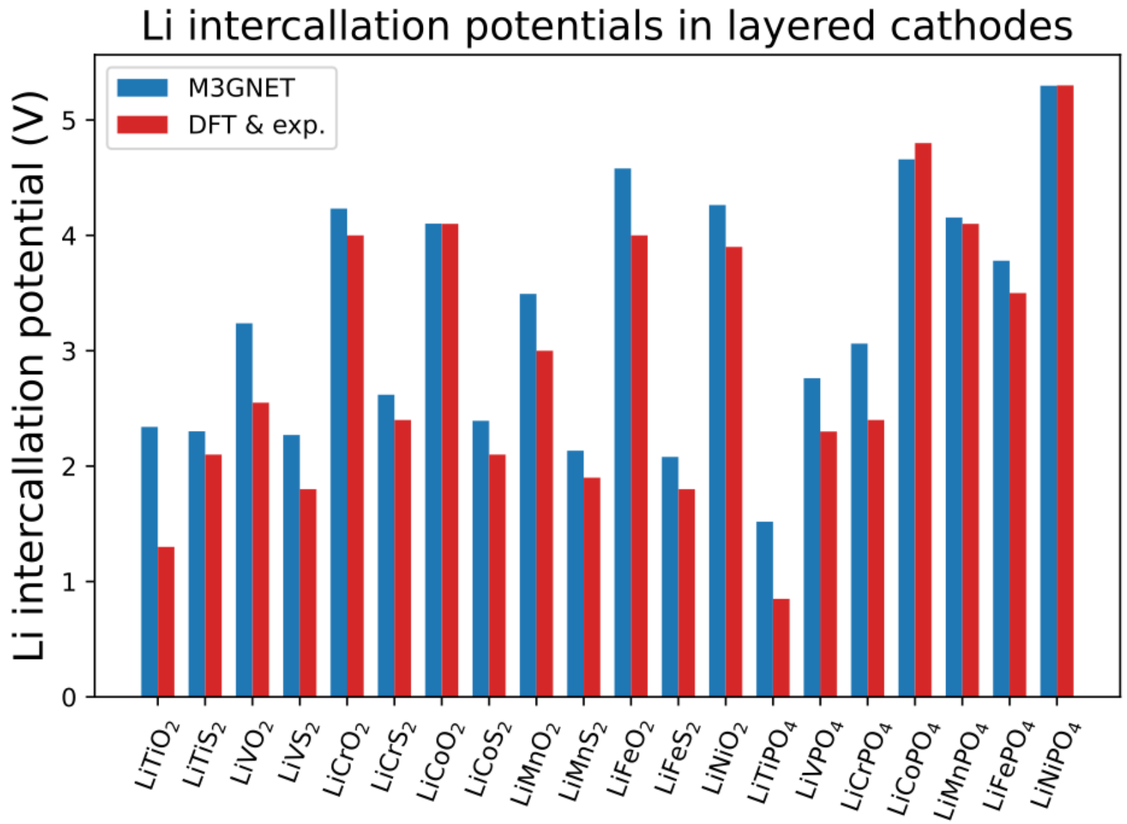


Md Jamil Hossain *et al. J. Electrochem. Soc.* **169 ,**110540 (2022)

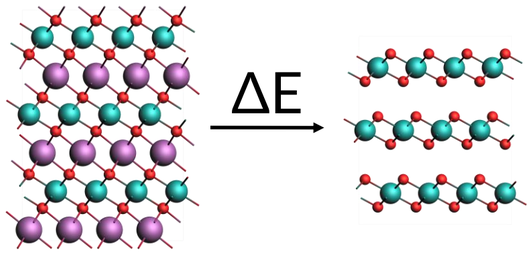
MLPotentials for (battery) materials

M3GNet, trained to Materials Project 1000x faster than DFT

C. Chen, S.P. Ong., Nature Comp. Sci. 2, 718–728 (2022)



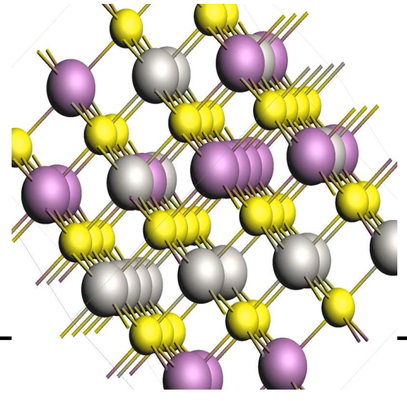
- Li intercalation potentials accurately predicted with DFT (~100 atoms)
- M3GNet reproduces DFT really well

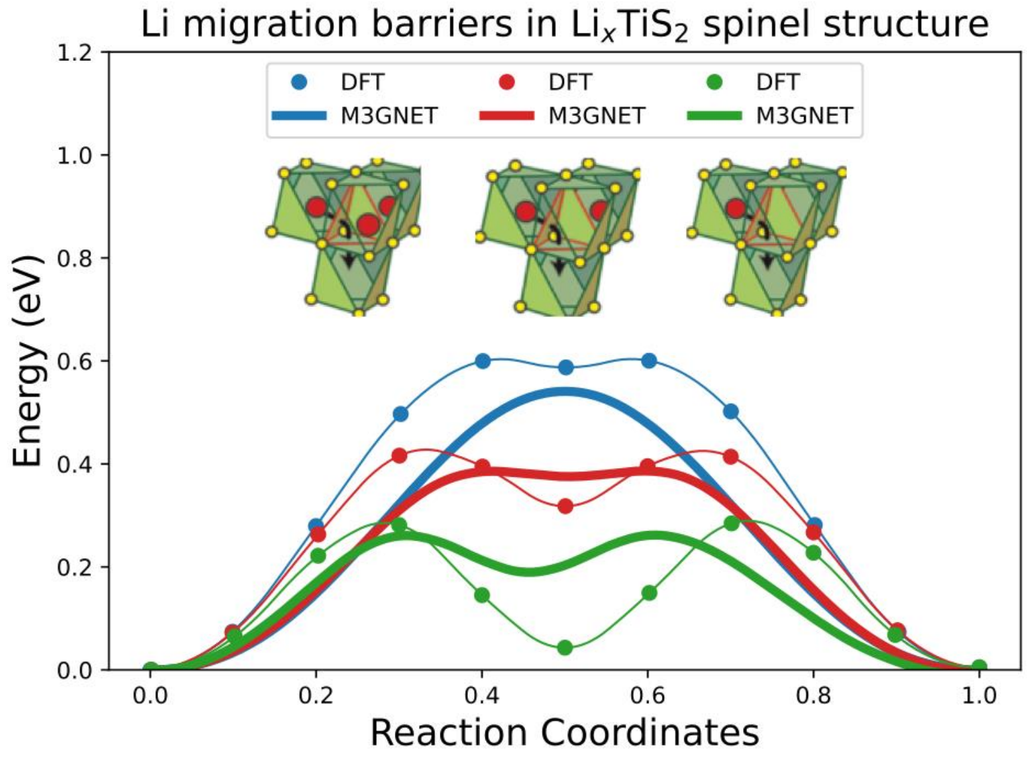


- Li potential
- Mechanical properties of electrode (volume change upon lithiation)

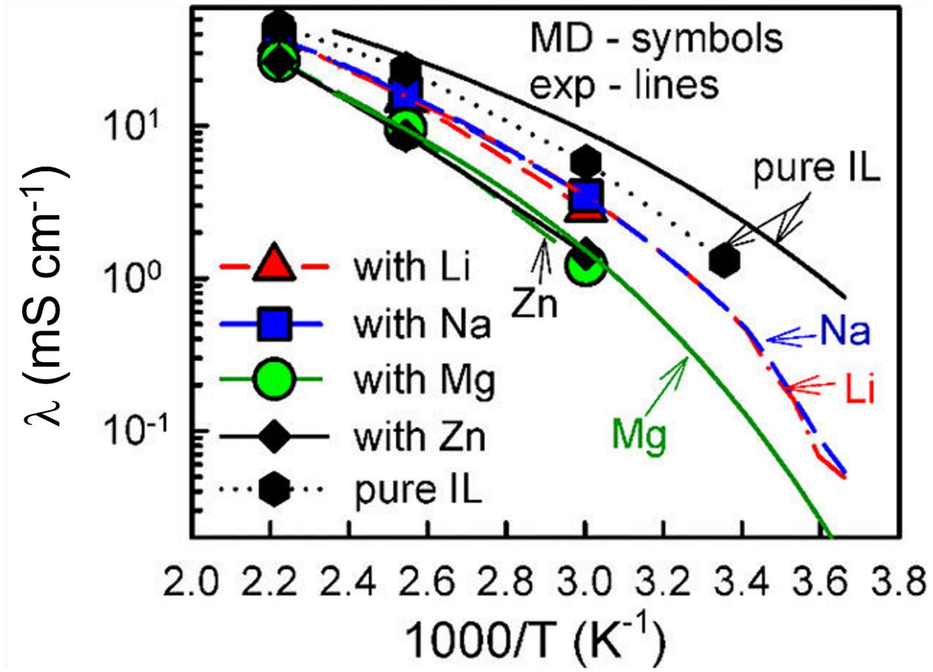
- Li diffusion through NEB or PES scan
- M3GNet can accelerate by 1000x
- (Dis)charge curves: GCMC

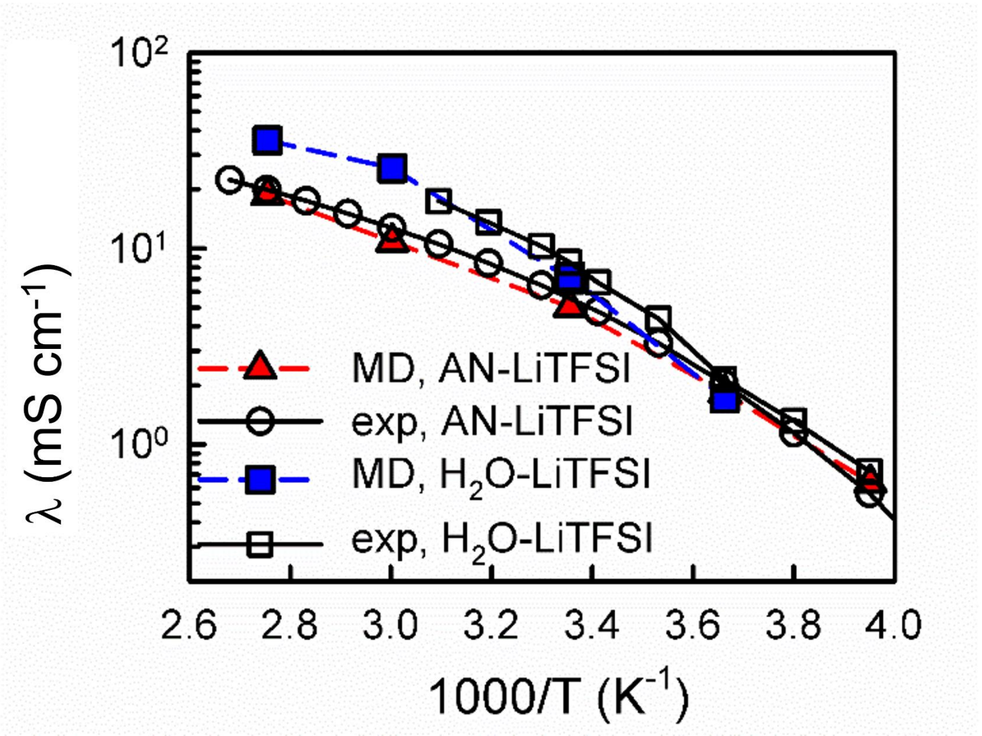
- Activation energy
- Diffusion (kinetics)

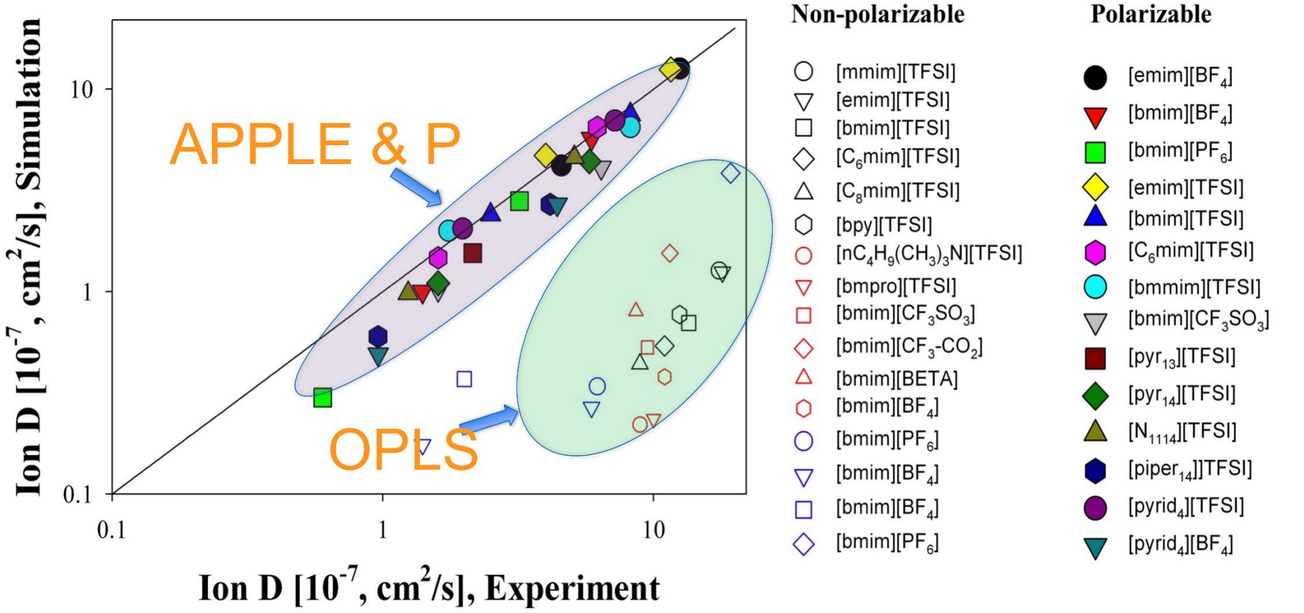




Diffusion, Conductivity with APPLE&P







Polarizable force field for batteries, ionic liquids, fuel cells

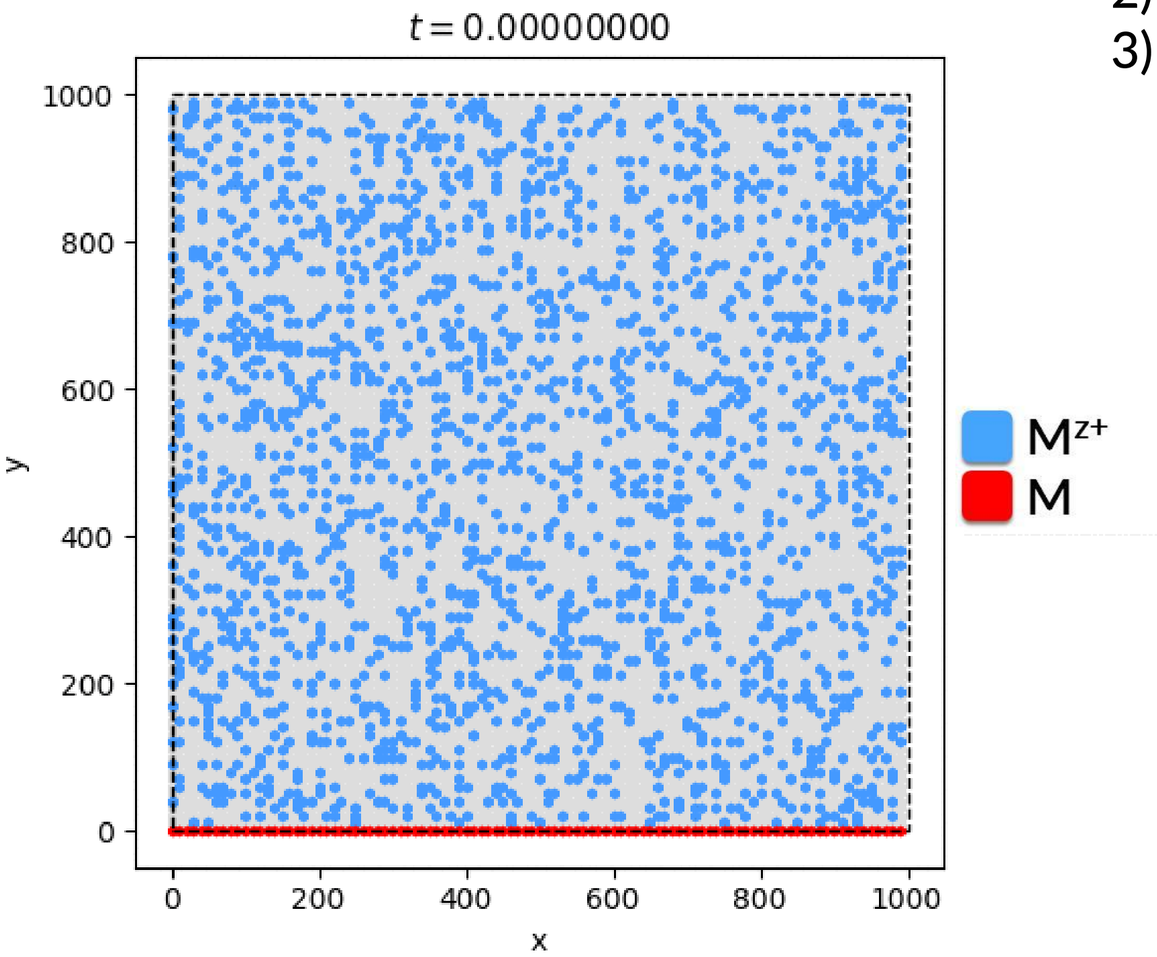
APPLE&P MD simulations: ion dynamics **within 15-20% from experiment**

More transferable than non-polarizable force fields with rescaled ion charges

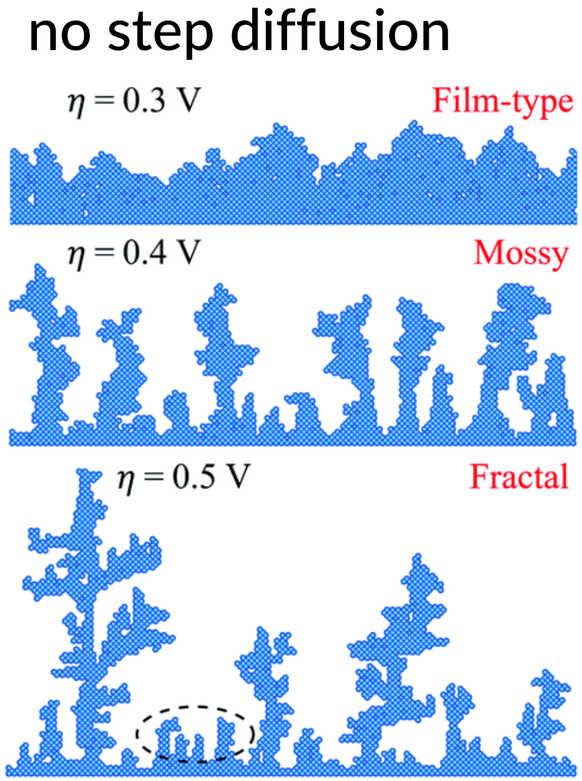
Chem. Rev. 2019, **119**, 7940

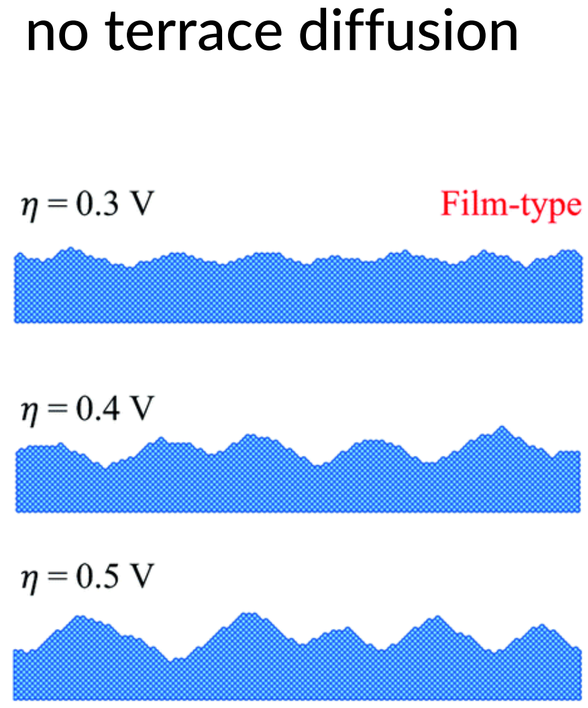
Kinetic Monte Carlo: SEI dendrite formation

Modified (py)Zacros kMC to study dendrite formation



3 Processes (rates can be computed with AMS):
1) Metal ion (**M^{z+}**) transport across electrolyte
2) Reduction at the solid-electrolyte interface (**M^{z+}->M**)
3) Diffusion of the metal (**M**) over the electrode surface

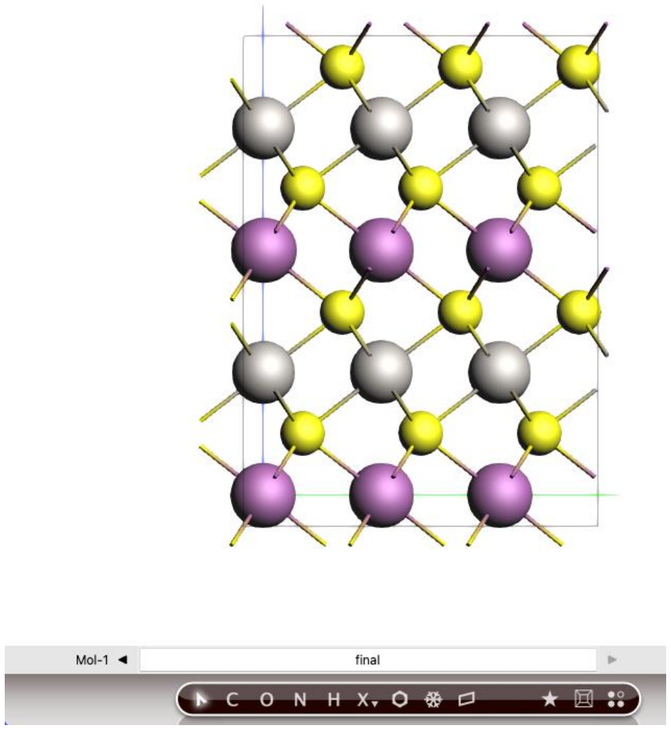


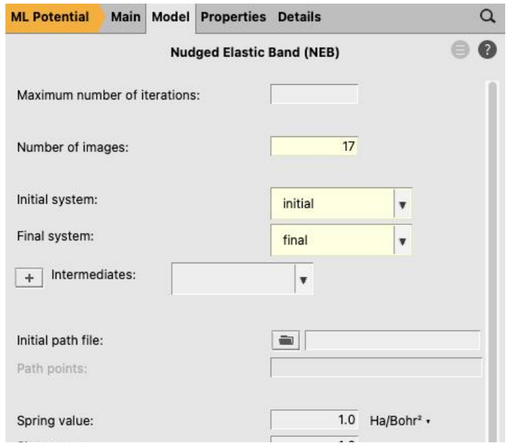


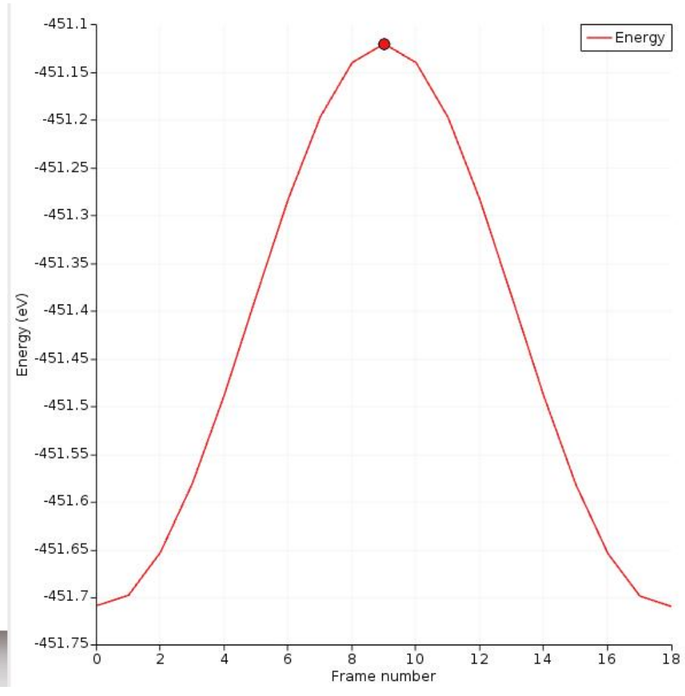
Inspired by **Surface diffusion manifestation in electrodeposition of metal anodes,** [PCCP 2020 (22), 11286]

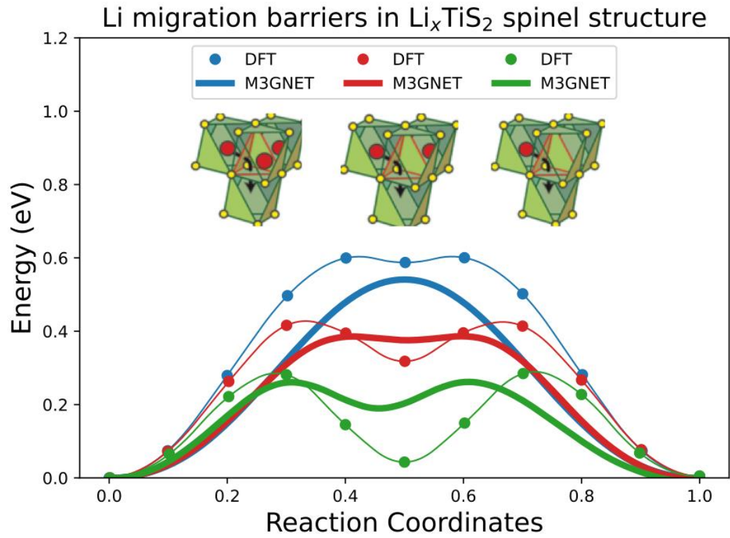
Demo: Li diffusion (tutorial)

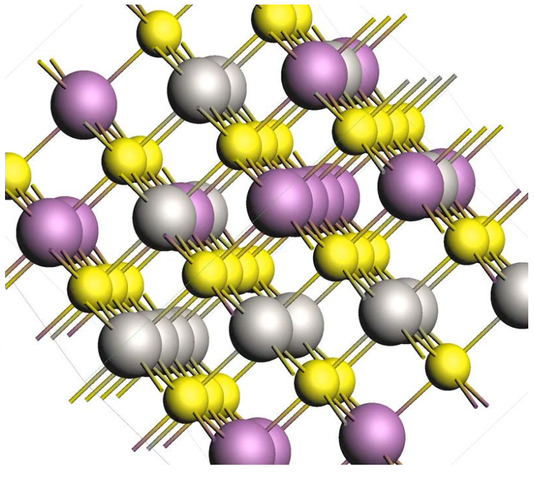
M3GNet, trained to Materials Project 1000x faster than DFT





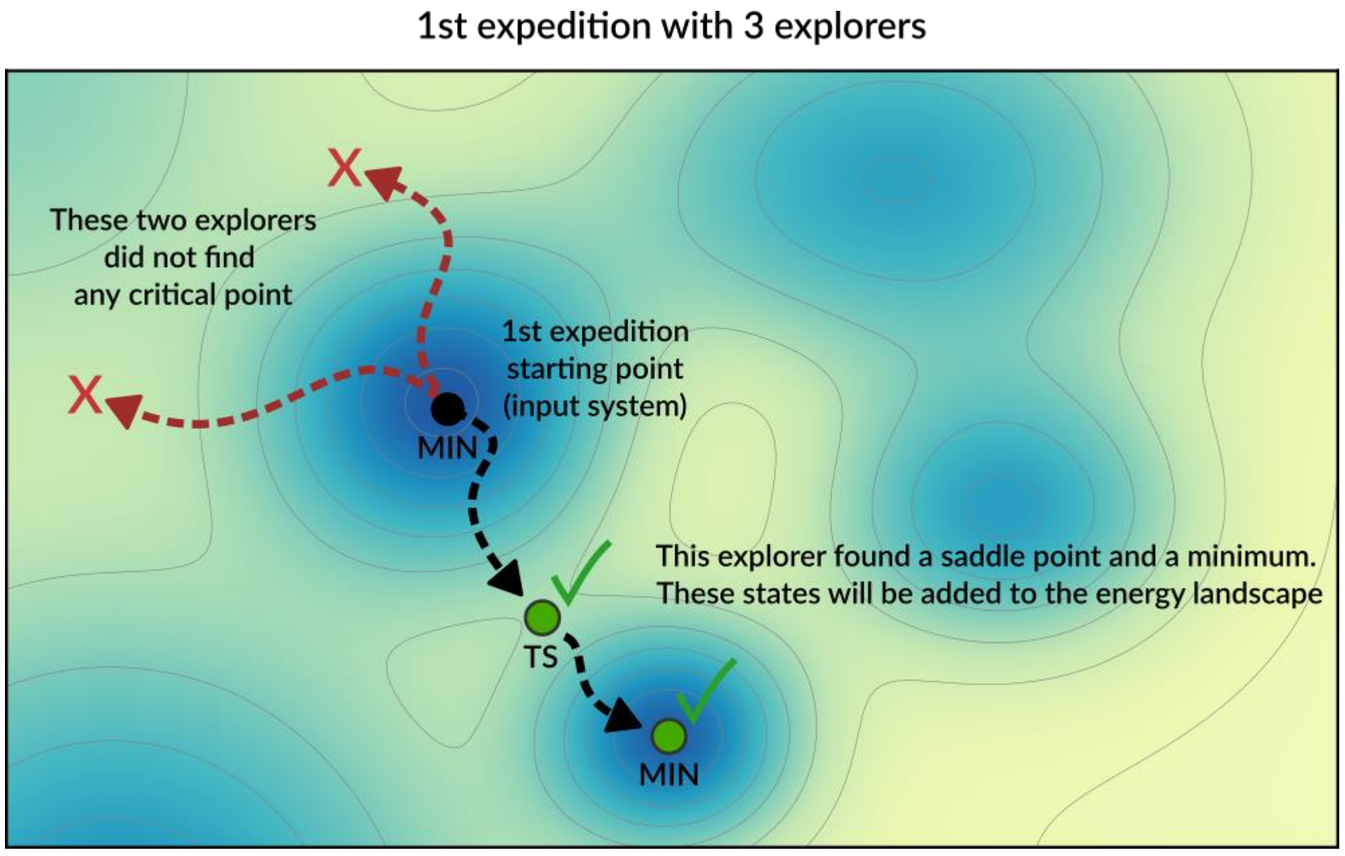


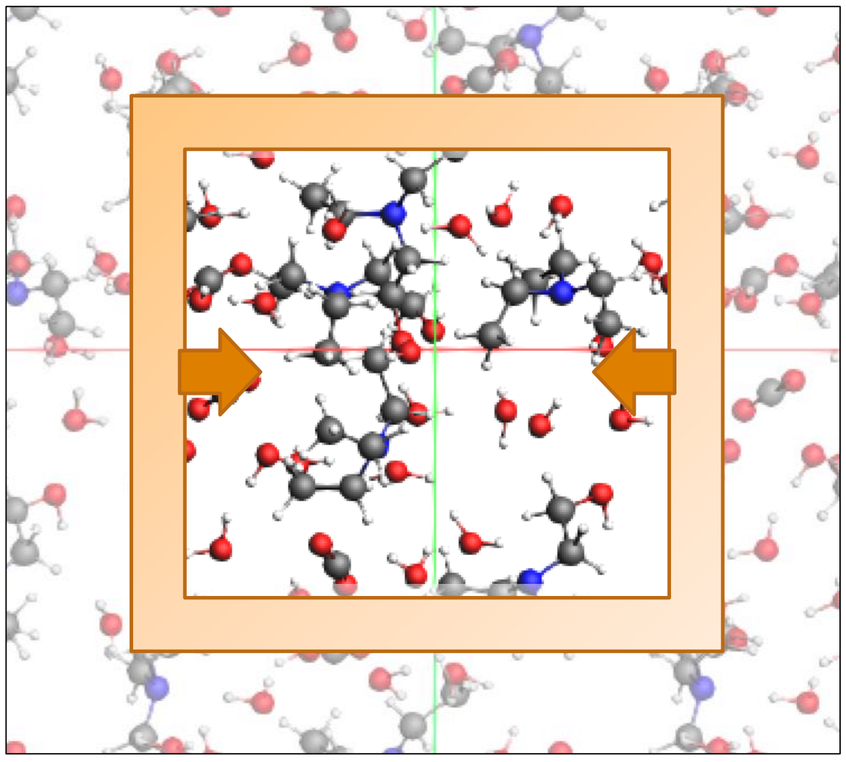




M3GNet: C. Chen, S.P. Ong., Nature Comp. Sci. 2, 718–728 (2022)

Reaction discovery

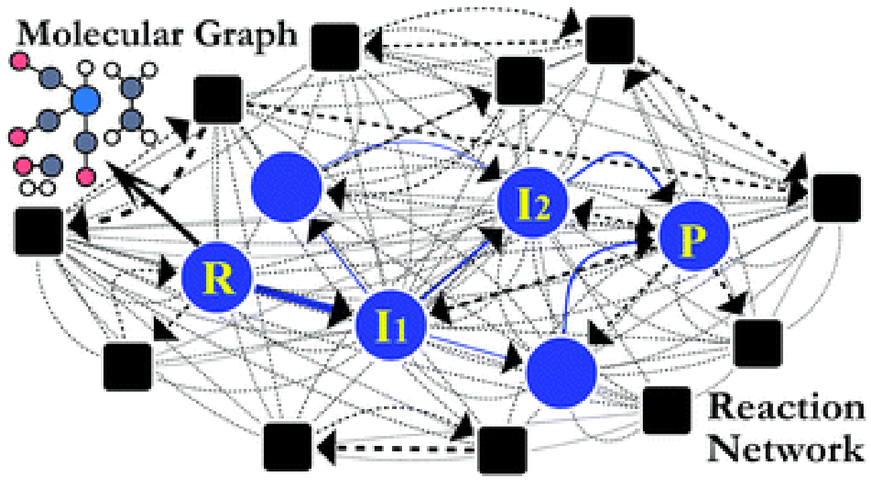


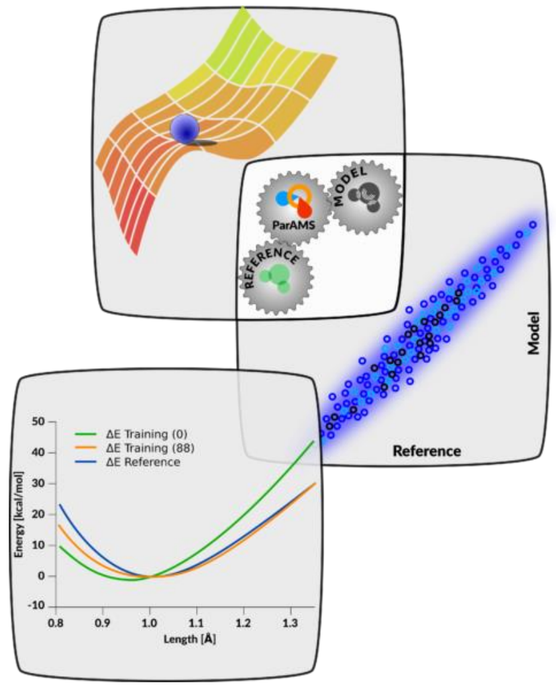


AutoCheMo: Automatic generation of Chemical Models

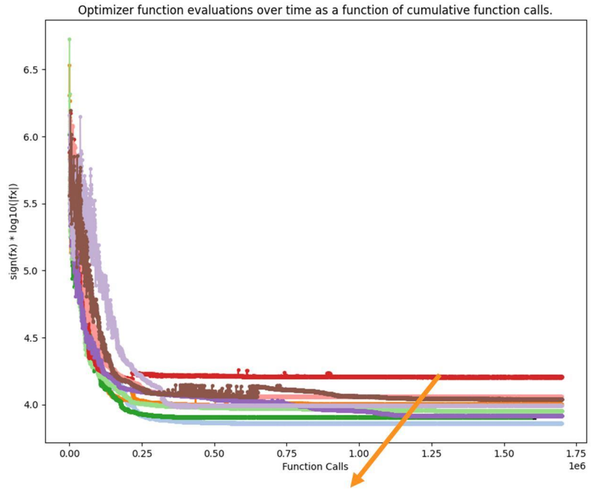
4 PhD projects, in collaboration with Universities of Gent and Aachen:

- Complex reaction networks, automatic rates — ChemTraYzer2
- Semi-automatic ReaxFF force field parameterization — ParAMS
- Efficient methods to estimate and optimize ReaxFF parameters — GloMPO
- Large amplitude motions — CIMCI

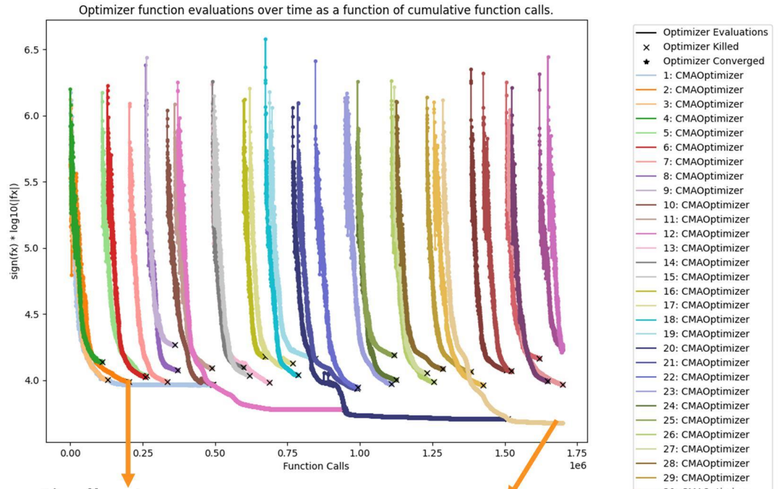




87 parameter Disulfide ReaxFF reparameterization



Time wasted in bad minima

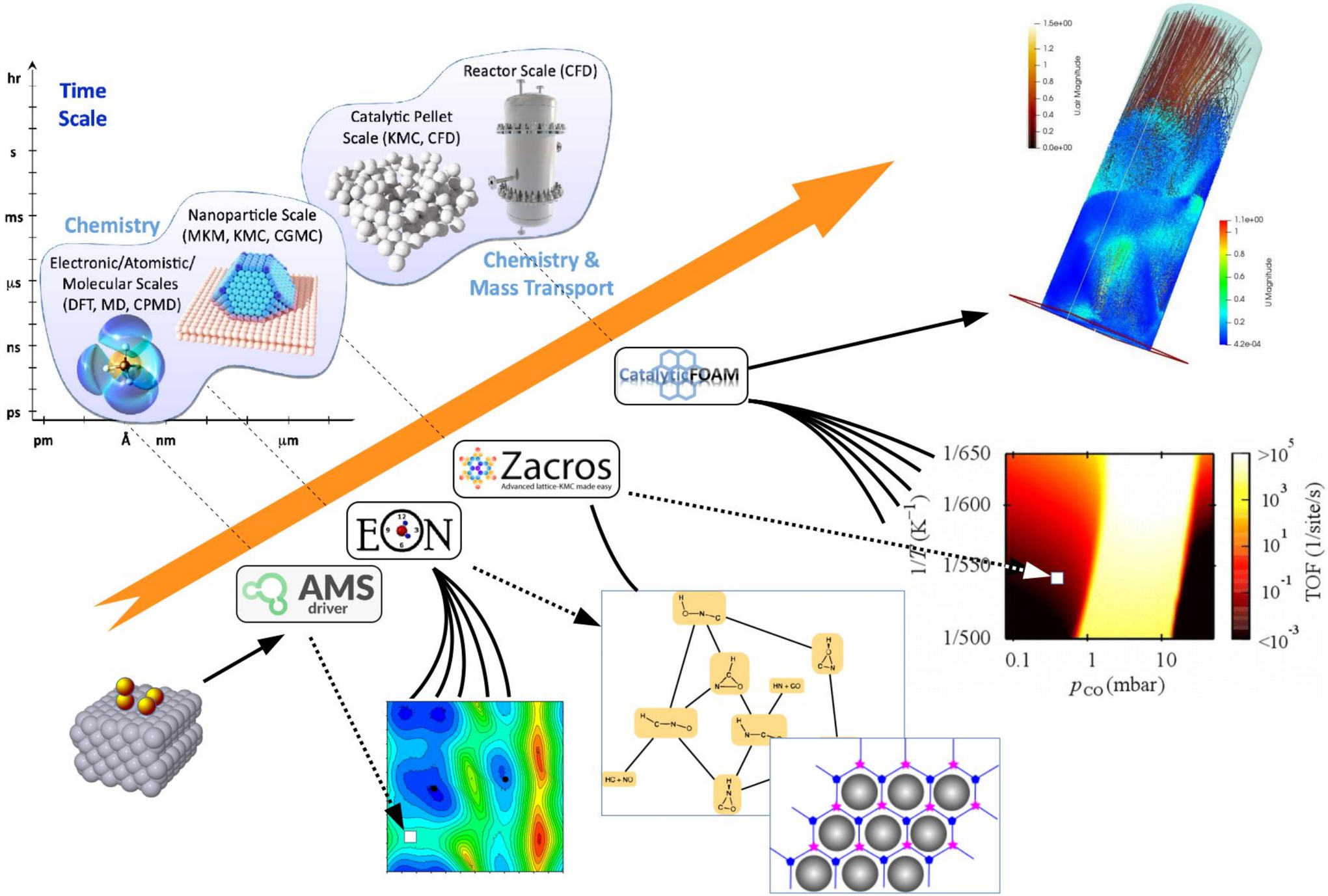


Automatically stops exploration of bad minima

More efficient use of function calls finds better answer in same time

Grant #814143, Finished Sept. 2022
with Verstraelen, Leonhard

ReaxPro: Multi-Scale Reactive Process Design



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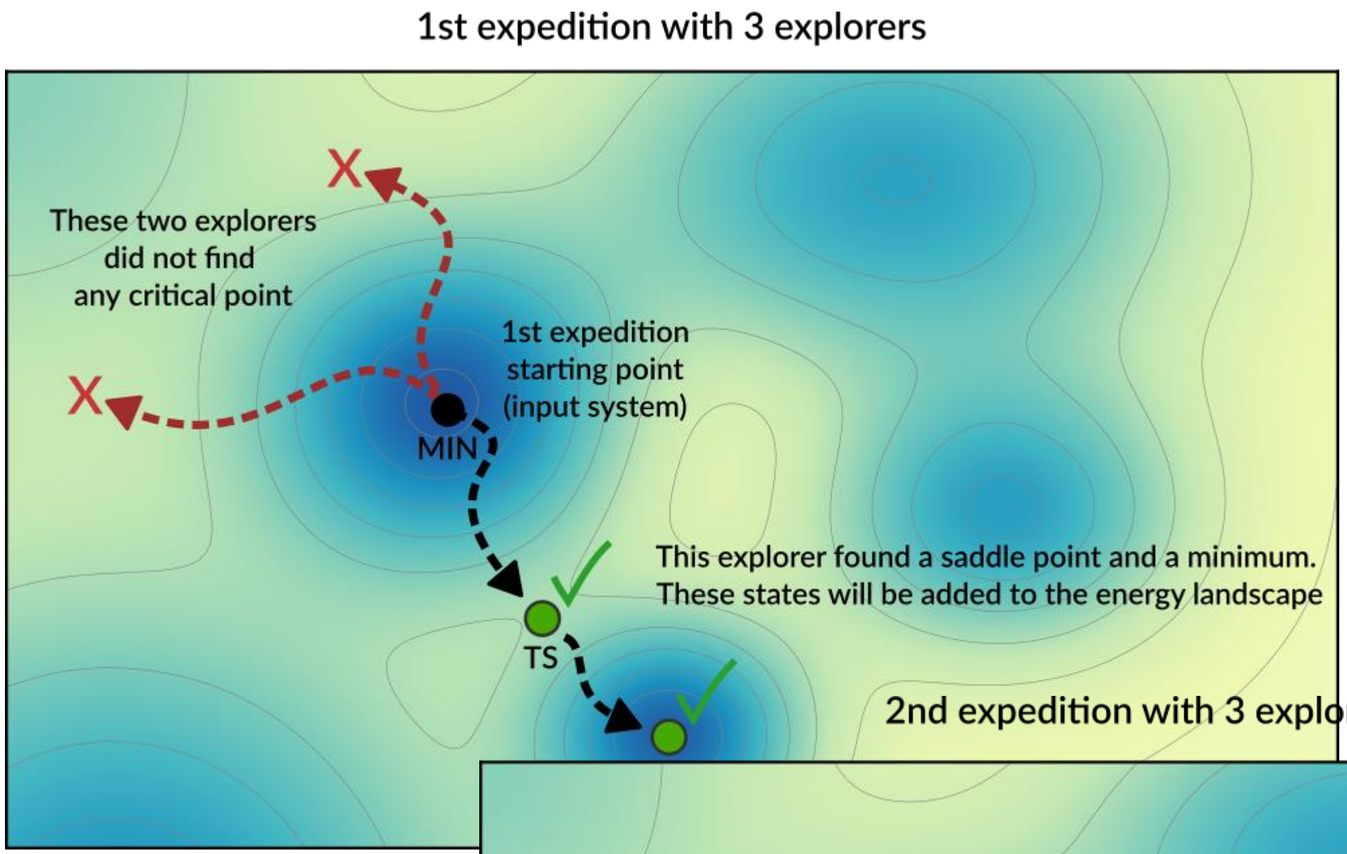
ReaxPro

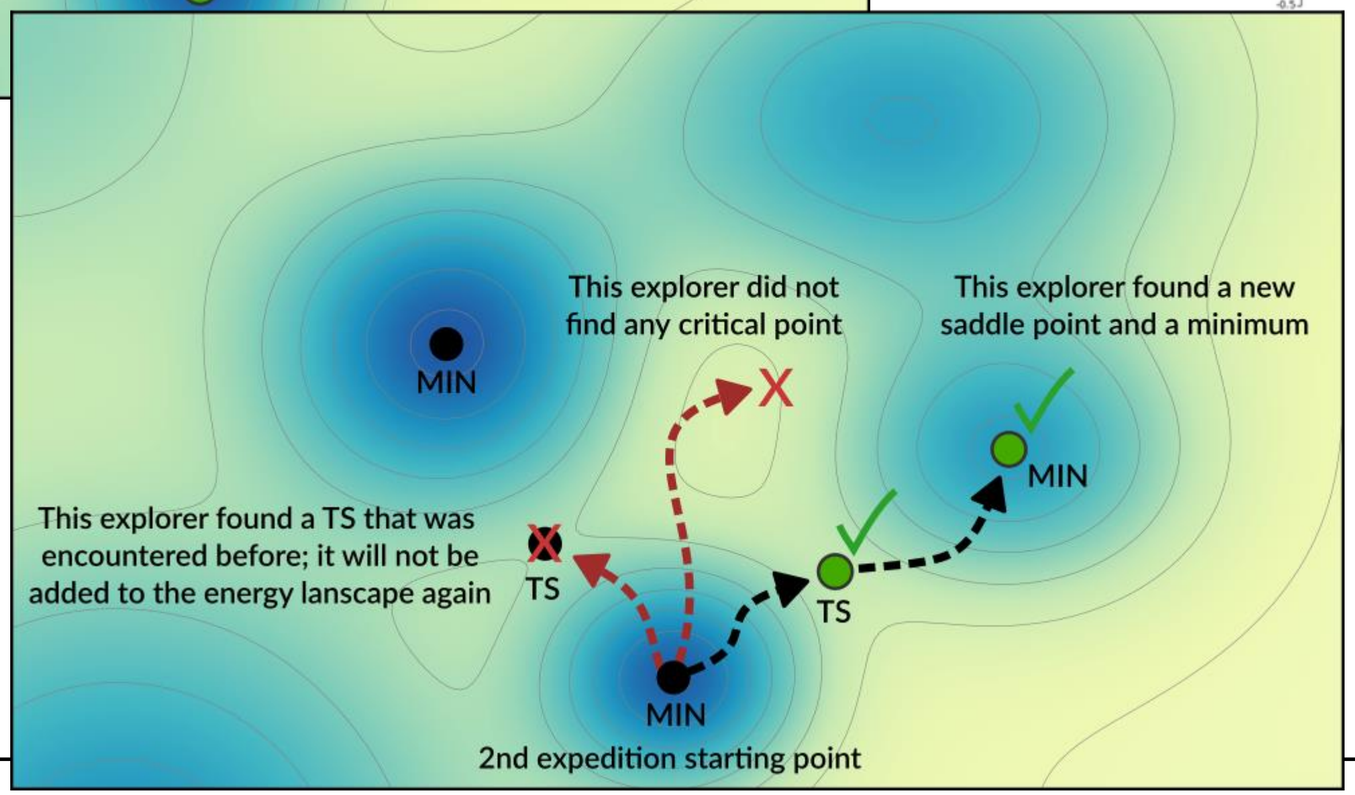
Accelerating reactive process innovation

LEIT - Grant Agreement No 814416

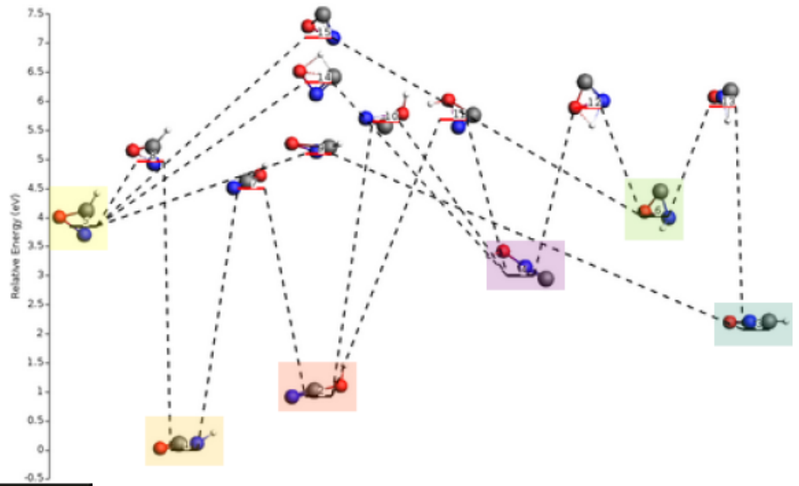
PES exploration

PES exploration

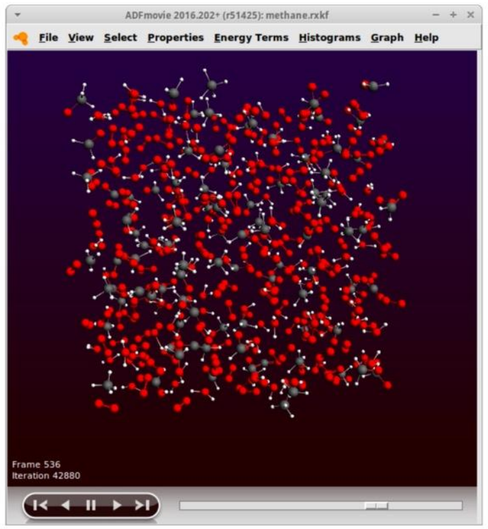


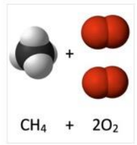


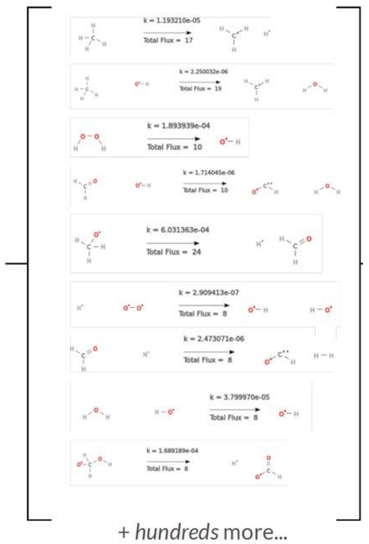

```
Task PESExploration

System
    Atoms
        H       -0.58691625       1.79642617       0.79110081
        O       -0.53563869       1.37408080      -0.08531432
        N       -0.54146683      -0.09761965       0.18986664
        C        0.58077340       0.40111238      -0.05052313
    End
End

PESExploration
    RandomSeed 100
    Job ProcessSearch
    NumExpeditions 500
    NumExplorers 4
End

Engine MOPAC
EndEngine
```



AutoReactPro: Automated Prediction Side Reactions for Process Design

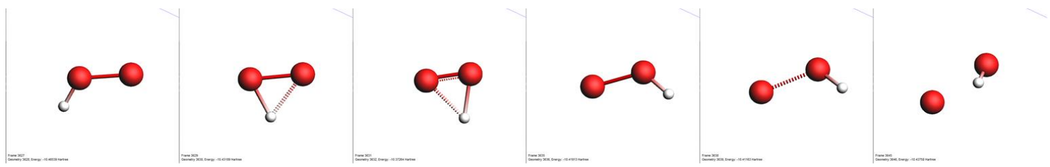






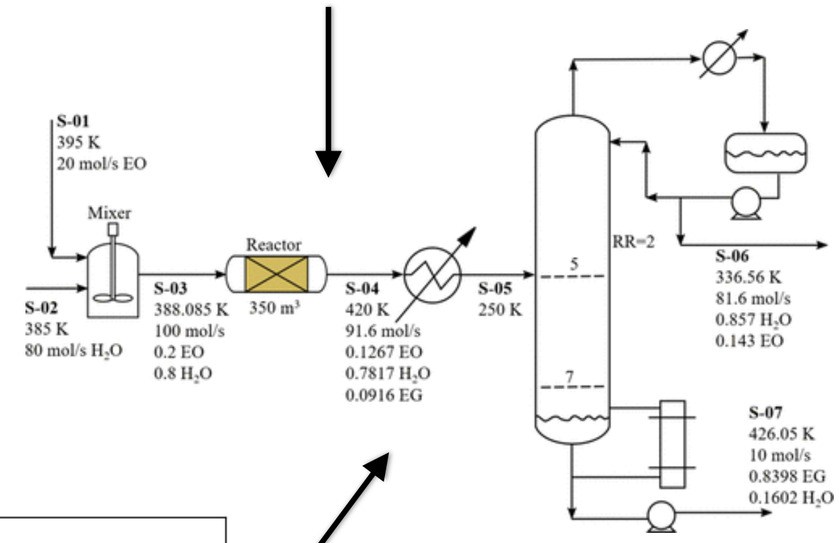
+ *hundreds* more...

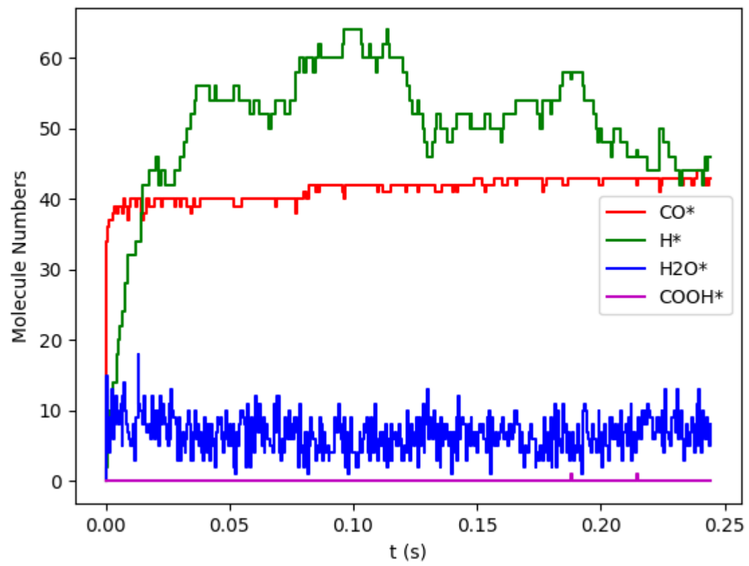
Automatically predict (side) reactions, improve rates



Reaction	Reaction Composition	Order	Rate constant k (cm^3, mol, s)
[O][O] + [H] => [O]O	O2 + H => HO2	2	1.407e+15
[O]O => [O][O] + [H]	HO2 => O2 + H	1	2.587e+12
[H][H] + [OH] => [H] + O	H2 + HO => H + H2O	2	3.881e+13
O[H]O => [OH] + O	H3O2 => HO + H2O	1	4.072e+13
[H] + [OH] => O	H + HO => H2O	2	1.903e+15

Thermodynamics (calc + exp)





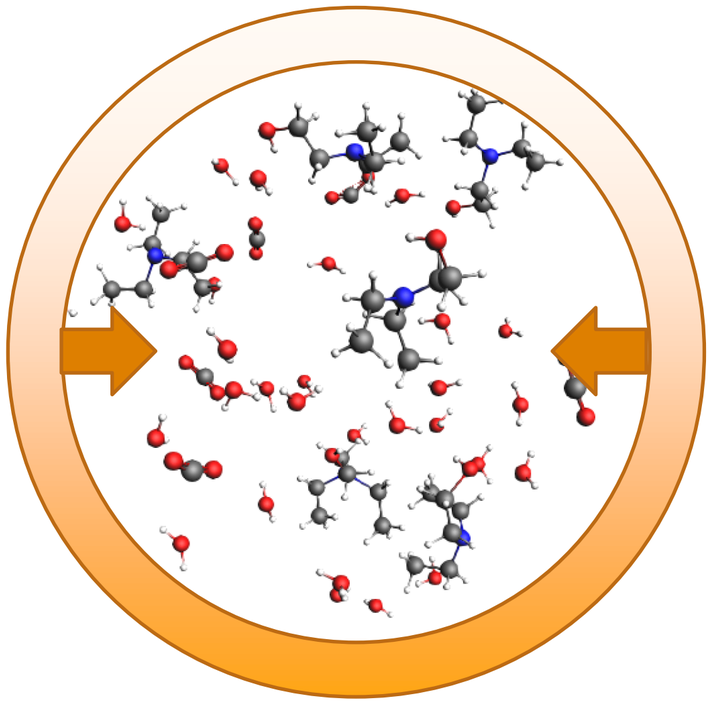
Kinetics

This project has received funding from the Eurostars-2 joint programme with co-funding from the European Union Horizon 2020 research and innovation programme

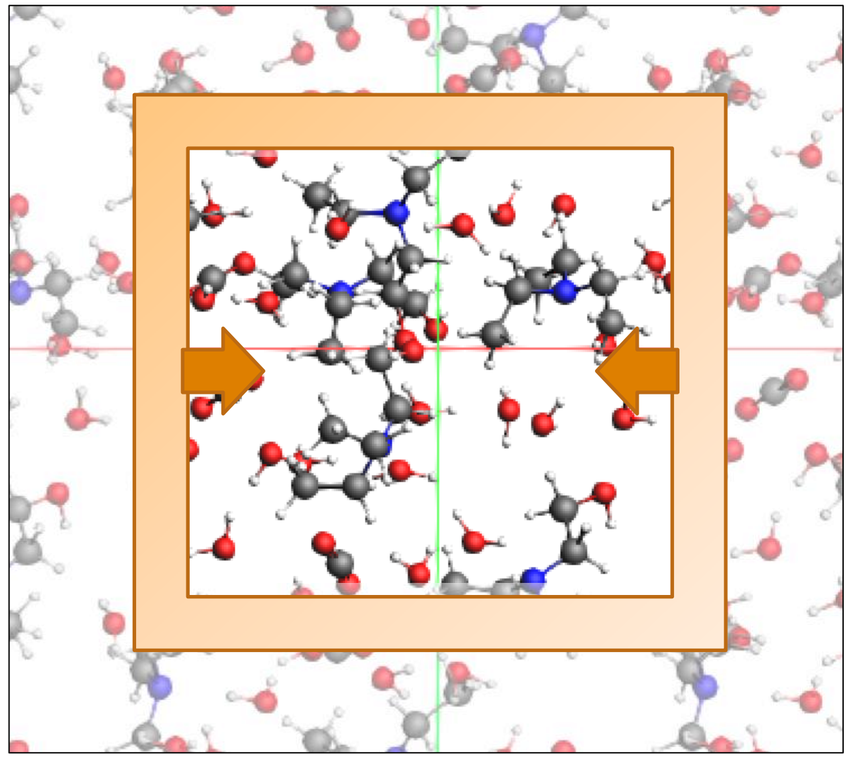
with Hafnium Labs

Nanoreactor

External Force



Coordinate Rescaling

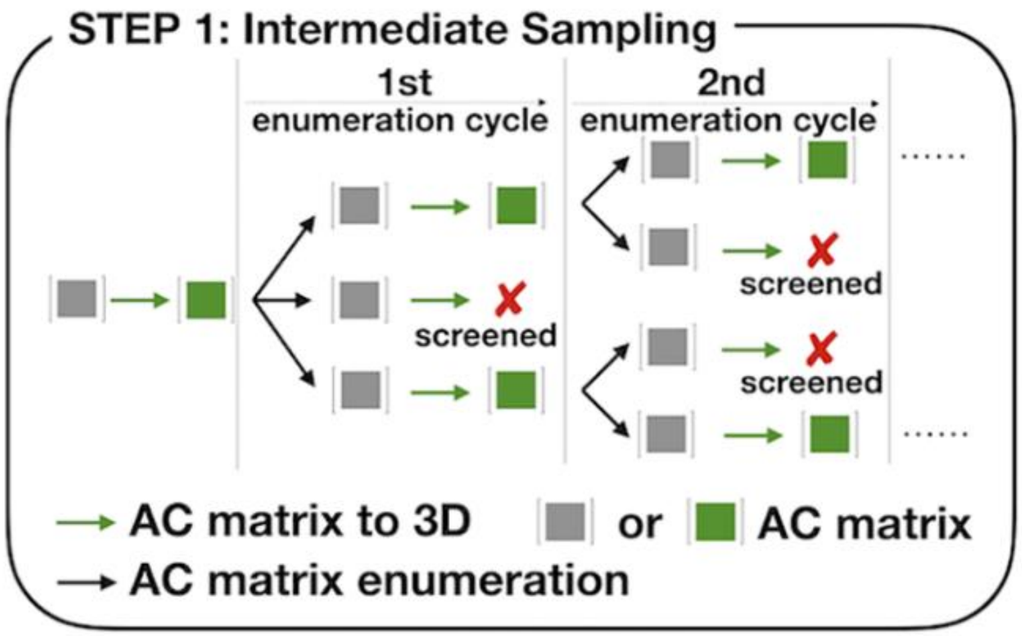


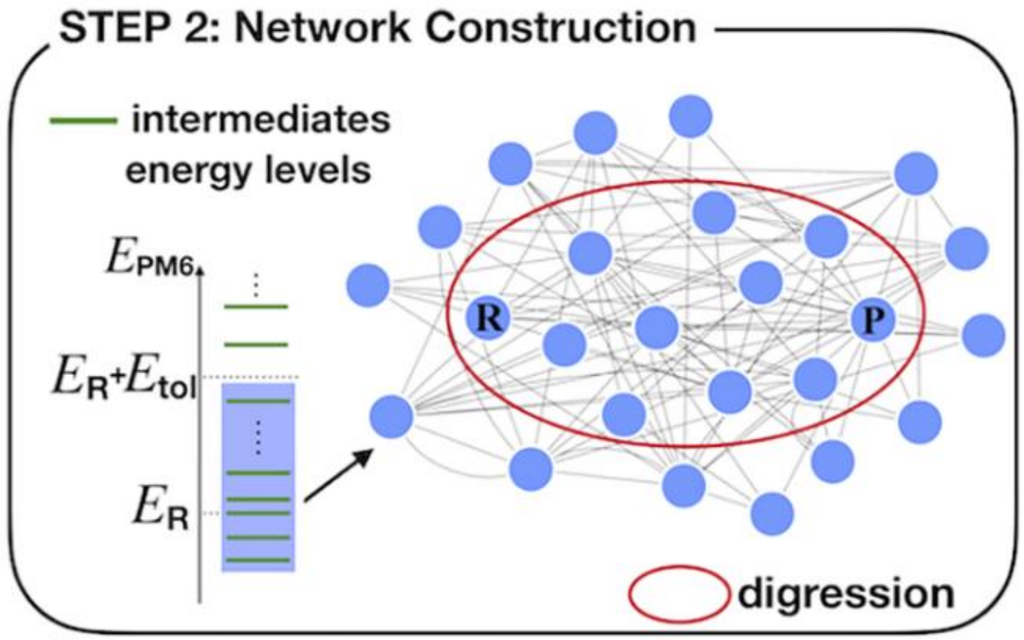
Discovering chemistry with an *ab initio* nanoreactor

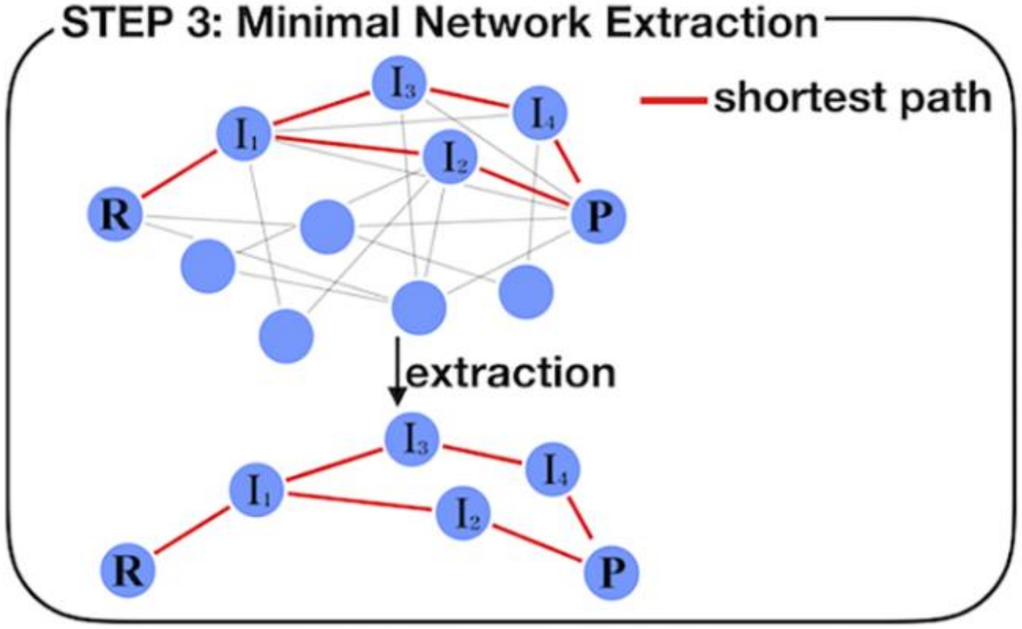
Lee-Ping Wang, Alexey Titov, Robert McGibbon, Fang Liu, Vijay S. Pande & Todd J. Martínez ✉

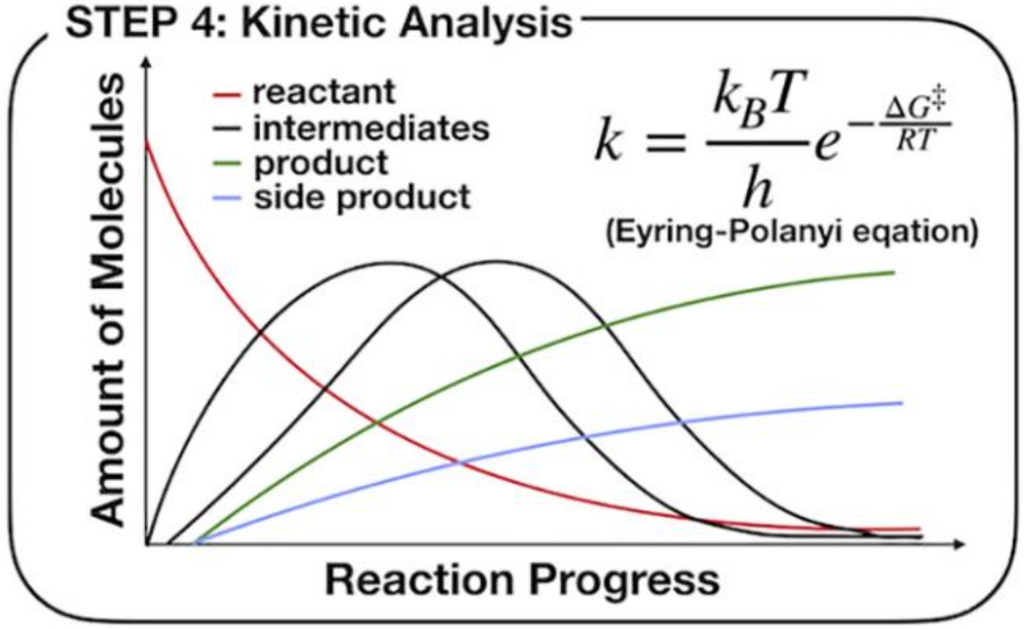
Nature Chemistry **6**, 1044–1048 (2014) | Cite this article

ACE-Reaction: Automatic Reaction Discovery



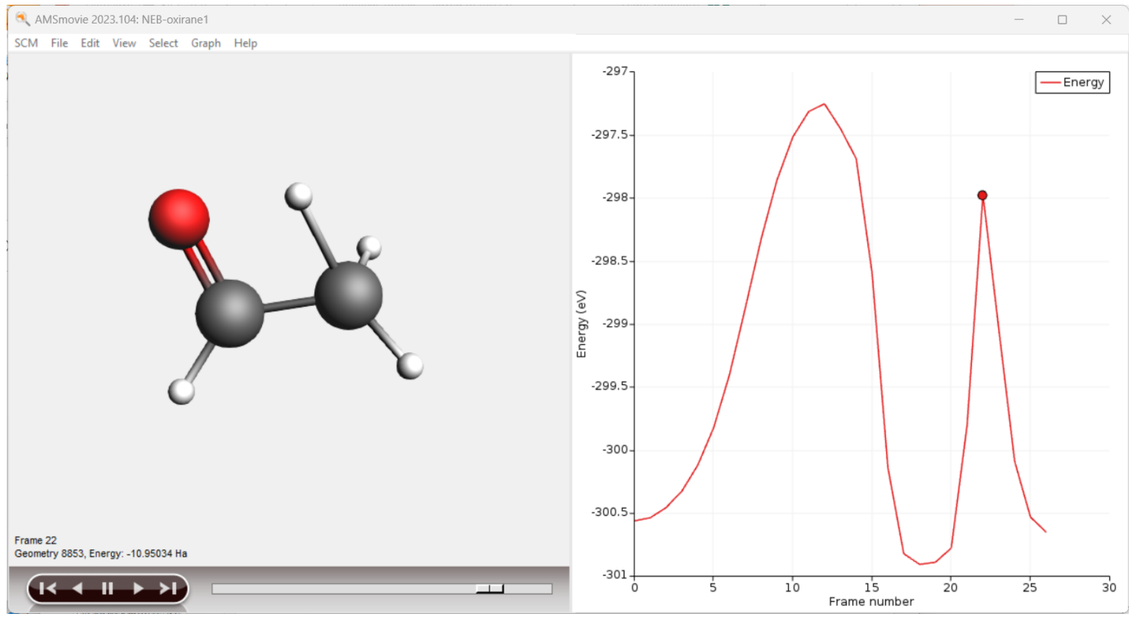




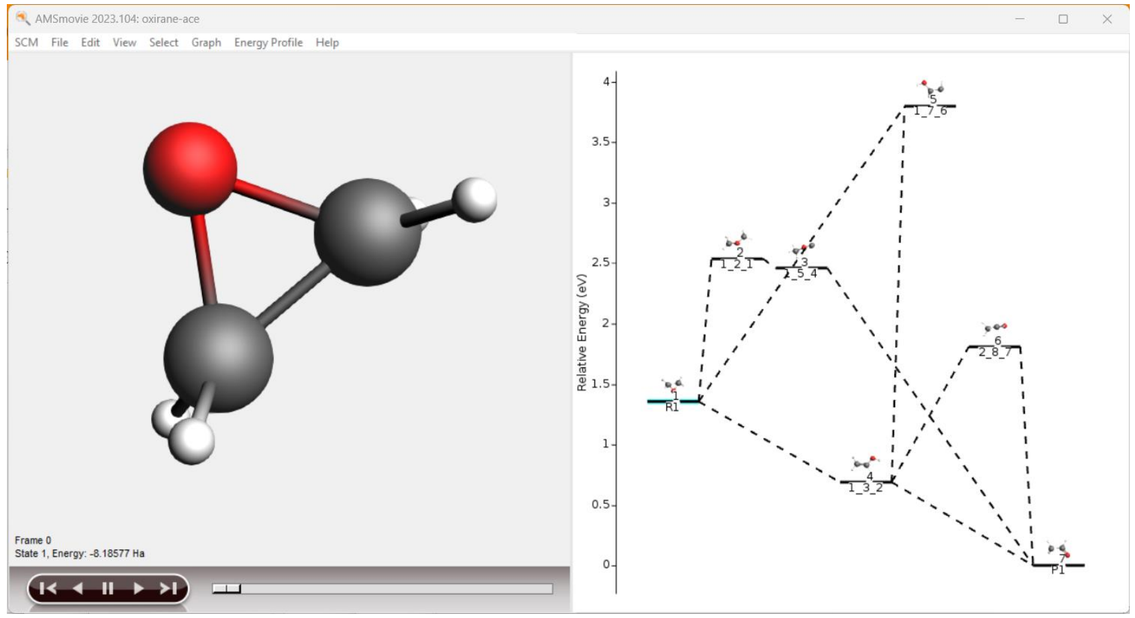


Y. Kim, J. W. Kim, Z. Kim and W. Y. Kim, Chem. Sci. 2018, 9, 825; JPCA 2019, 123, 4796.

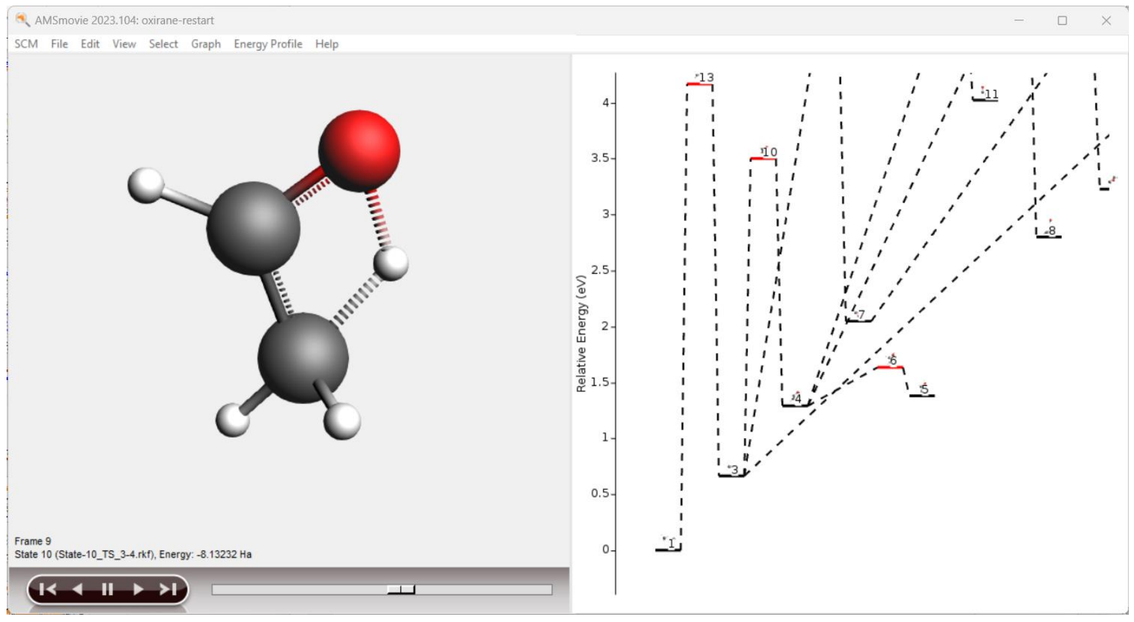
Demo reactivity exploration: oxirane



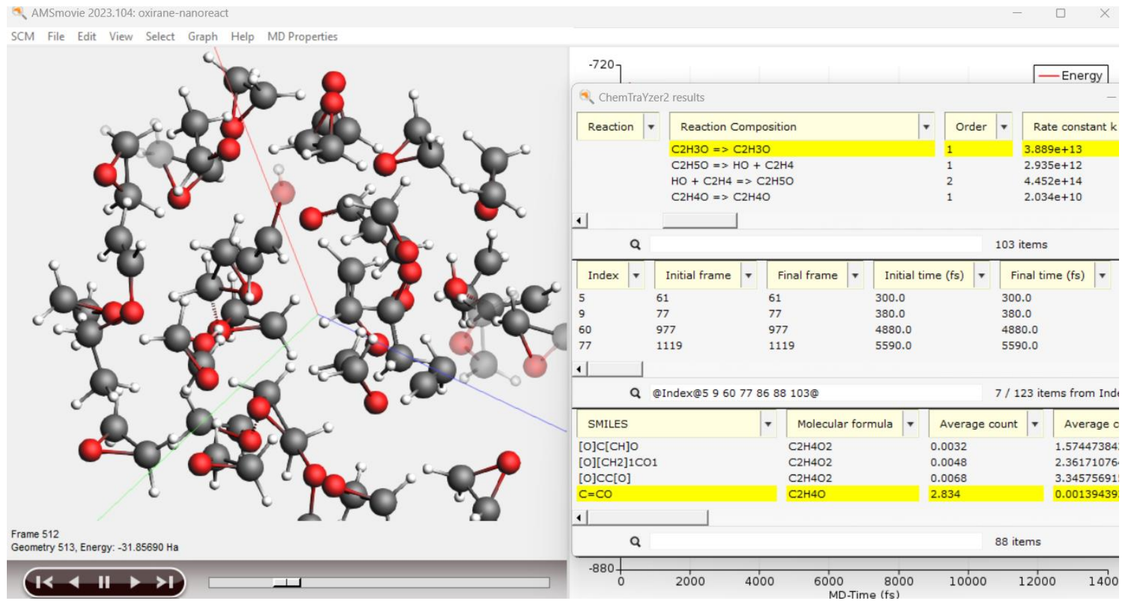
NEB



ACE-Reaction



PES exploration

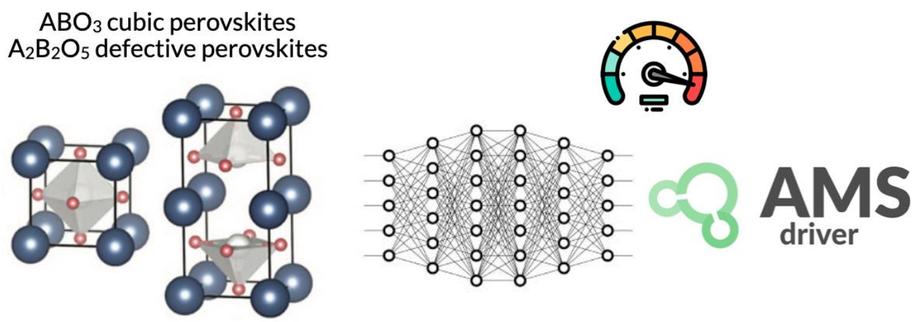


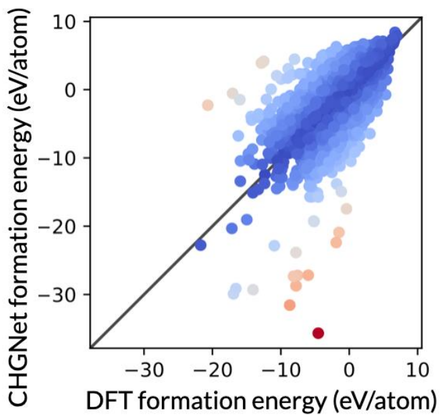
Nanoreactor

Files in Reactions-oxirane directory

Ongoing developments in AMS

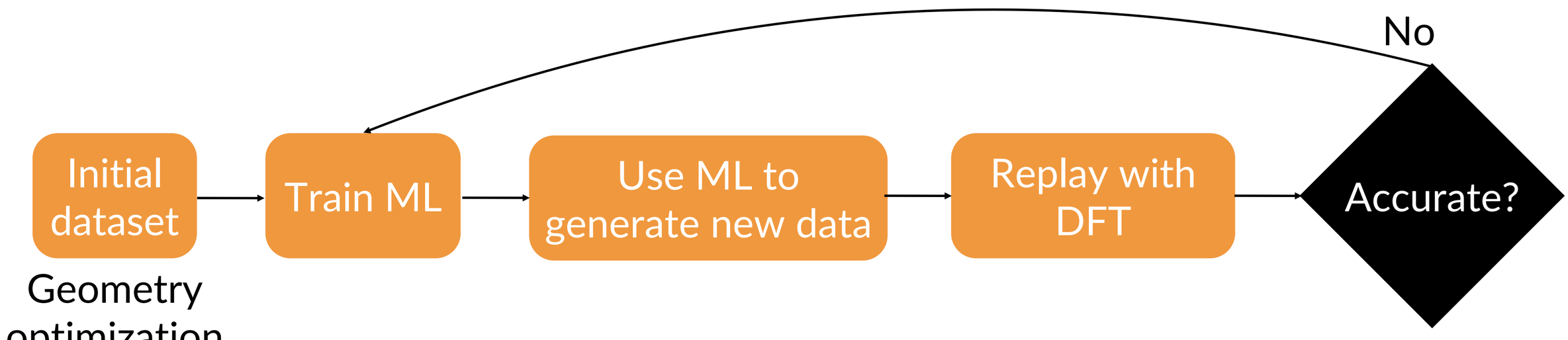
- OLEDs: faster deposition, exciton couplings, GW + polarizable embedding
- Machine learning potentials
  - Reactive potentials: CHGNet, ANI-xnr, Open Catalyst Project
  - On-the-fly learning: NEquIP, FLARE
- Further integration Quantum ESPRESSO (phonons, Raman(?), ParAMS, …)
- Charged periodic systems (defects, electrochemistry??)





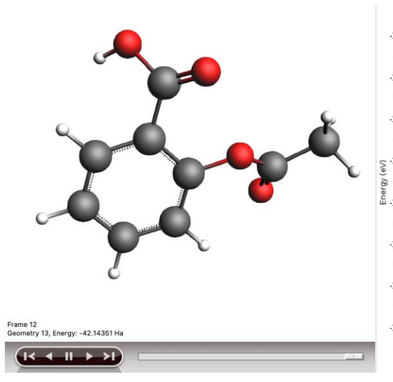
Training MLP with ParAMS

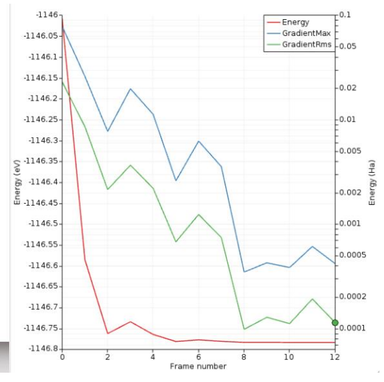
Active learning workflow



Geometry optimization

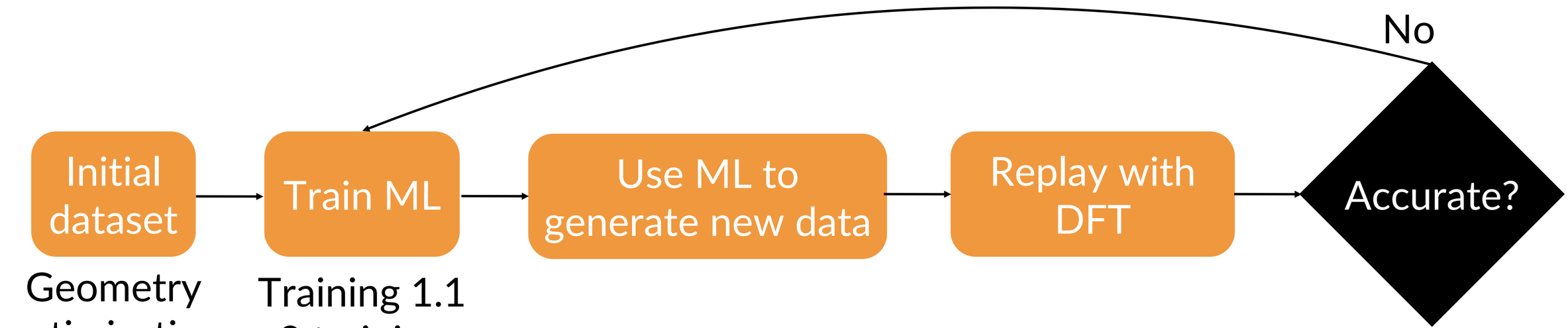
~10 steps

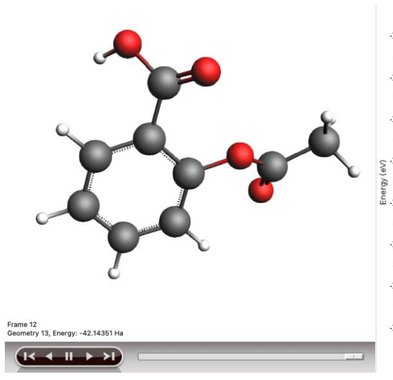


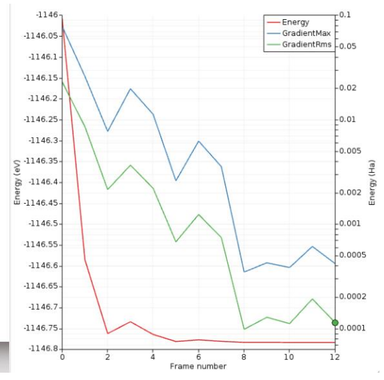


Training MLP with ParAMS

Active learning workflow

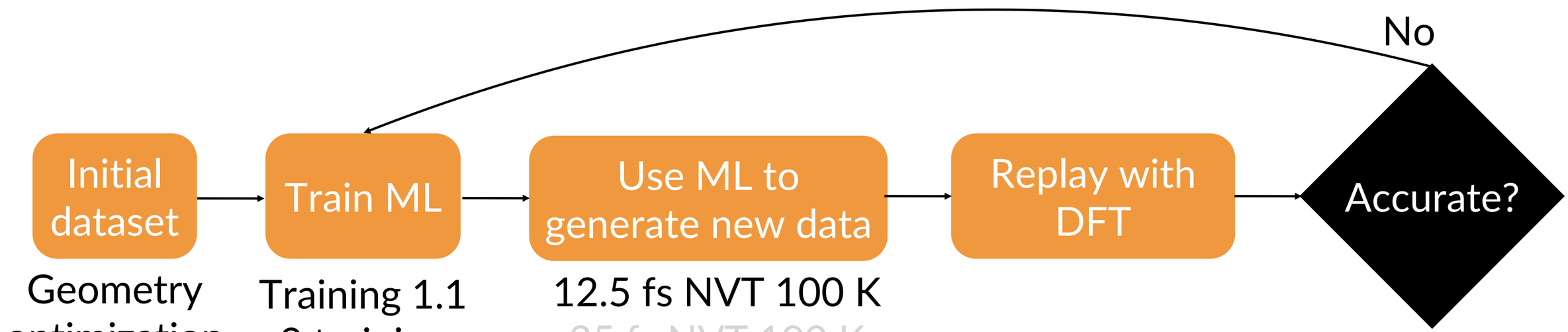


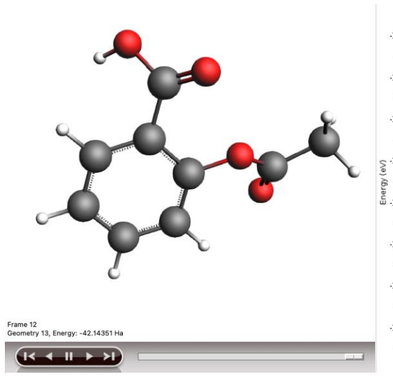


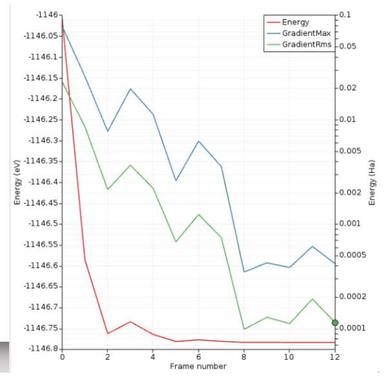


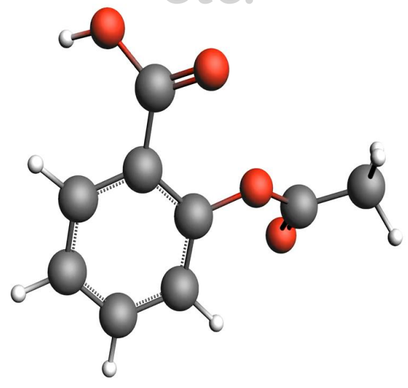
Training MLP with ParAMS

Active learning workflow



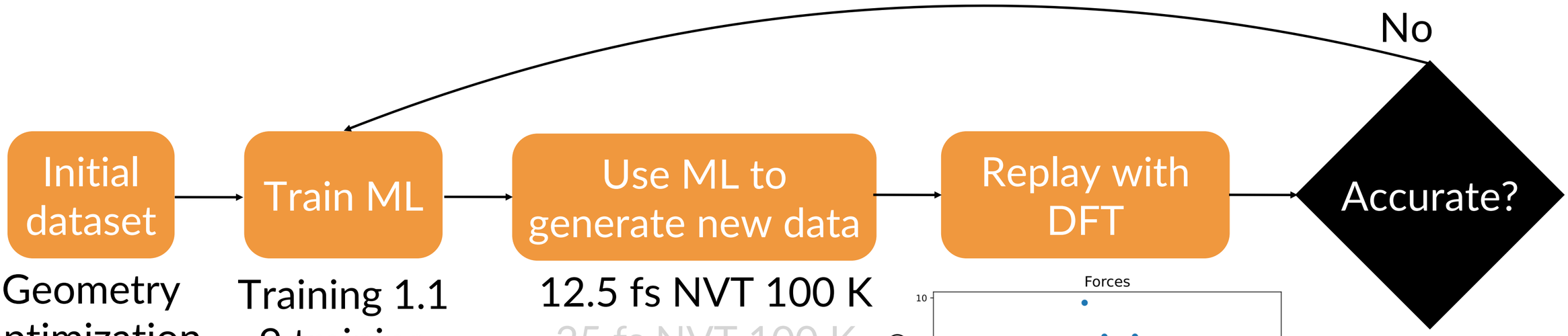


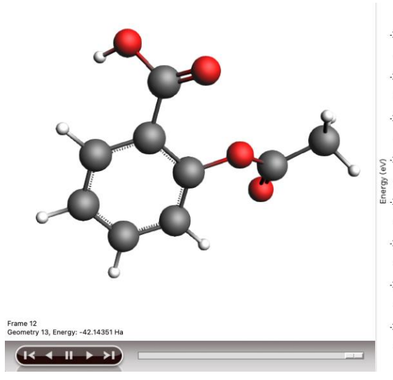


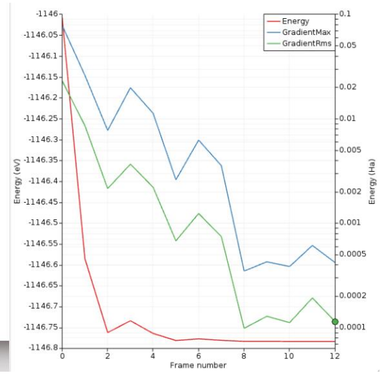


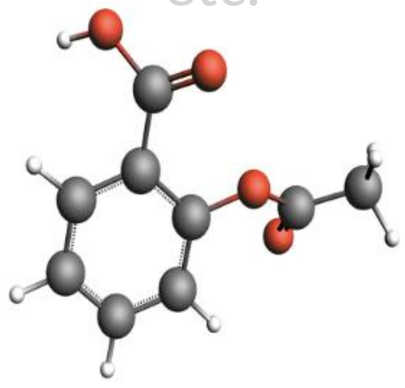
Training MLP with ParAMS

Active learning workflow





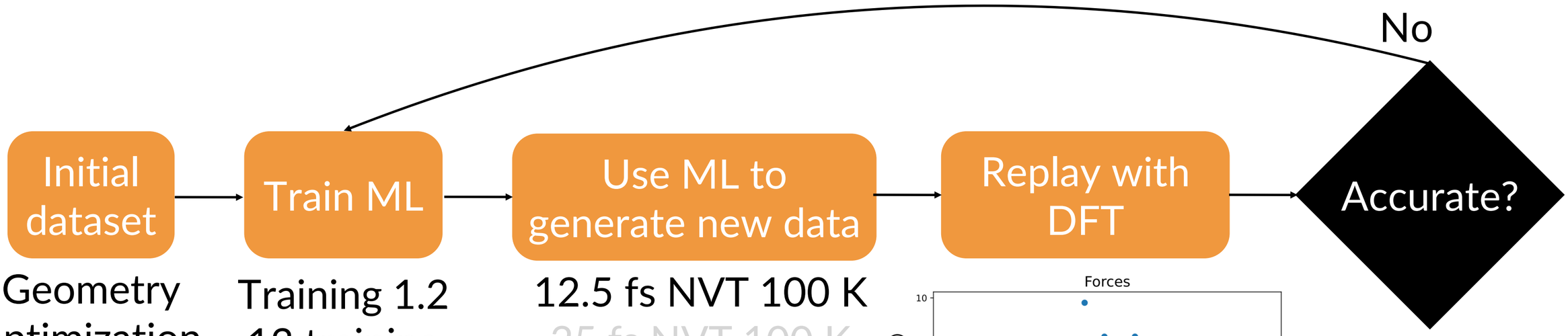


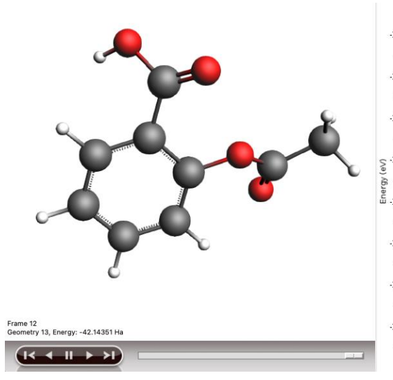


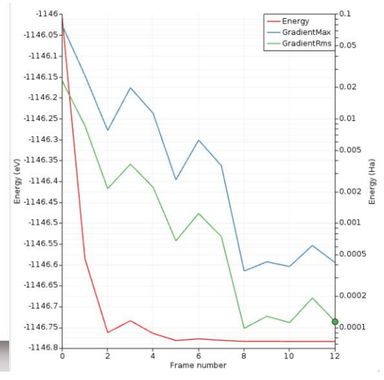
MAE = 1.83 eV/Å

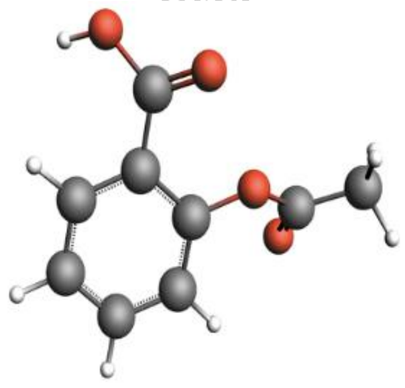
Training MLP with ParAMS

Active learning workflow





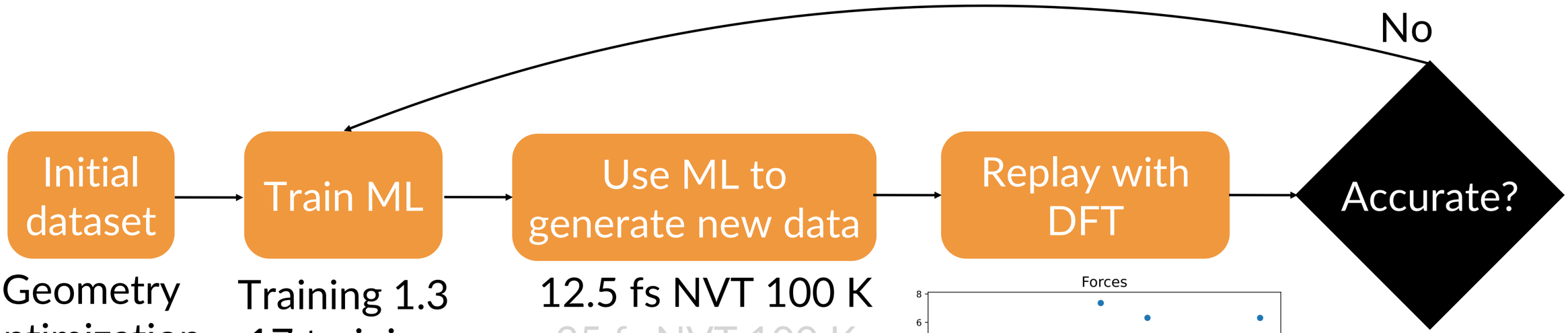


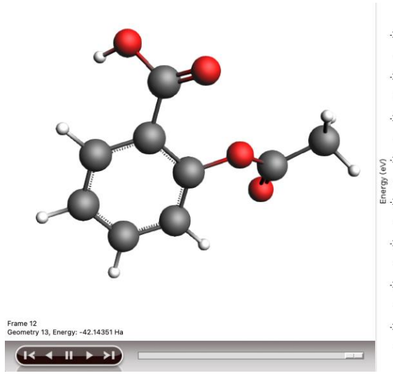


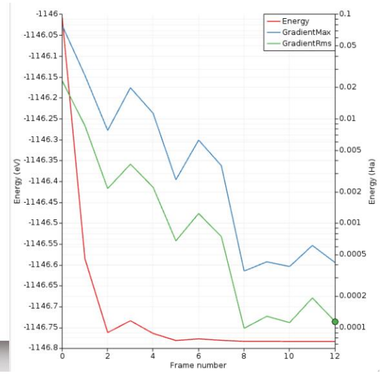
MAE = 1.83 eV/Å

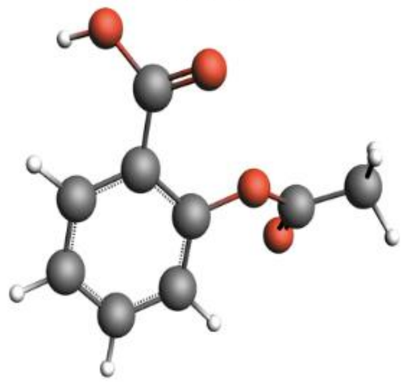
Training MLP with ParAMS

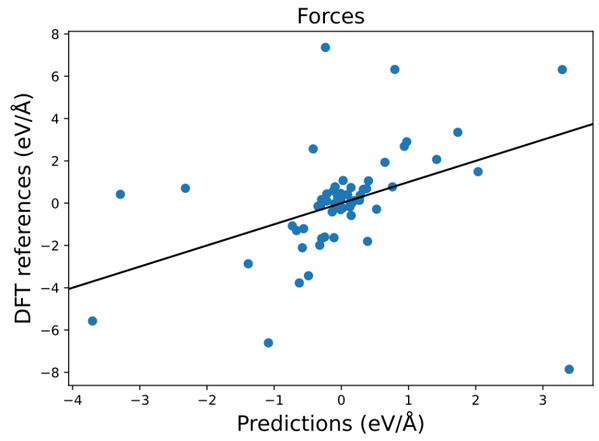
Active learning workflow







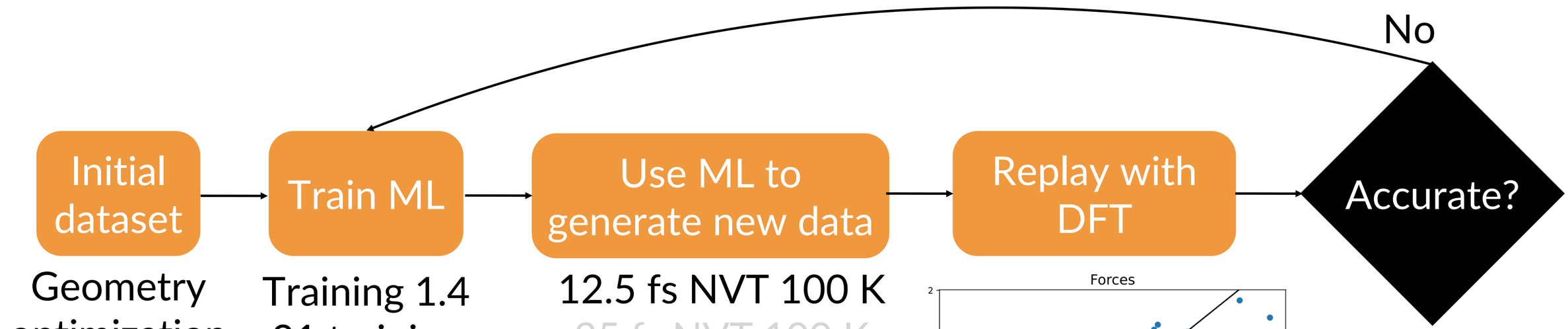


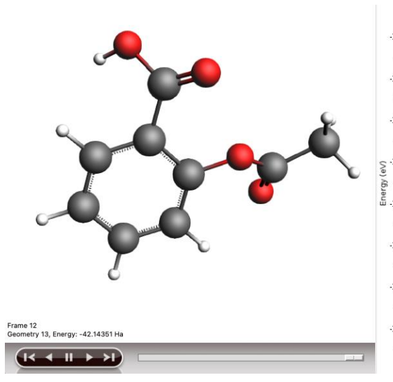


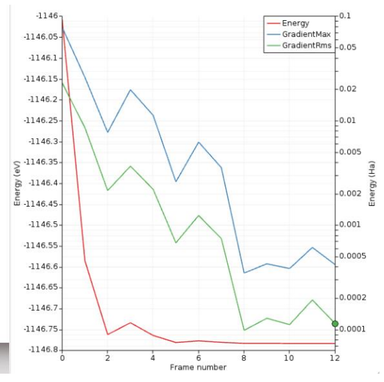
MAE = 1.32 eV/Å

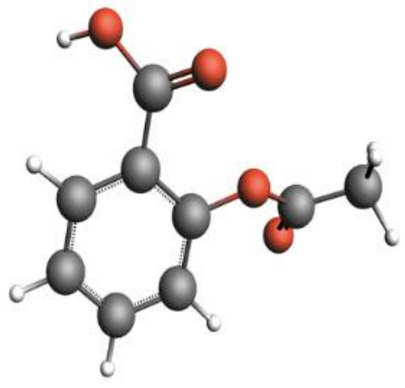
Training MLP with ParAMS

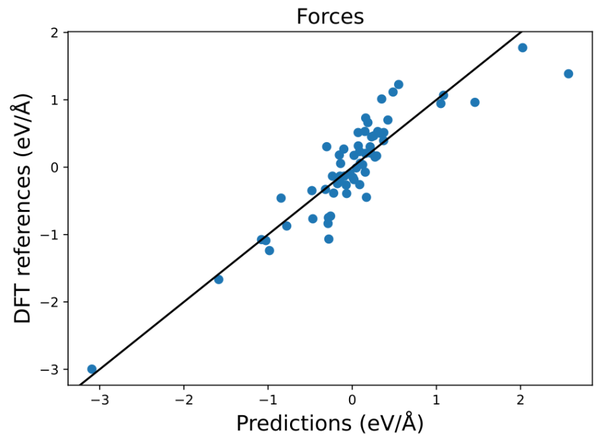
Active learning workflow







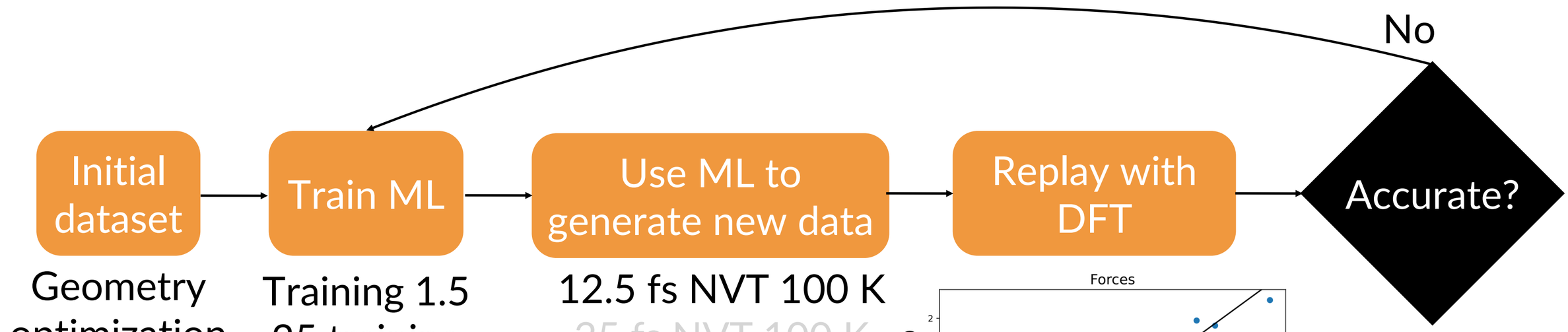


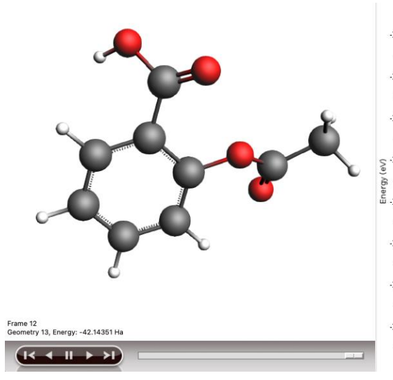


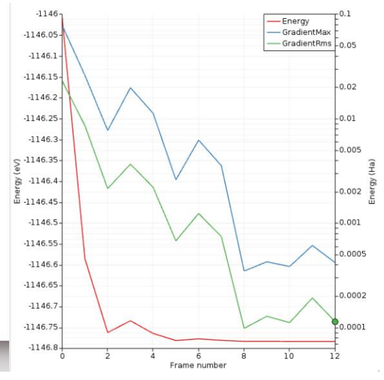
MAE = 0.26 eV/Å

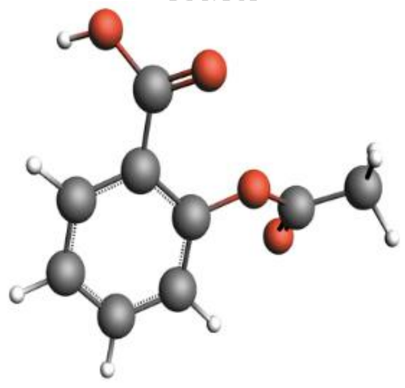
Training MLP with ParAMS

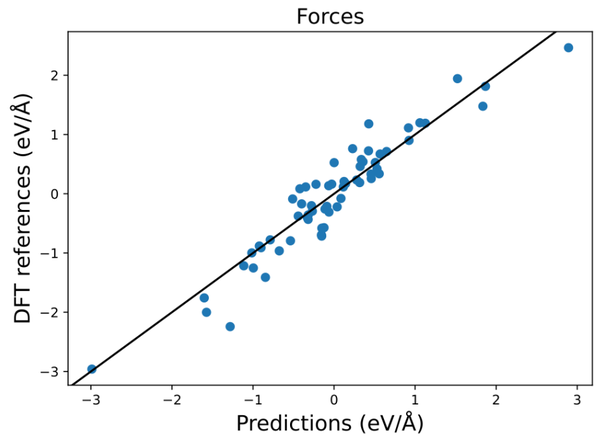
Active learning workflow







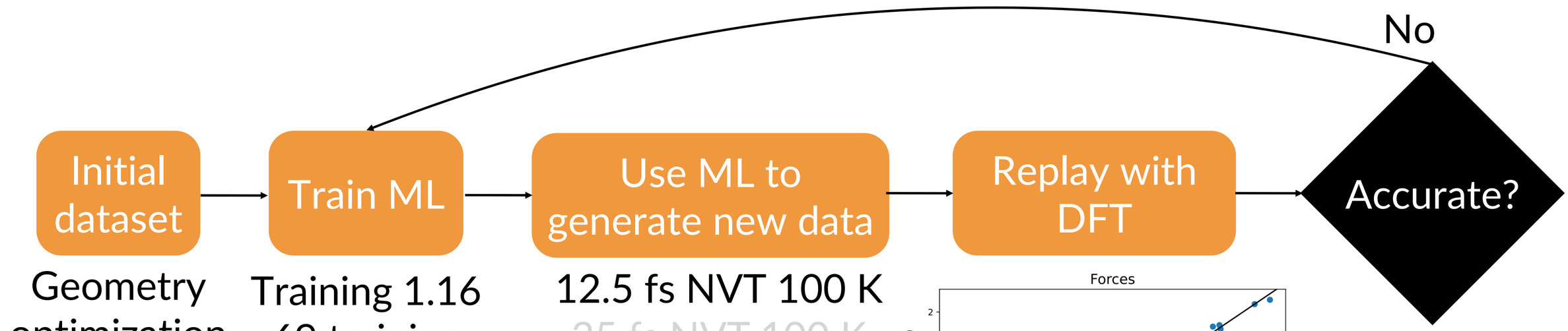




MAE = 0.25 eV/Å

Training MLP with ParAMS

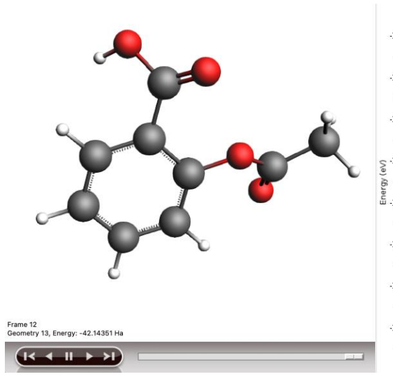
Active learning workflow

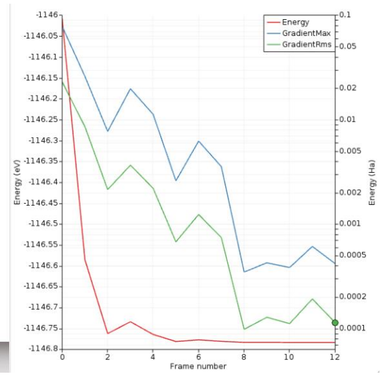


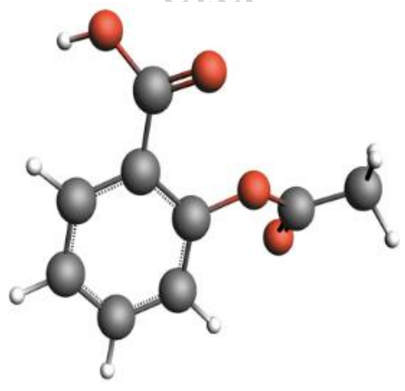
Geometry optimization ~10 steps

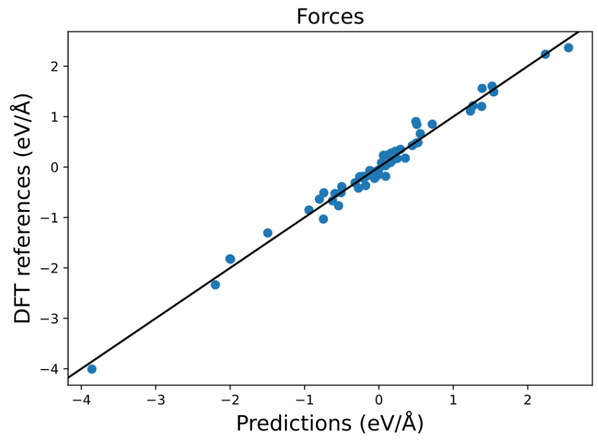
Training 1.16
69 training
20 validation

12.5 fs NVT 100 K
25 fs NVT 100 K
50 fs NVT 100 K
etc.





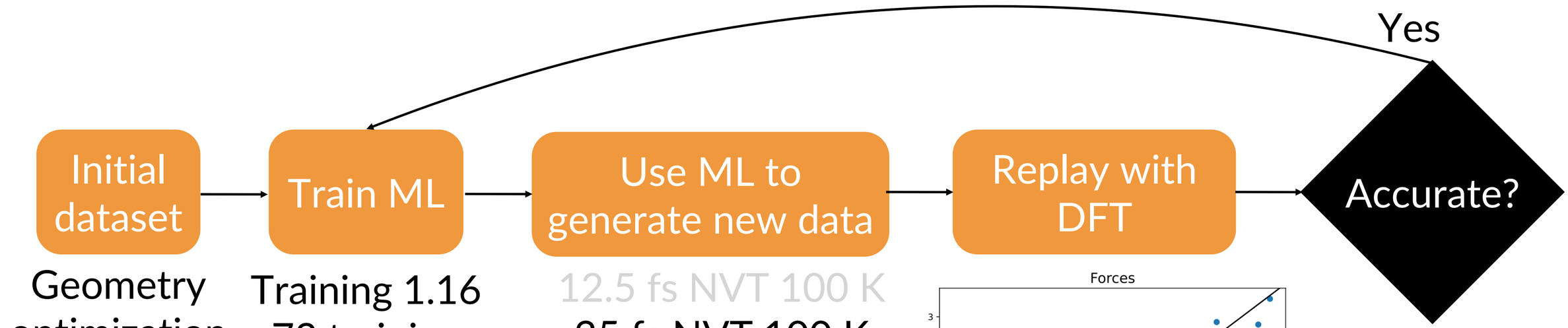




MAE = 0.10 eV/Å

Training MLP with ParAMS

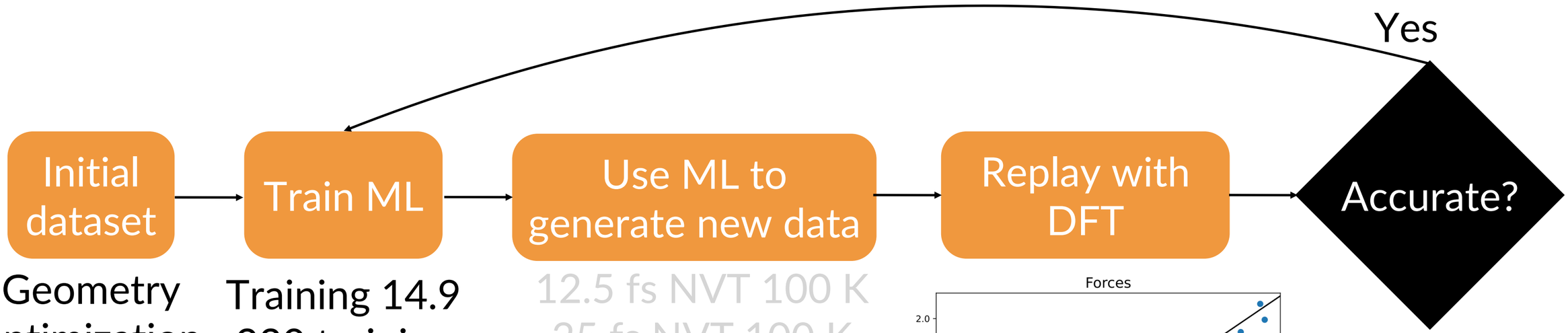
Active learning workflow

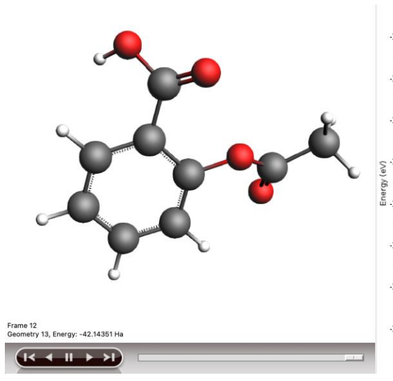


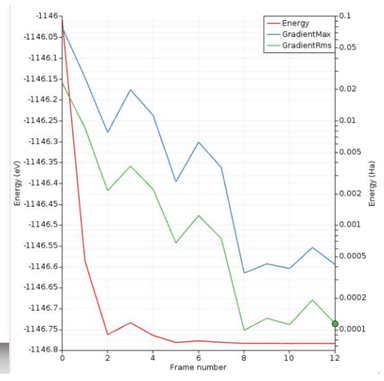
MAE = 0.18 eV/Å

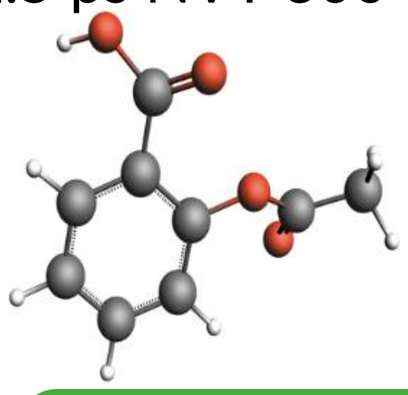
Training MLP with ParAMS

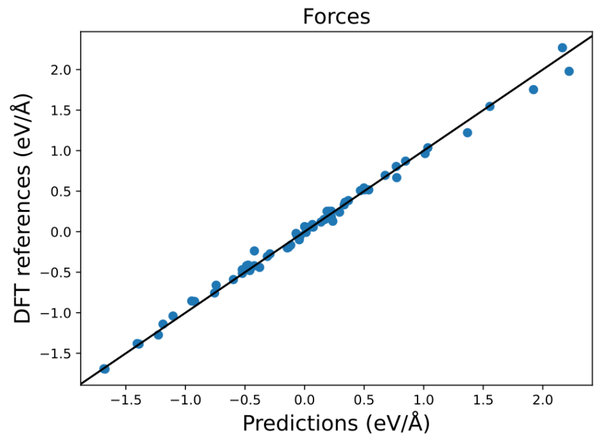
Active learning workflow



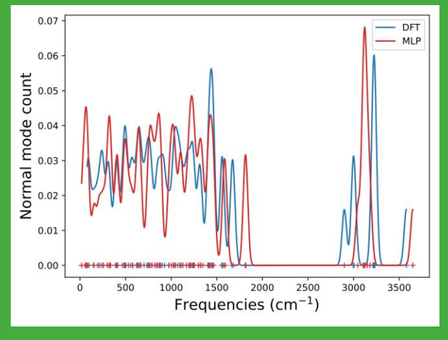




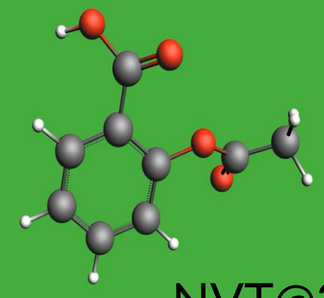




MAE = 0.05 eV/Å



Final model

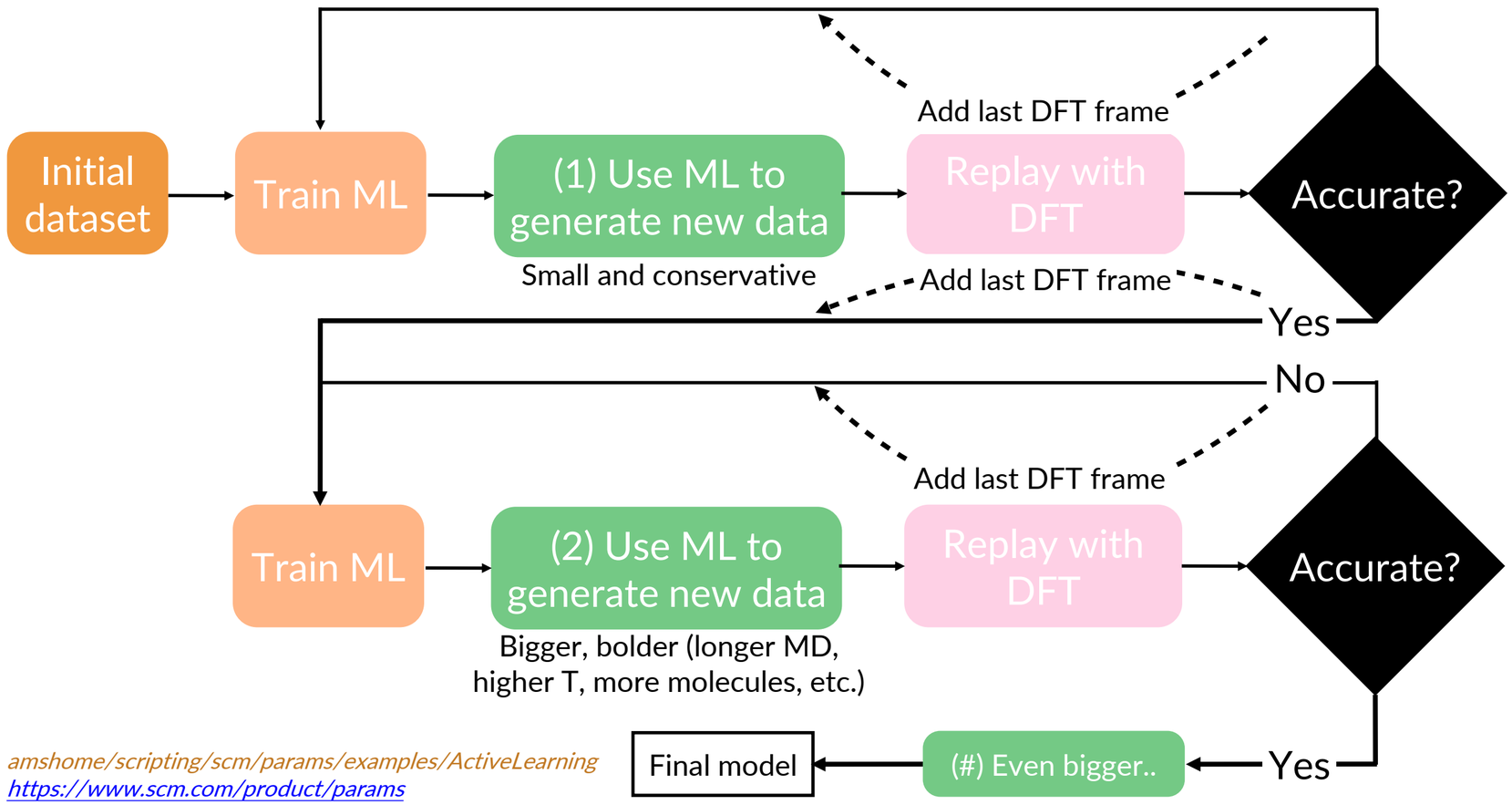


NVT@300K

Training MLP with ParAMS

Summary

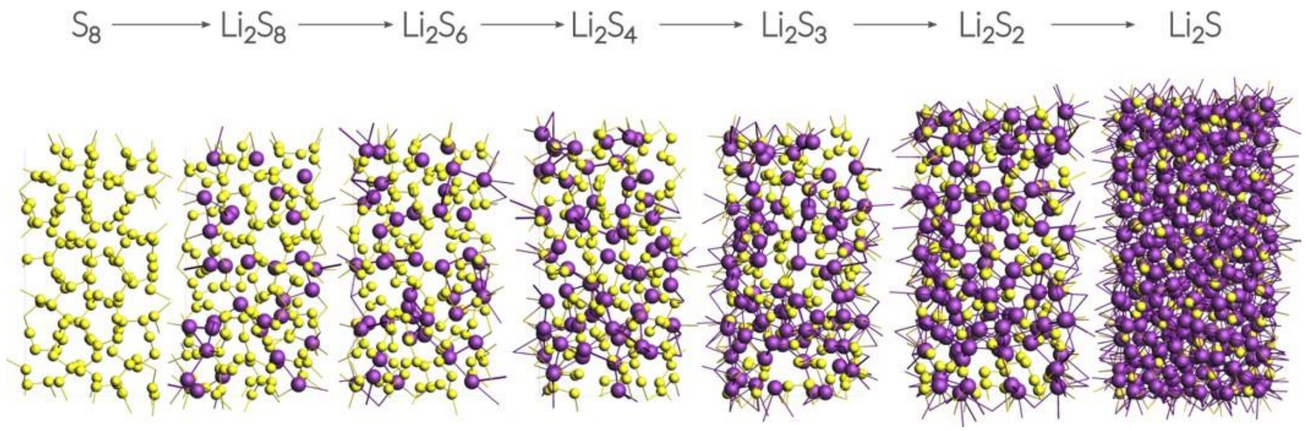
- Compute the initial training set of reference calculations
- Select the ML model to optimize (nequip, flare)
- Define the series of test tasks (default/custom)
- Run an interactively follow the training procedure
  - MAE plot
  - Parity plot
  - Dynamics



amshome/scripting/scm/params/examples/ActiveLearning
https://www.scm.com/product/params

매우 감사합니다!
Let us help you accelerate your R&D!

Important properties?
Most exp. costs/time?
Need help setting up?
Errors?



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