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Software for Chemistry & Materials

ipam institute for pure & applied mathematics

Workshop III: Complex Scientifi Workflows at Extreme Computational Scales

MAY 1 - 5, 2023

Revolutionizing Catalysis Industry through Automated Multiscale Modeling and Active Exploration of Chemical Space

Nestor F. Aguirre
Scientific Software Developer
aguirre@scm.com

Background: SCM, ADF & AMS

- AMOL/ADF: first DFT code for chemistry (1970s)
  Baerends@VU (>'73), Ziegler@Calgary(+) (>'75)

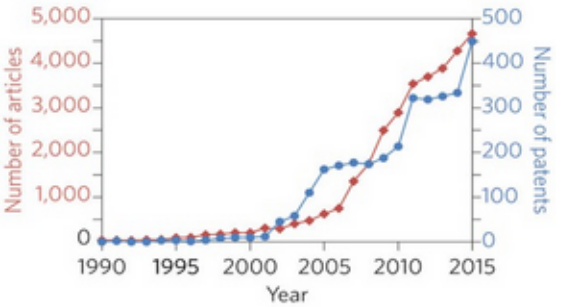
- 1980s: Mitsui, Shell, Akzo, Unilever: training@Amsterdam
  - Tom Ziegler => Ziegler-Natta catalysts, hydroformulation
  - BAND for periodic systems

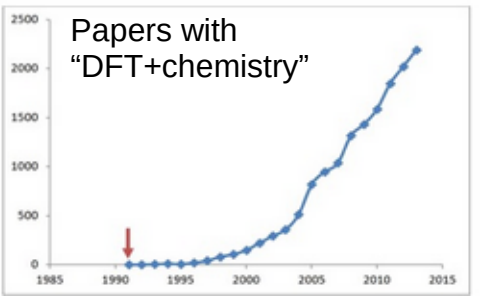
- SCM: Spin-off company 1995
  - To keep supporting users

- 2010s: DFTB, ReaxFF, COSMO-RS (Albemarle, DSM)

- 2019: Multi-scale: ReaxPro (BASF, Dow, Shell, JM)

- 2022: 24 people (19 senior PhD's) + 3 EU fellows
  Many academic collaborators & EU networks
  SCM: development, debug, port, optimize, & support





The SCM team celebrating 25 years (2020)

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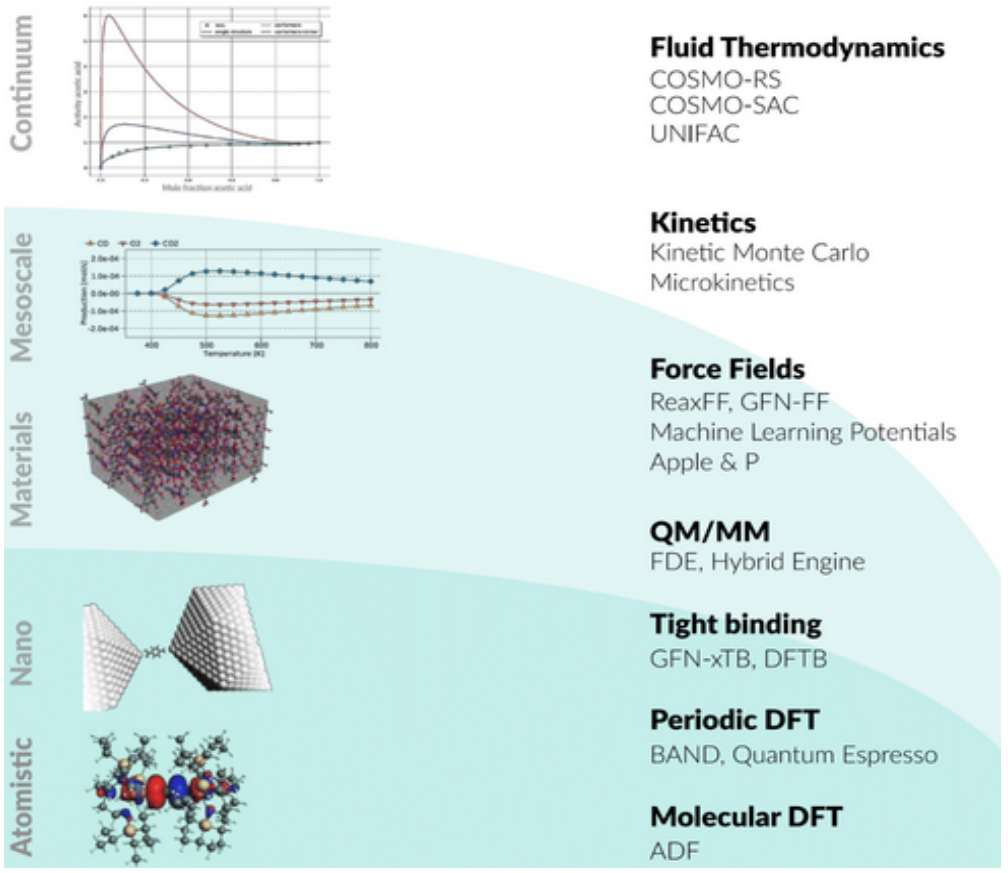
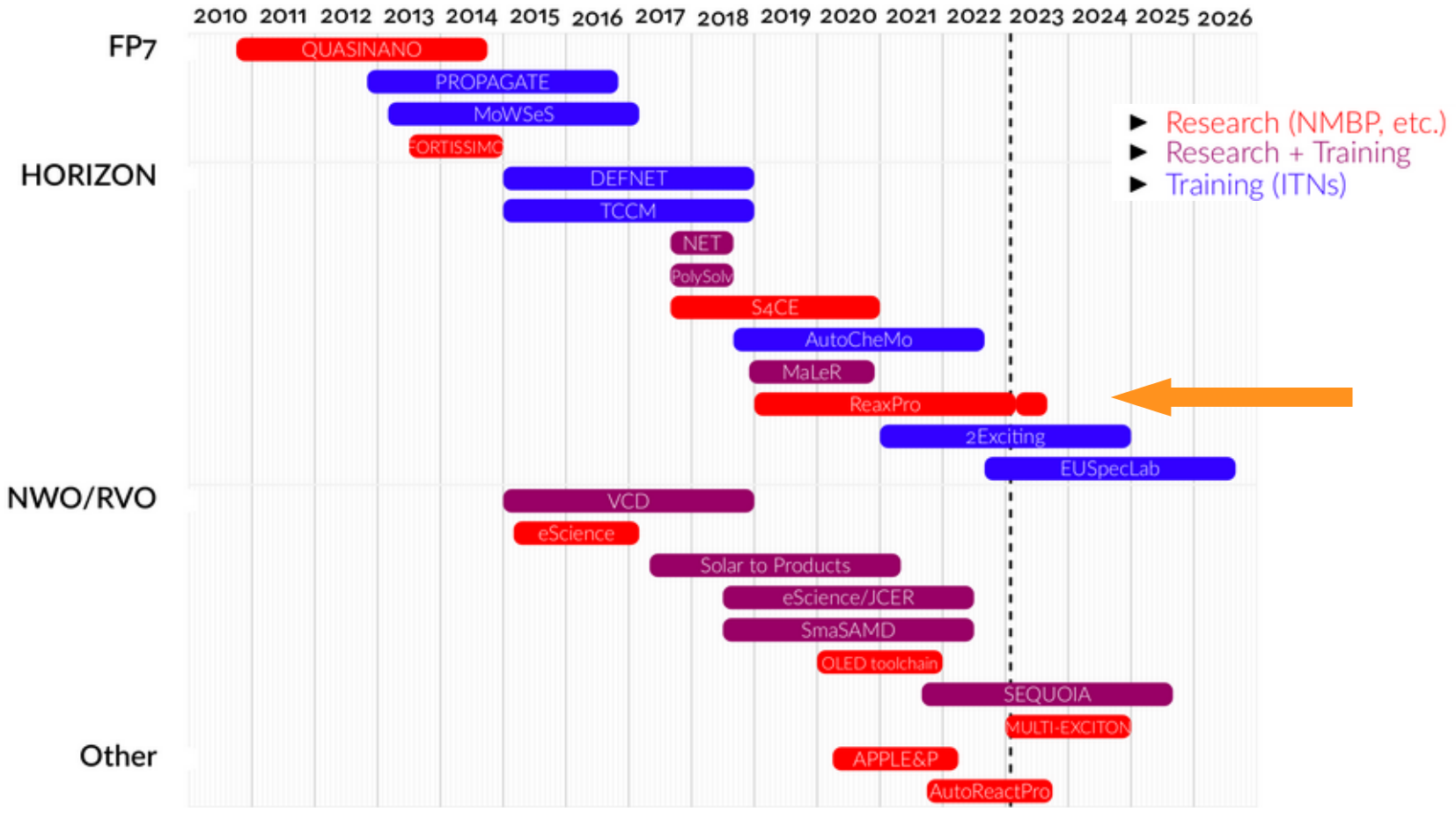
Amsterdam Modeling Suite



- Integrated GUI
- Python scripting (workflows)
- Tools: parametrization, reaction mapping & analysis
- AMSdriver:
  MD, MC, PES exploration
  - Hybrid: multi-layer,
  - QM/MM, QM/QM'
  - Automated reaction
  - Network mapping
  - Analysis, properties

(EU) collaborations



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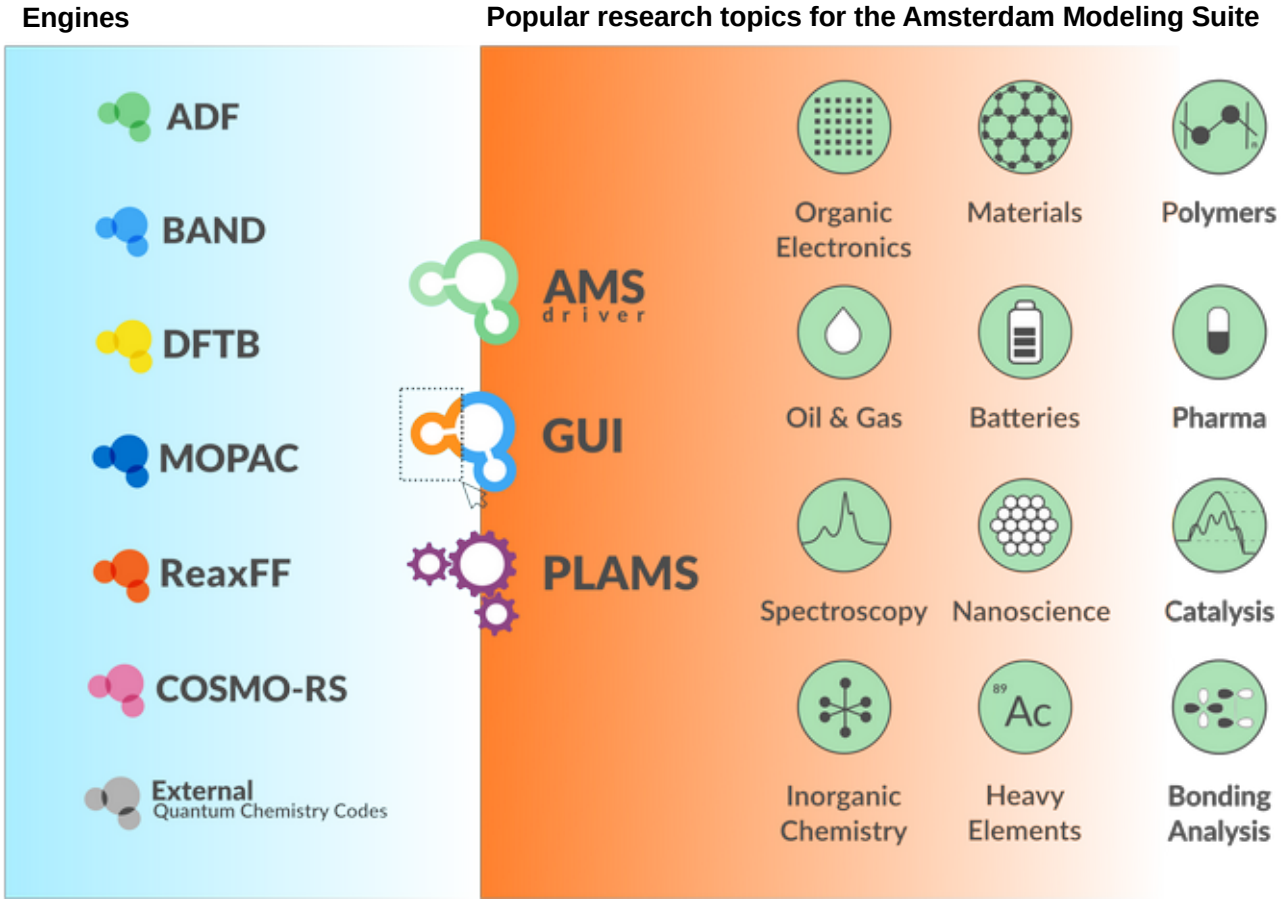
Software for Chemistry & Materials

Joint Code Development

- We collaborate with academic groups developing code.
- They provide code and/or know-how (algorithms, test sets, etc).
- We focus on usability (e.g. GUI), performance (optimization, parallelization, etc.), long-term maintenance and support.
- We integrate and distribute code.
- Academic developers get increased visibility and outreach, citations, software licenses, etc.
- And they keep their intellectual property.

AMS2023 (www.scm.com)



AMS driver is a powerful central tool in the Amsterdam Modeling Suite for complex potential energy tasks, such as molecular dynamics, Monte Carlo, PES scans, and finding transition states.

The AMS driver provides efficient and reliable implementations for common tasks like geometry optimization or transition state searches as well as more advanced modeling and simulation options like Grand Canonical Monte Carlo, force bias Monte Carlo, and the molecule gun.

Revolutionizing Catalysis Industry through Automated Multiscale Modeling and Active Exploration of Chemical Space

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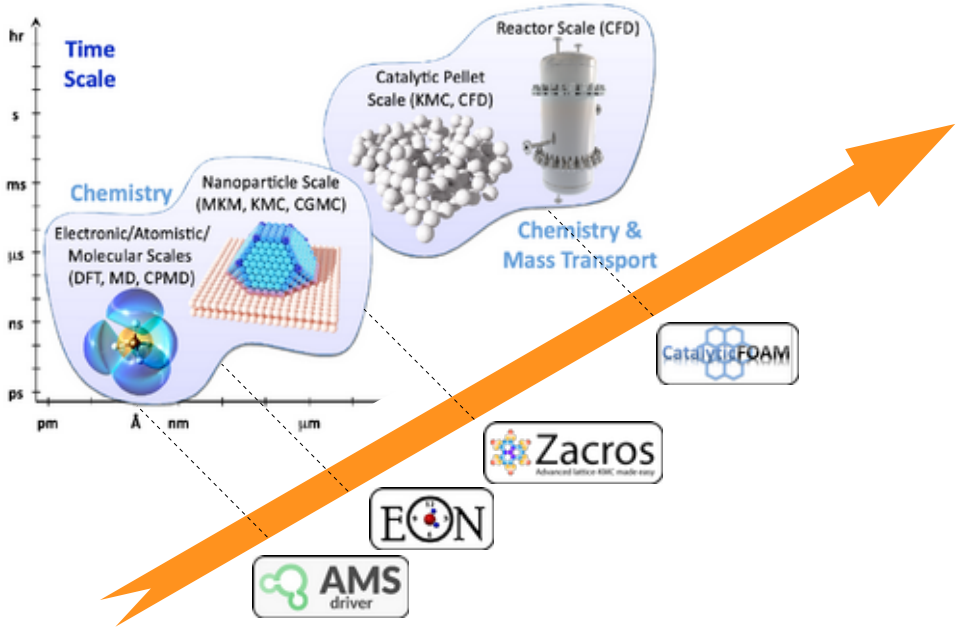
The ReaxPro Project

http://www.reaxpro.eu



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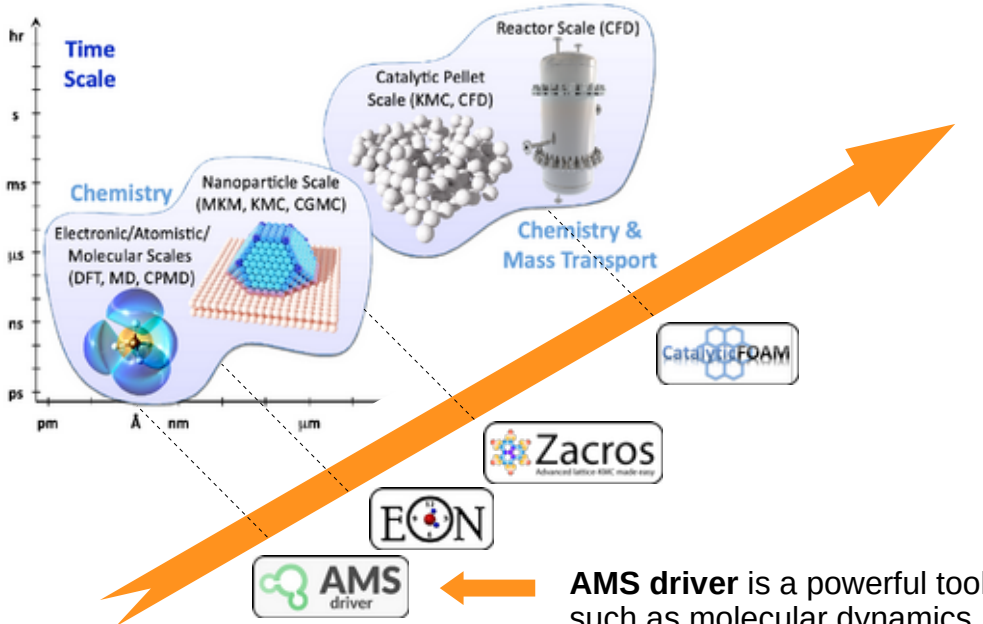
This project has received funding from the European Union's Horizon 2020 research and innovation programme under the grant agreement No 814416

The ReaxPro Project

http://www.reaxpro.eu



AMS driver is a powerful tool for potential energy tasks, such as molecular dynamics, Monte Carlo, and finding transition states with our atomistic modules (engines) such as ADF, BAND, DFTB, MOPAC, ReaxFF, Machine Learning Potentials, and Force Field.

`https://www.scm.com/product/ams/`

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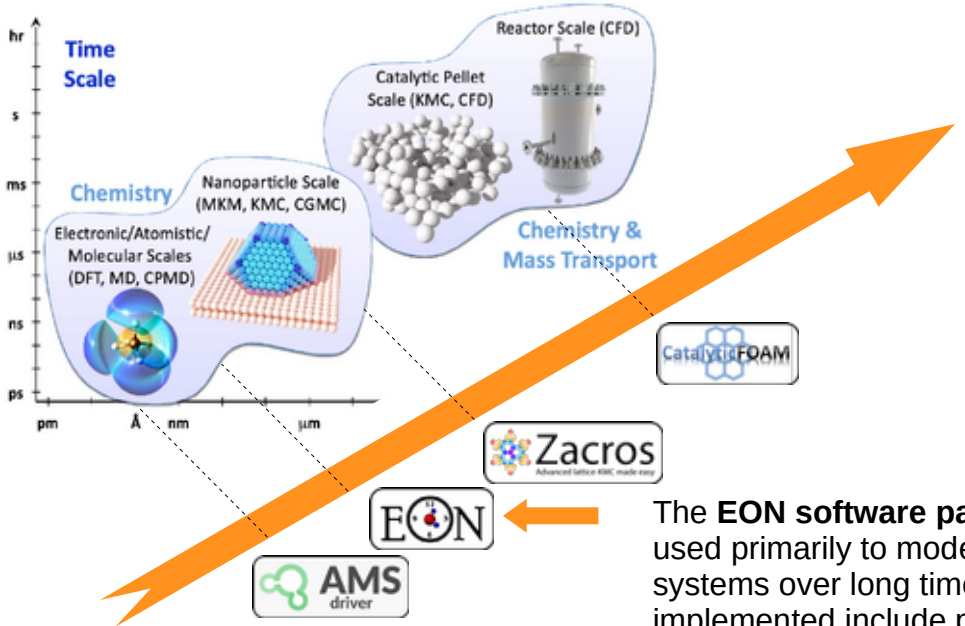

The **EON software package** contains a set of algorithms used primarily to model the evolution of atomic scale systems over long time scales. The algorithms currently implemented include parallel replica dynamics, hyperdyamics, adaptive kinetic Monte Carlo, and basin hopping. The EON software is a collaboration between the Henkelman and Jónsson research groups.

`https://theory.cm.utexas.edu/eon/`

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S. T Chill, M. Welborn, R. Terrell, L. Zhang, J.-C. Berthet, A. Pedersen, H. Jónsson and G. Henkelman. EON: software for long time simulations of atomic scale systems, Modelling Simul. Mater. Sci. Eng. 22 055002 (2014).

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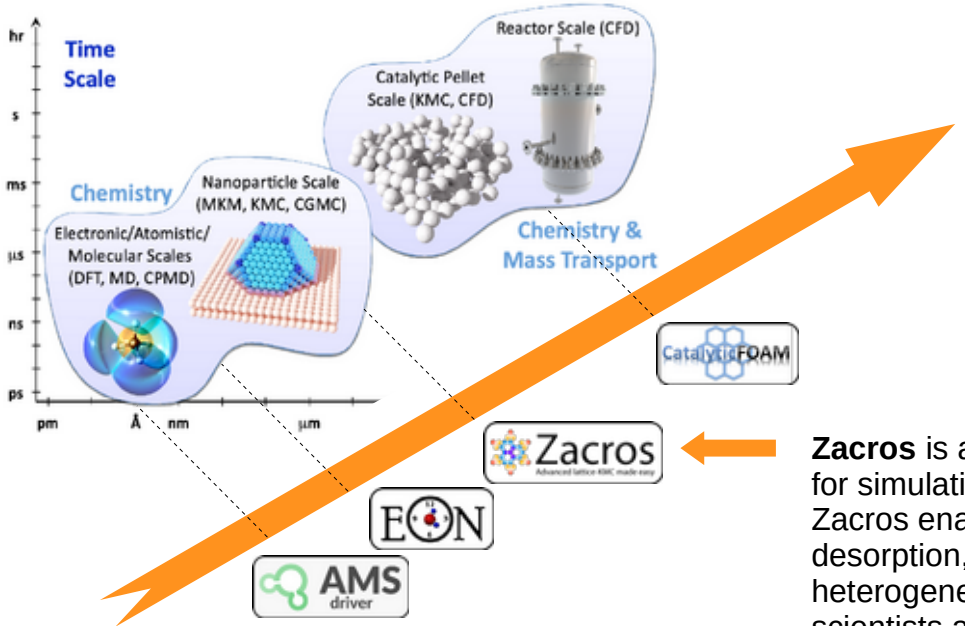

Zacros is a Kinetic Monte Carlo (KMC) software package, for simulating molecular phenomena on catalytic surfaces. Zacros enables to perform dynamic modeling of adsorption, desorption, surface diffusion, and reaction processes on heterogeneous catalysts. Zacros is developed by a team of scientists at UCL, led by Dr Michail Stamatakis,

`https://zacros.org/`

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Stamatakis, M. and D. G. Vlachos, A Graph-Theoretical Kinetic Monte Carlo Framework for on-Lattice Chemical Kinetics., The Journal of Chemical Physics, 134(21): 214115.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the grant agreement No 814416

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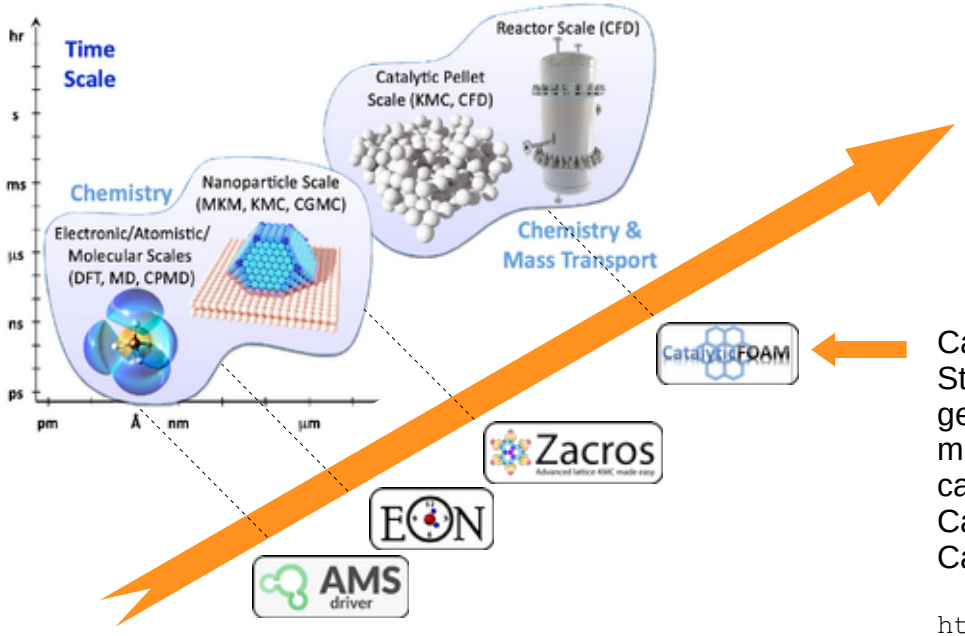

CatalyticFOAM allows for the solution of Navier-Stokes equations for complex and general geometries for reacting flows at surfaces, based on microkinetic descriptions of the surface reactivity. catalyticFoam has been developed in the Multiscale Catalysis Group of the Laboratory of Catalysis and Catalytic Processes of Politecnico di Milano.

`https://www.catalyticfoam.polimi.it/`
`https://github.com/multiscale-catalysis-polimi/catalyticFoam`

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Maestri, M. and Cuoci, A. (2013) Coupling CFD with detailed microkinetic modeling in heterogeneous catalysis. Chemical Engineering Science. Volume 96. Pages 106-117. doi.org/10.1016/j.ces.2013.03.048.

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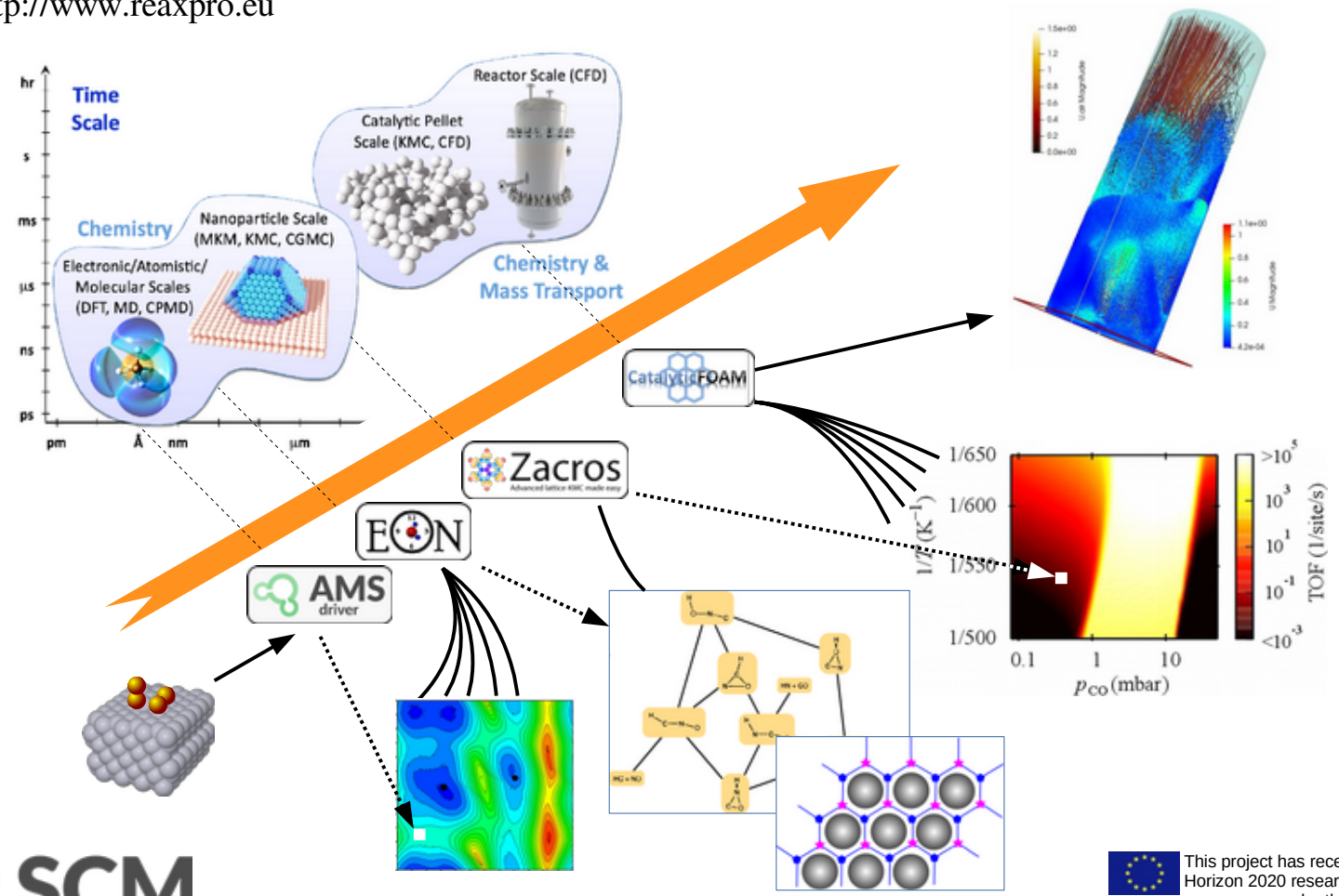

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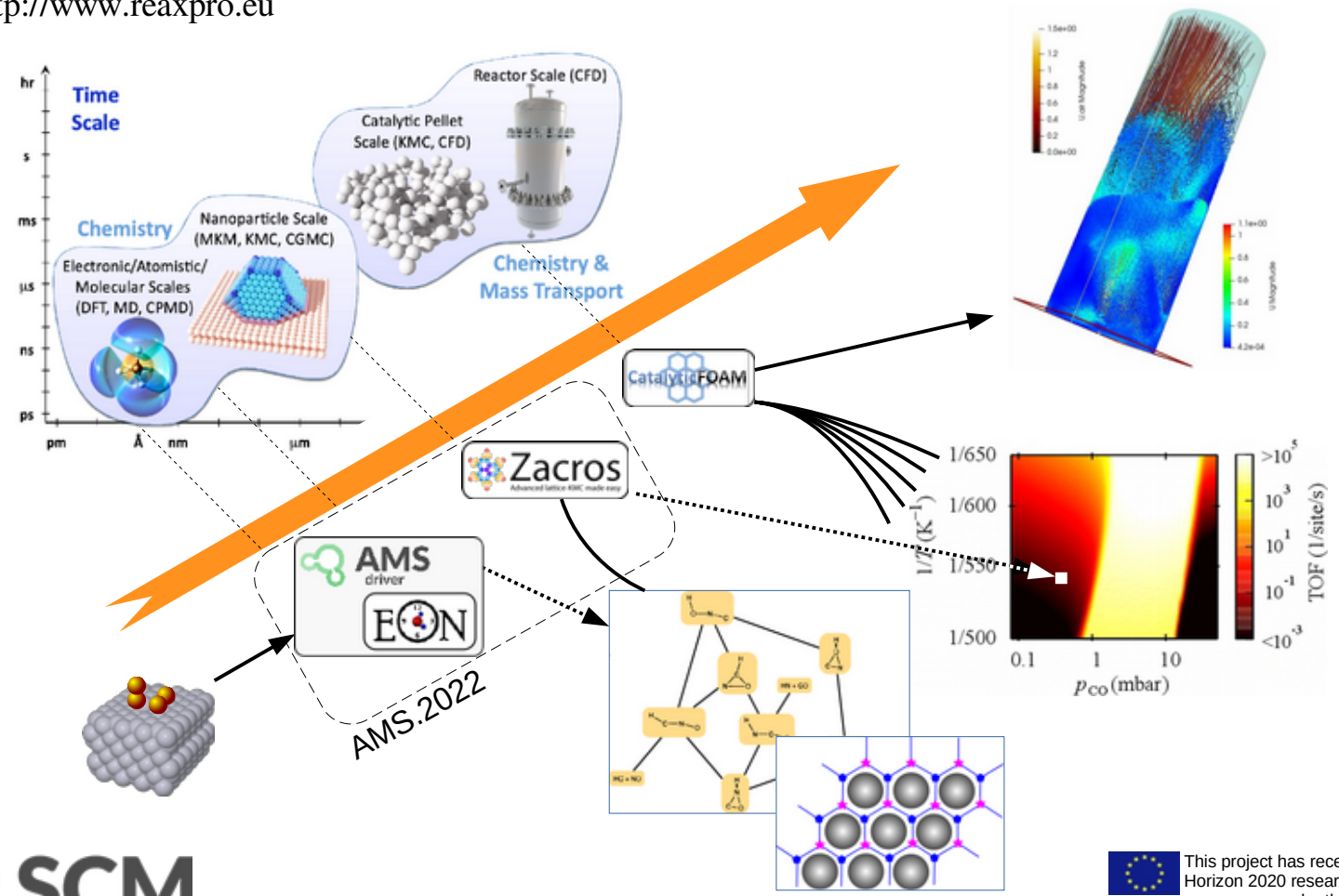

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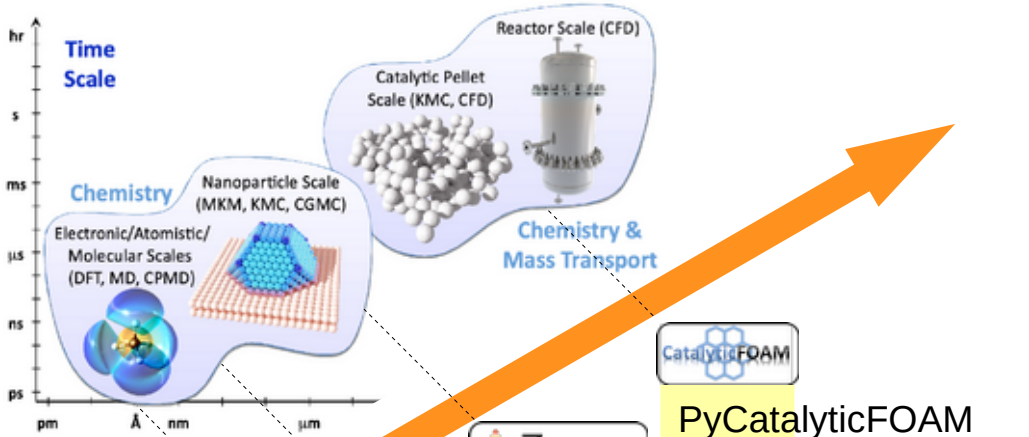

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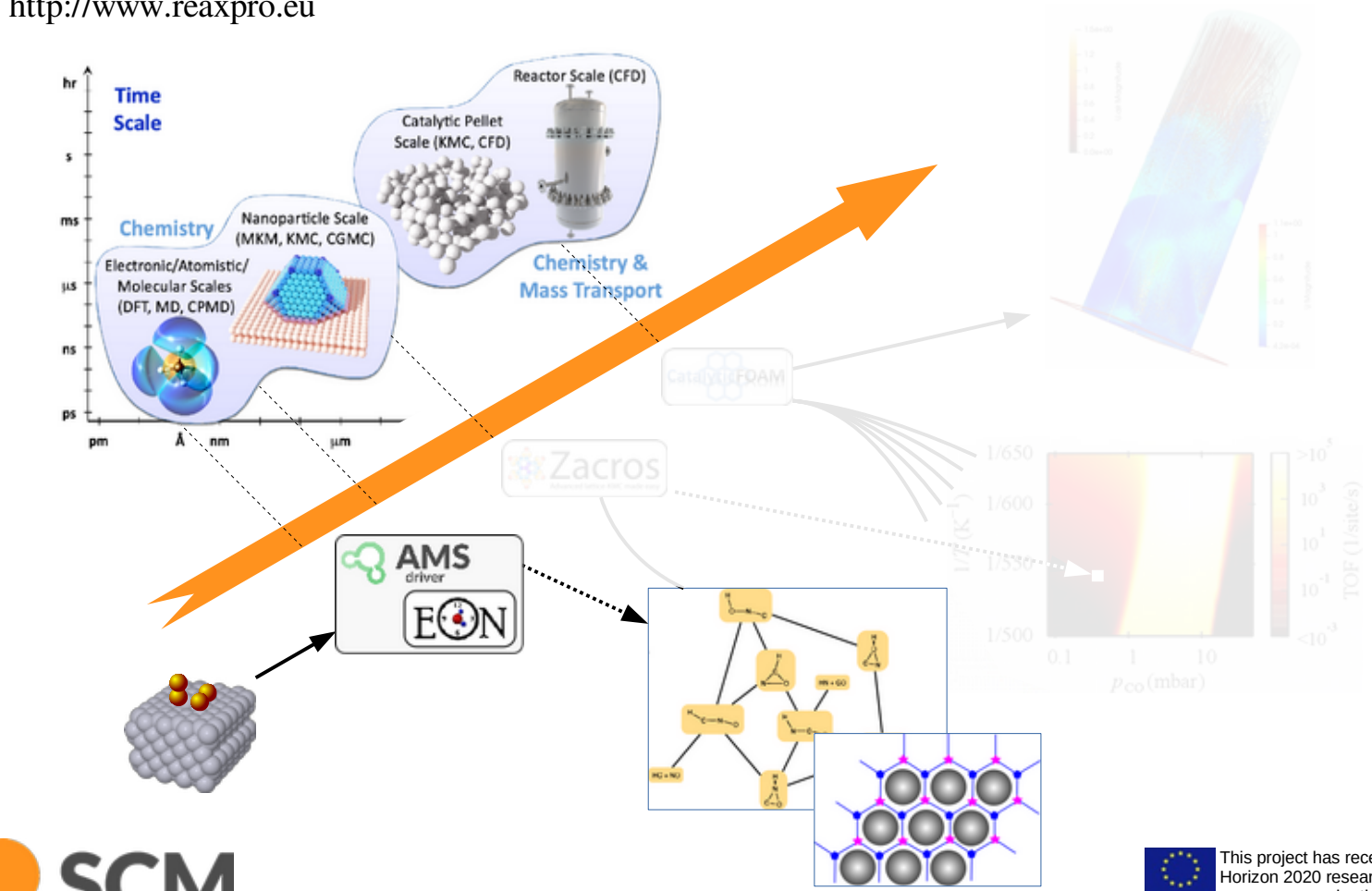

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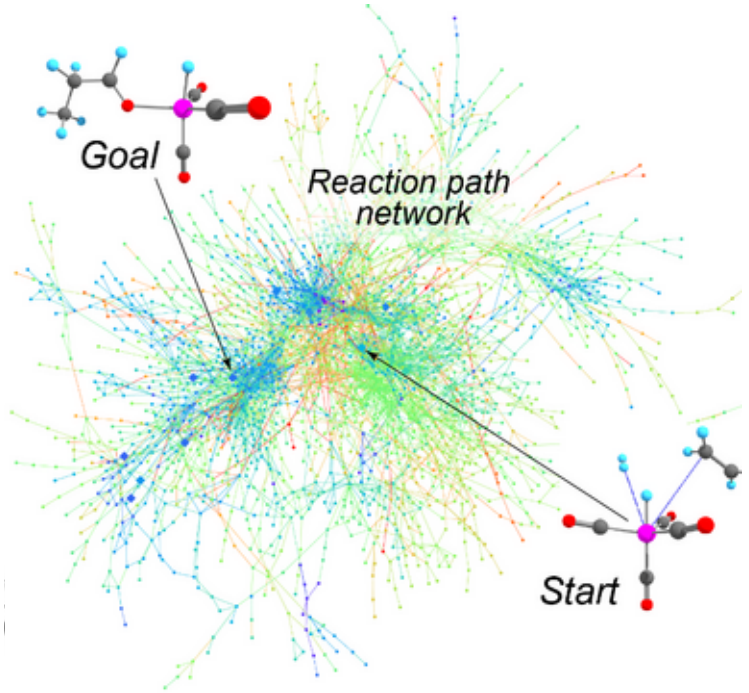
Automated Exploration of Energy Landscapes



The reaction path network for the $HCo(CO)_3 + CO + H_2 + C_2H_4$ system obtained by the SC-AFIR search. 2601 local minima.

Determination of accurate rate coefficients remains a key challenge for a wide variety of chemical research areas.

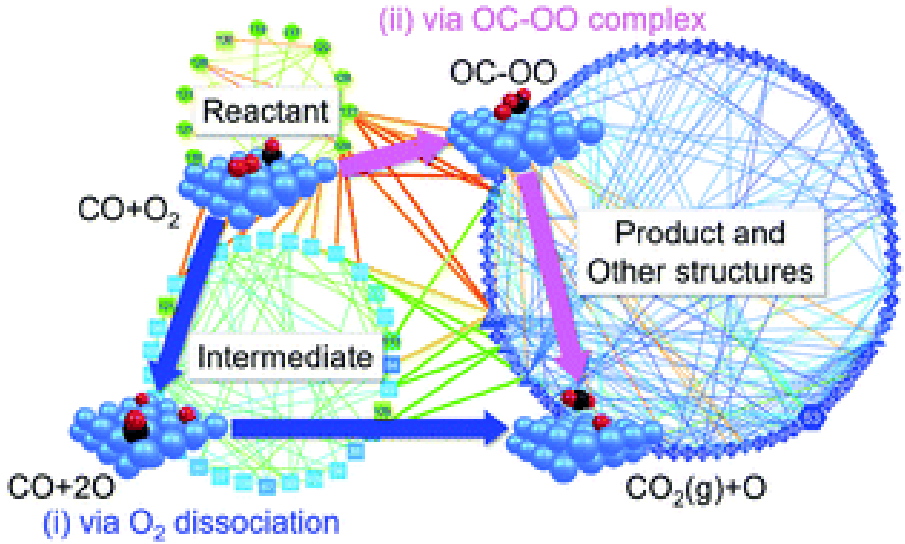
Main problems:

- The complexity of mapping the possible reaction channels.
- The traditionally used strategies often incorporate several manual actions and need chemical expert knowledge.
- It is expensive to calculate accurate ab initio parameters (typically energies, frequencies, and geometries)

It is necessary to create tools that automatically search for reaction pathways and calculate the rate coefficients.

Figure taken from: https://www.icredd.hokudai.ac.jp/research/1591asdasd
Hatanaka, M., Yoshimura, T., Maeda, S.
New Directions in the Modeling of Organometallic Reactions 2020, 57-80

Automated Exploration of Energy Landscapes for Catalytic Processes



The reaction path network for CO oxidation on Pt(111).
$CO + O_2 \rightarrow CO_2$
139 MIN + 572 TS

Additional problems:

- The structural variety and size of the systems
- The vast amount of small transformation steps that need to be considered.
- Structural changes of the catalyst occur during the reaction.
- Structural rearrangements during reactions on surfaces significantly differ from their gas-phase counterparts.

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Understanding CO oxidation on the Pt(111) surface based on a reaction route network
K. Sugiyama, Y. Sumiya, M. Takagi, K. Saita. S. Maeda
Phys. Chem. Chem. Phys., 2019,**21**, 14366-14375

PESExploration in AMS

```
PESExploration
  Job ProcessSearch
  NumExpeditions 25
  NumExplorers 3
End
```

EON Jobs available from AMS:

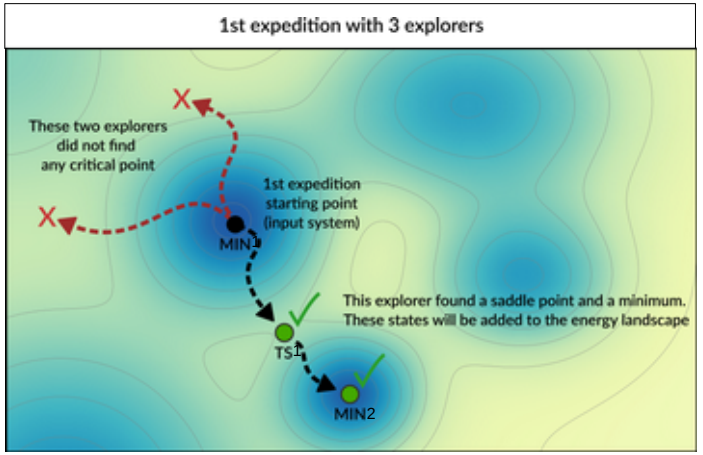
- ProcessSearch
- BasinHopping
- SaddleSearch
- NudgedElasticBand
- MolecularDynamics
- ParallelReplica

Jobs AMS original:

- LandscapeRefinement
- BindingSites

G. Henkelman and H. Jónsson, A dimer method for finding saddle points on high dimensional potential surfaces using only first derivatives, J. Chem. Phys. 111, 7010-7022 (1999).

PESExploration in AMS

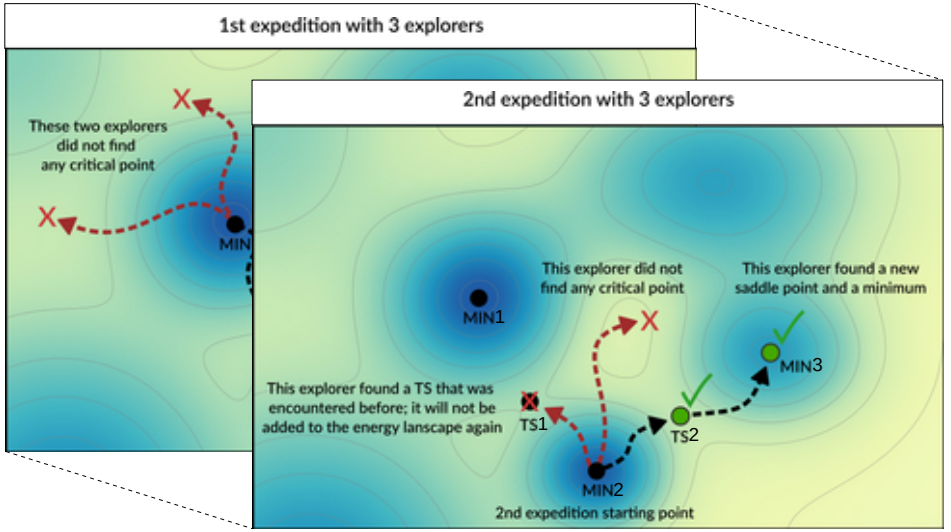


ProcessSearch uses the dimer method (min-mode following) for finding nearby saddle points without knowledge of the final or transition state. The method only makes use of first derivatives of the potential energy.

```
PESExploration
  Job ProcessSearch
  DynamicSeedStates T
  NumExpeditions 25
  NumExplorers 3
  CalculateFragments T
End
```

G. Henkelman and H. Jónsson, A dimer method for finding saddle points on high dimensional potential surfaces using only first derivatives, J. Chem. Phys. 111, 7010-7022 (1999).

PESExploration in AMS




```
PESExploration
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  DynamicSeedStates T
  NumExpeditions 25
  NumExplorers 3
  CalculateFragments T
End
```
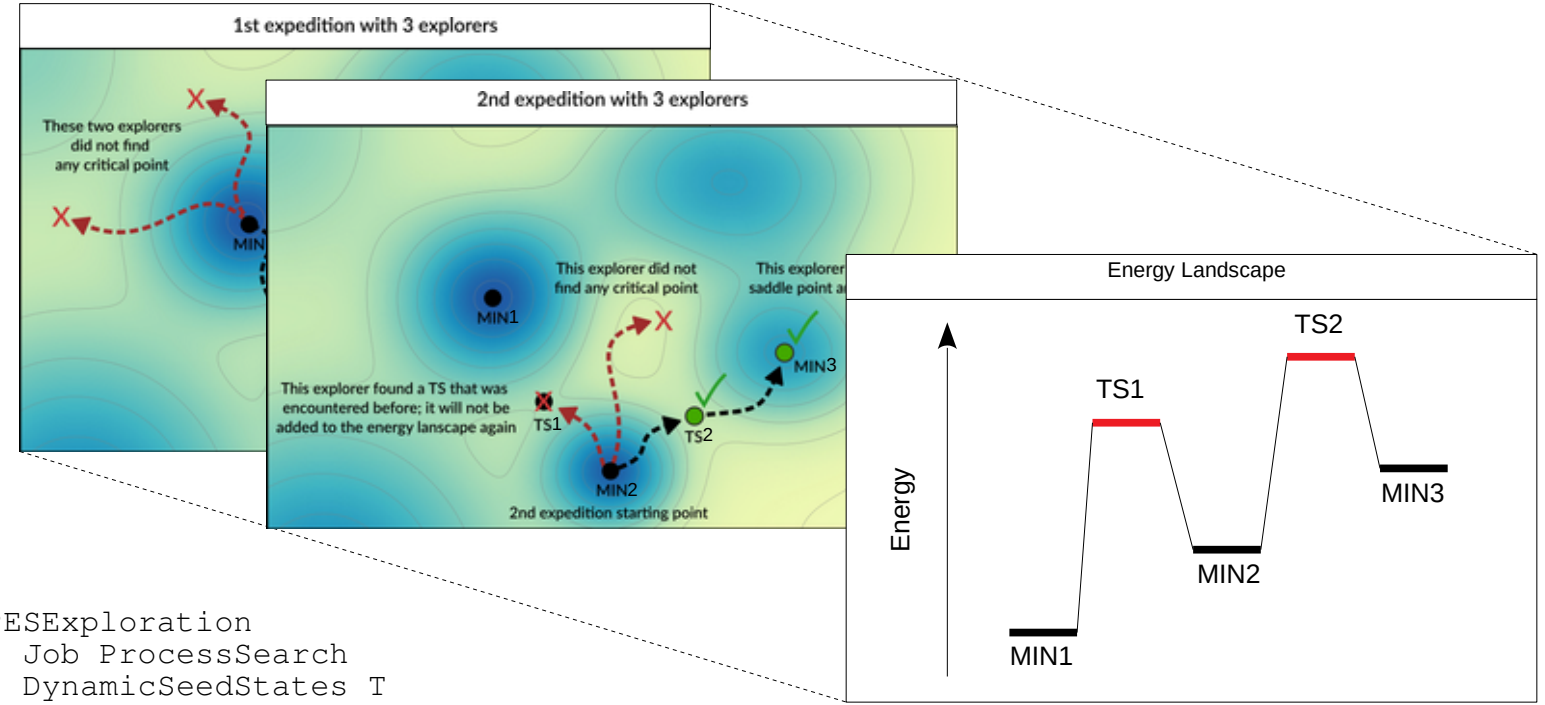

PESExploration in AMS




```
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  DynamicSeedStates T
  NumExpeditions 25
  NumExplorers 3
  CalculateFragments T
End
```
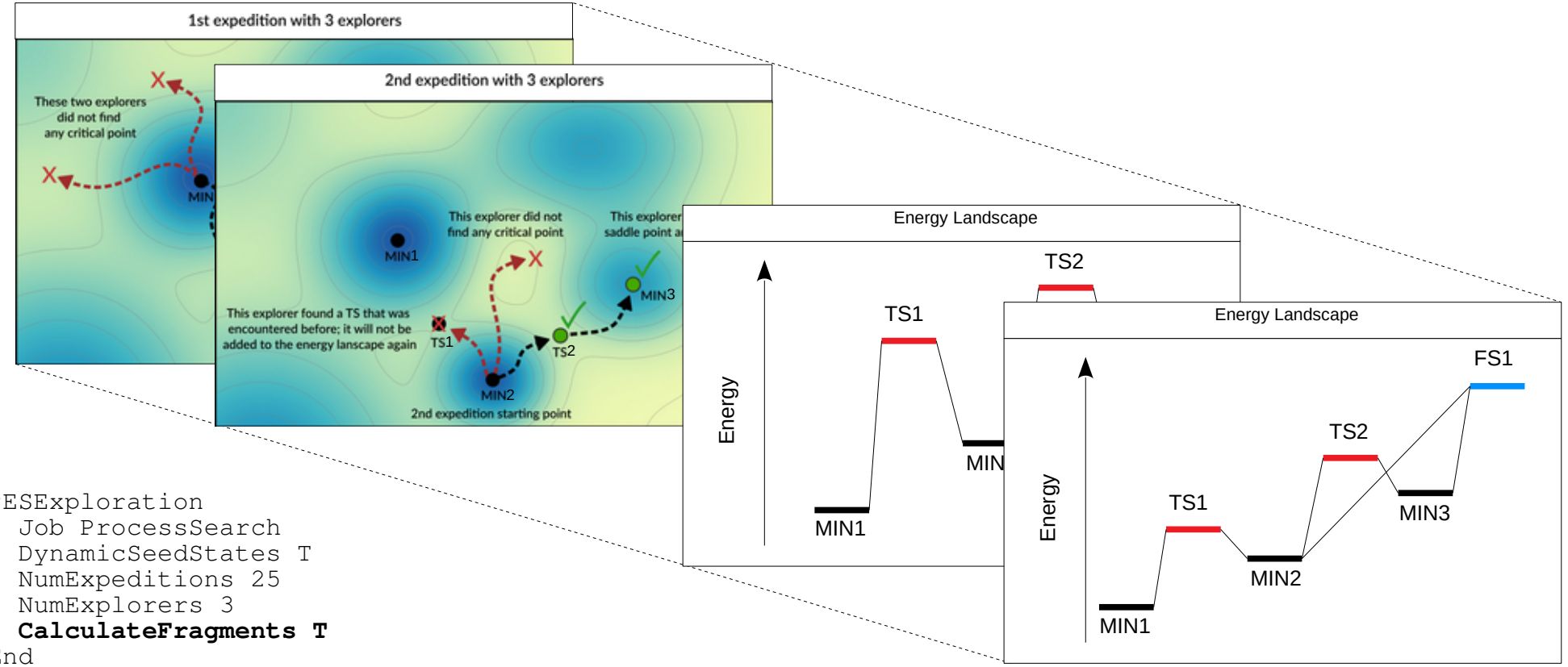
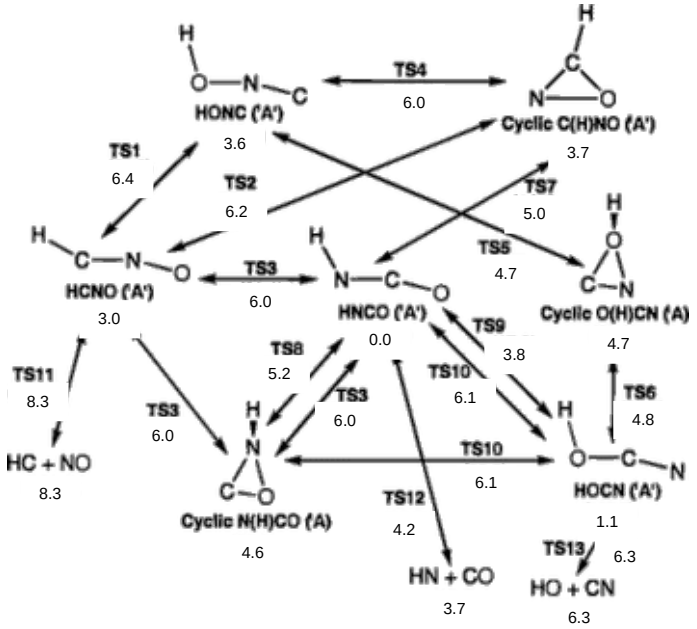

PESExploration in AMS




```
PESExploration
  Job ProcessSearch
  DynamicSeedStates T
  NumExpeditions 25
  NumExplorers 3
  CalculateFragments T
End
```

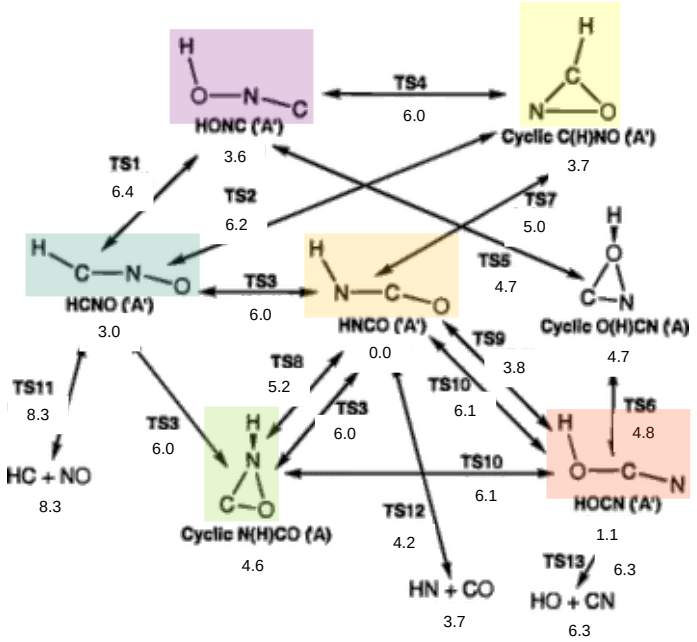
Isomerization of CHNO

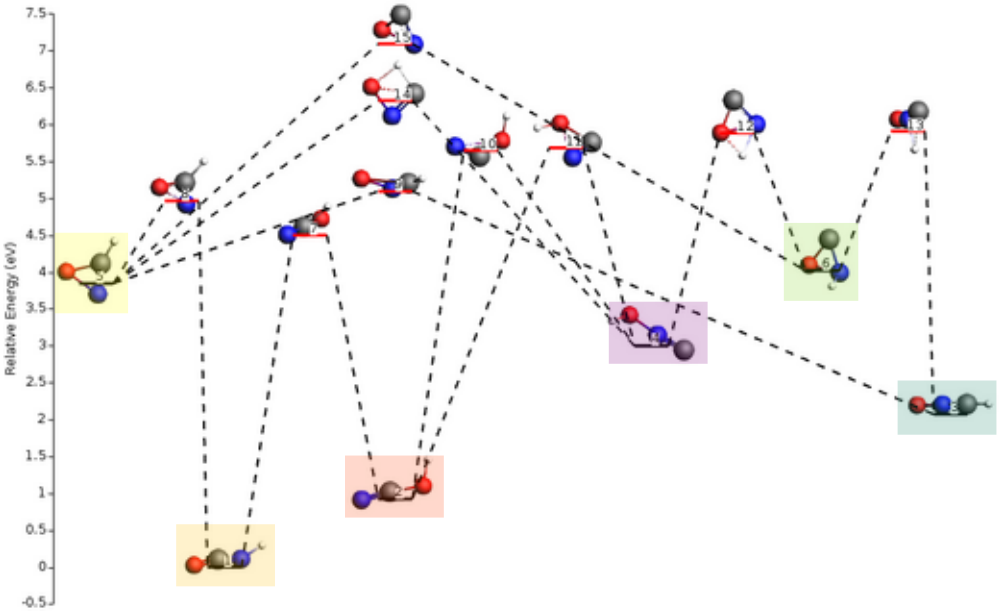



```
Task PESExploration

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
```

W. A. Shapley, and G. B. Bacskay. A Gaussian-2 Quantum Chemical Study of CHNO: Isomerization and Molecular Dissociation Reactions, J. Chem. Phys. A. **103** (1999) 6624-6631. doi:10.1021/jp990294e

Isomerization of CHNO

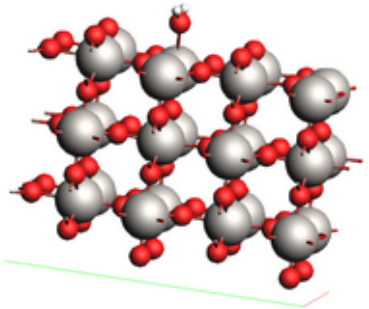




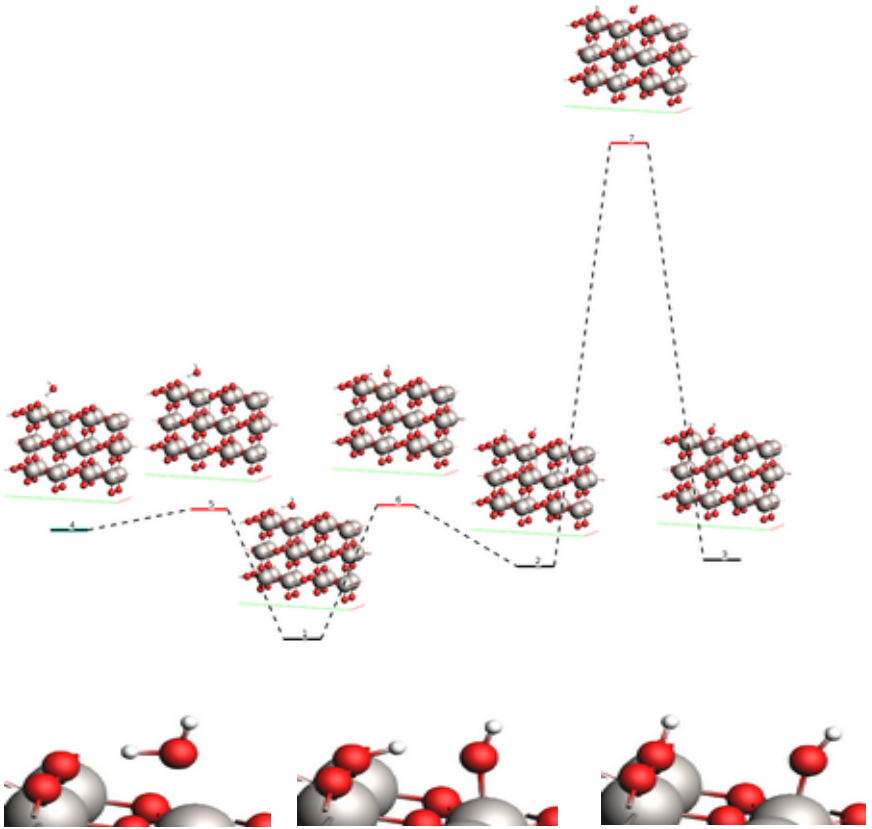
W. A. Shapley, and G. B. Bacskay. A Gaussian-2 Quantum Chemical Study of CHNO: Isomerization and Molecular Dissociation Reactions, J. Chem. Phys. A. **103** (1999) 6624-6631. doi:10.1021/jp990294e

Splitting Water on rutile TiO_2(110)

Input System



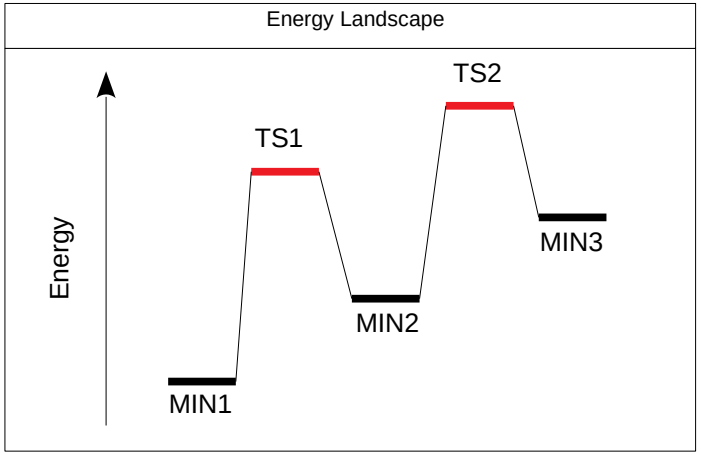
Engine: ReaxFF (TiO2bio.ff)

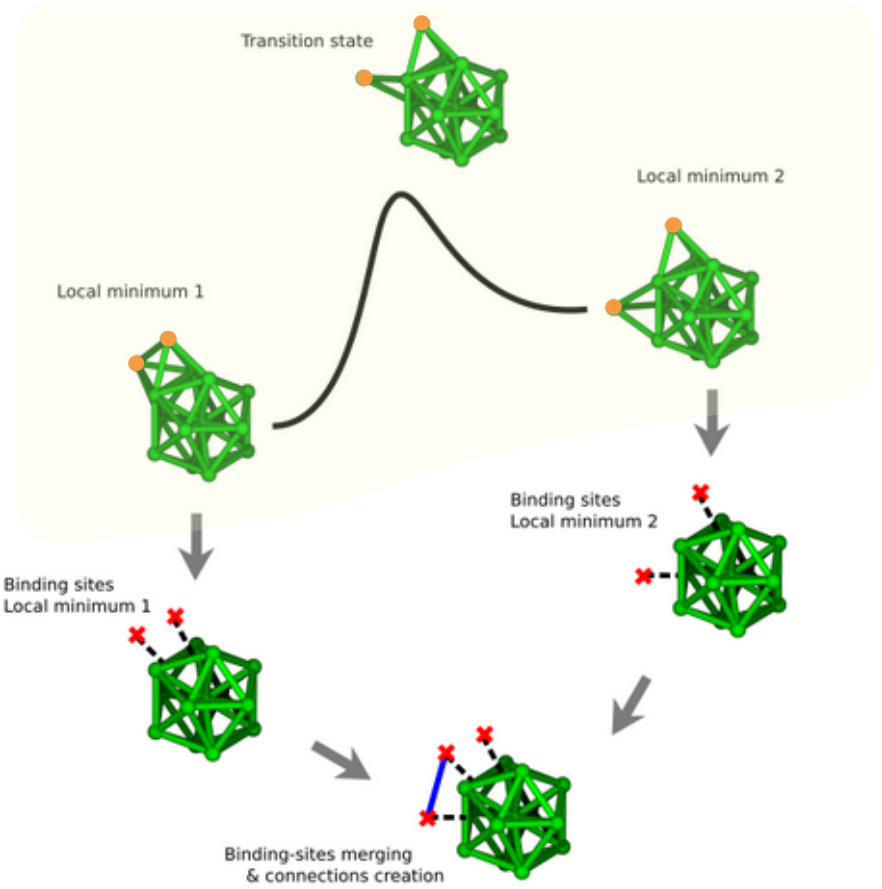


H. Xu, R. Q. Zhang, A. M. C. Ng, A. B. Djurišić, H. T. Chan, W. K. Chan, and S. Y. Tong
Splitting Water on Metal Oxide Surfaces
J. Phys. Chem. C 2011, **115**, 40, 19710–19715

Binding Sites

A binding site is a small fraction of the catalyst surface which is catalytically active and might be composed of an atom or an ensemble of atoms. They are generally situated at surface defects such as corners, edges, and other crystalline discontinuities.





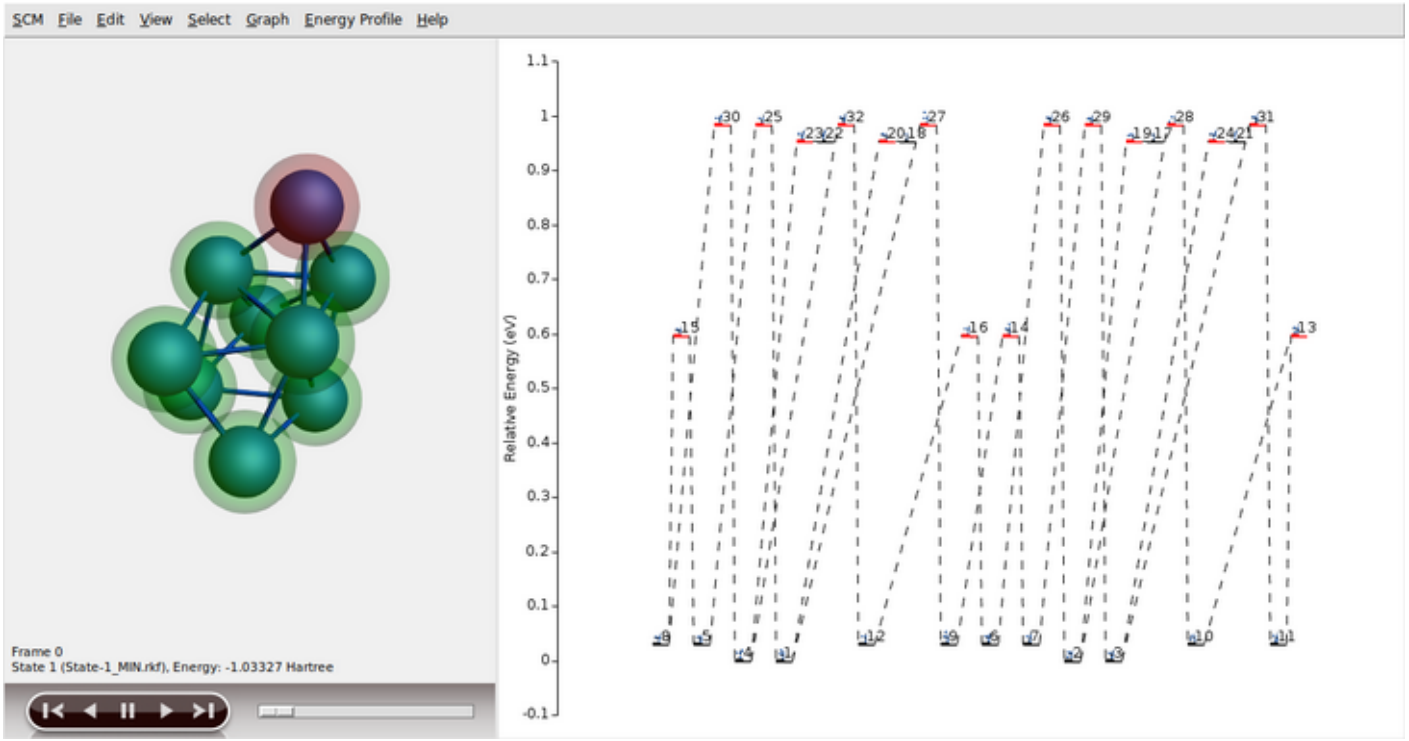
Binding Sites: Case Co_8+Co

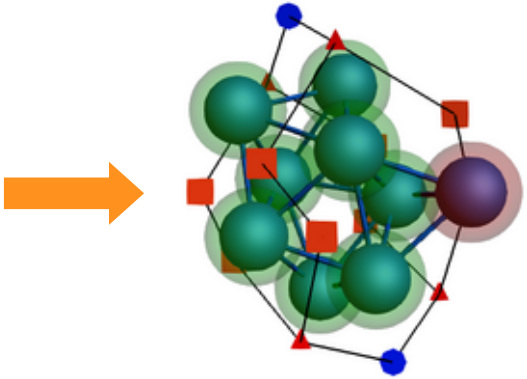
https://www.scm.com/doc/Tutorials/StructureAndReactivity/PESExpClusterGrowthCo8.html

Input System

Energy Landscape

Binding Sites





PLAMS: python interface

https://github.com/SCM-NV/PLAMS

```
mol = scm.plams.Molecule( 'CO-Pt111.xyz' )

sett = scm.plams.Settings()
sett.input.ams.Task = 'PESExploration'
sett.input.ams.PESExploration.Job = 'ProcessSearch'
sett.input.ams.PESExploration.NumExpeditions = 10
sett.input.ams.PESExploration.NumExplorers = 4
...
job = scm.plams.AMSJob(molecule=molO, settings=sett)
results = job.run()

for state in results.get_energy_landscape():
    print("Energy = ", state.energy)
    print("Geometry = ", state.molecule)
    if state.isTS:
        print("Forward  barrier = ", state.energy - state.reactants.energy)
        print("Backward barrier = ", state.energy - state.products.energy)
...
```

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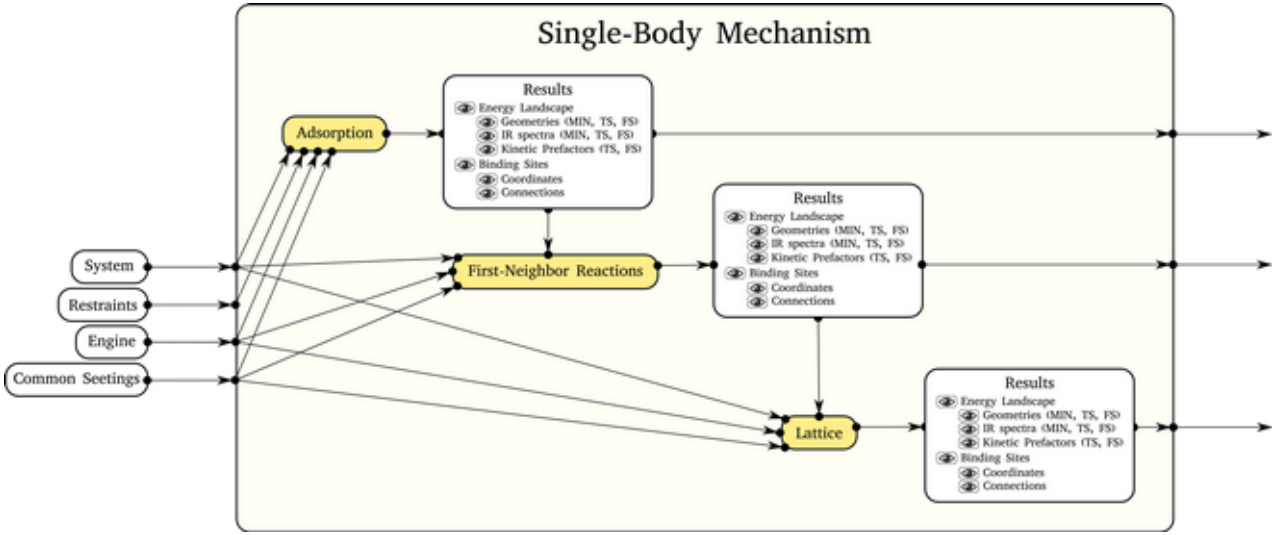
PLAMS: python interface

https://github.com/SCM-NV/PLAMS



Adsorption:

PESExploration
  ProcessSearch
  +DynamicSeedStates = F
  +CheckSymmetry = T
  +Restraints

First-Neighbor Reactions:

PESExploration
  ProcessSearch
  +DynamicSeedStates = F
  +CheckSymmetry = T

Lattice:

PESExploration
  LandscapeRefinement
  +GenerateSymmetryImages = T
  +RelaxFromSaddlePoint = T
  +CheckSymmetry = F

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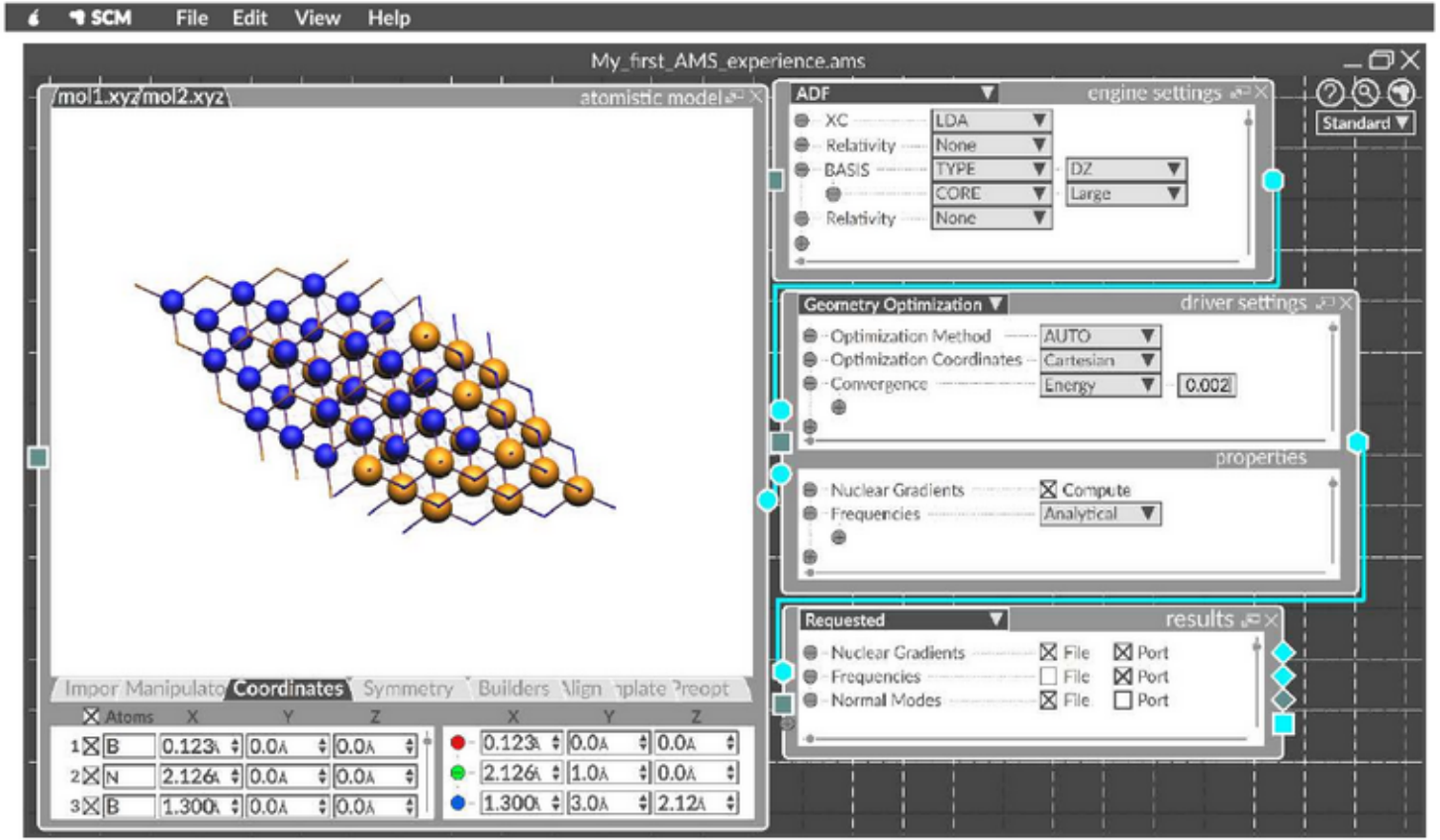
AMS workflows 2024?



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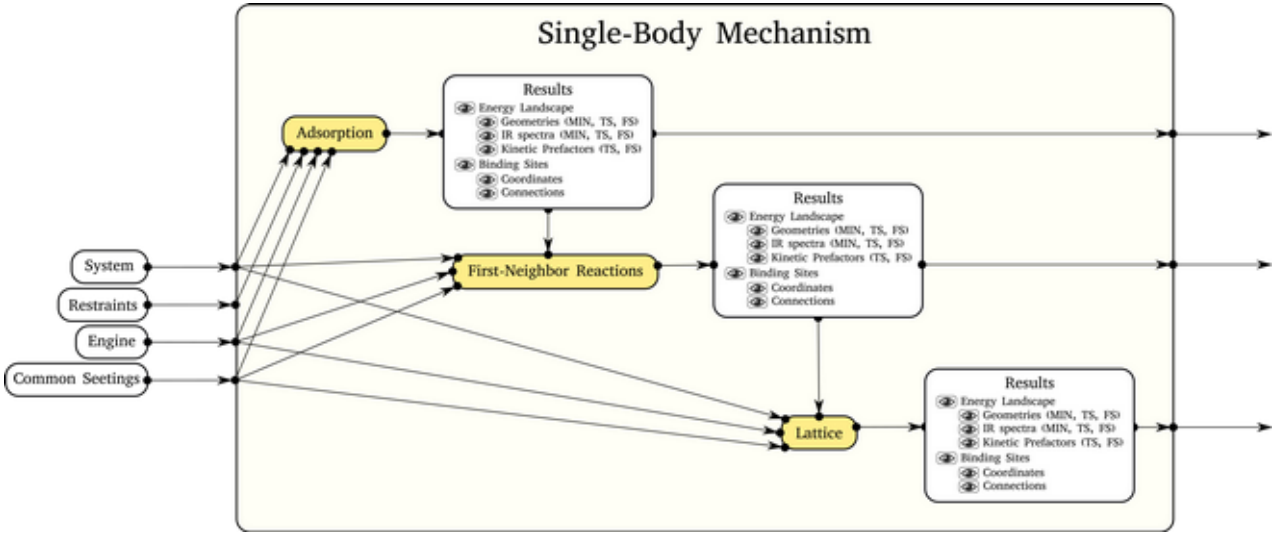

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  +CheckSymmetry = T

Lattice:

PESExploration
  LandscapeRefinement
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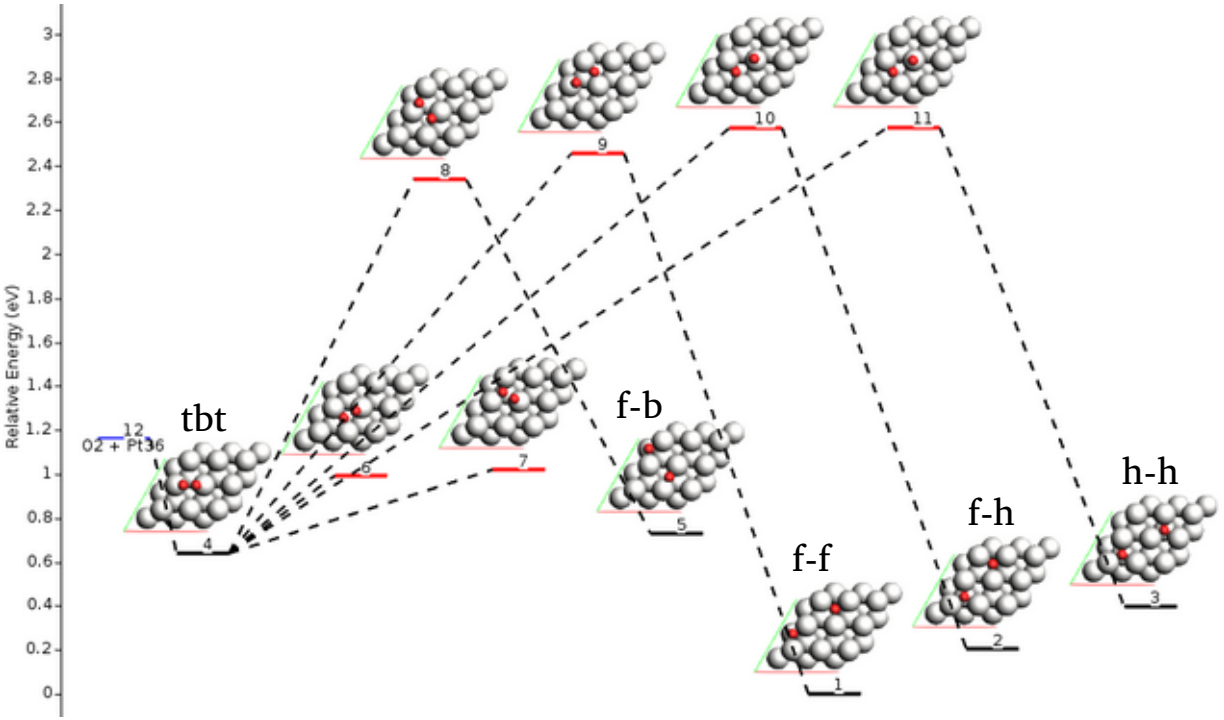
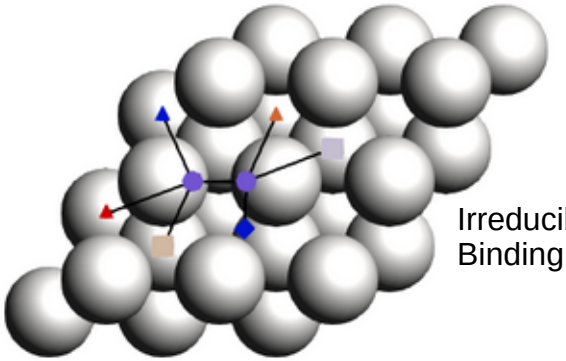
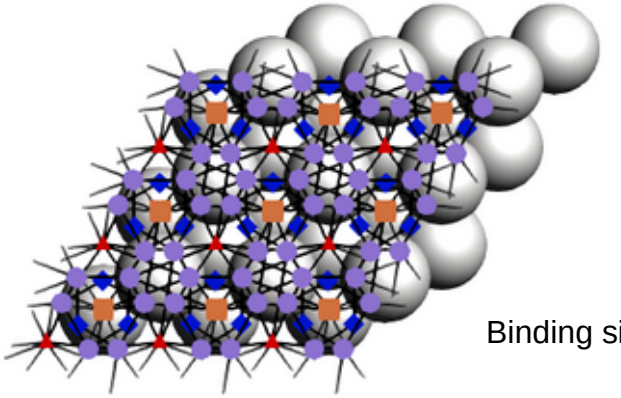
Single-Body Mechanism for O_2-Pt(111)



Irreducible-Symmetry Energy Landscape



Irreducible-Symmetry
Binding sites



Binding sites

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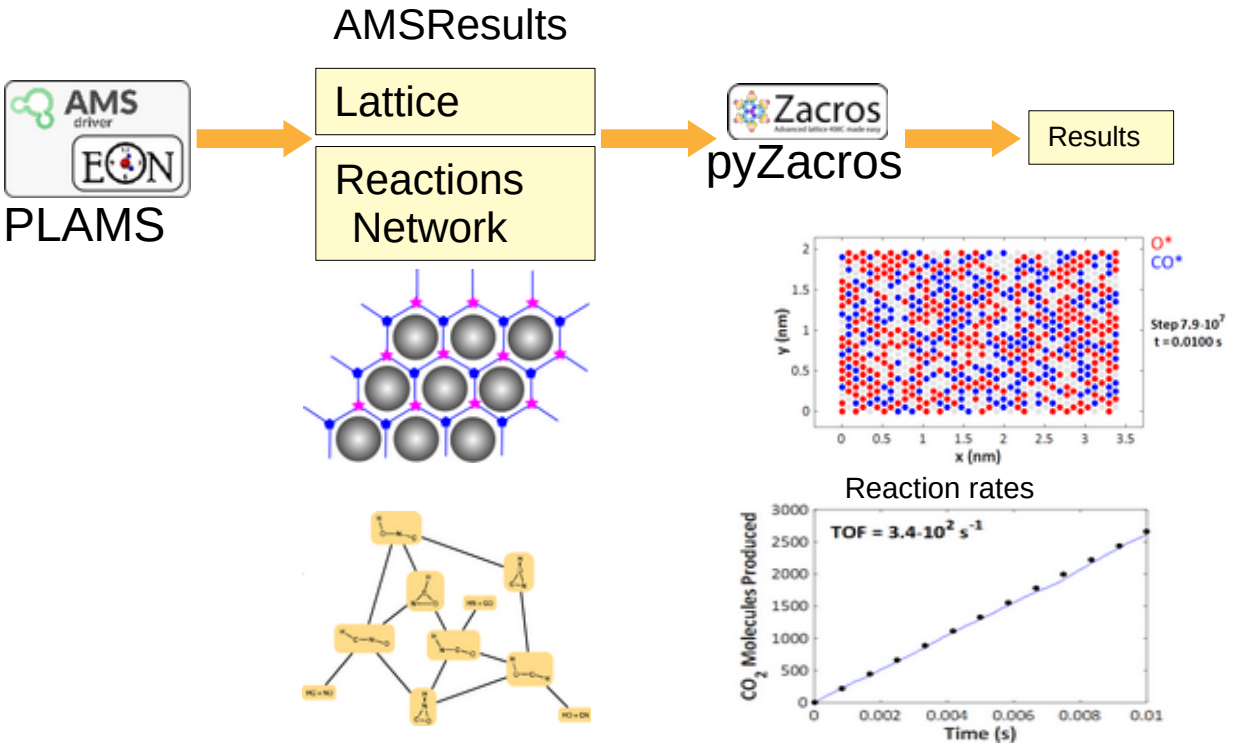

Zacros enables to perform dynamical modeling of adsorption, desorption, surface diffusion, and reaction processes on heterogeneous catalysts.

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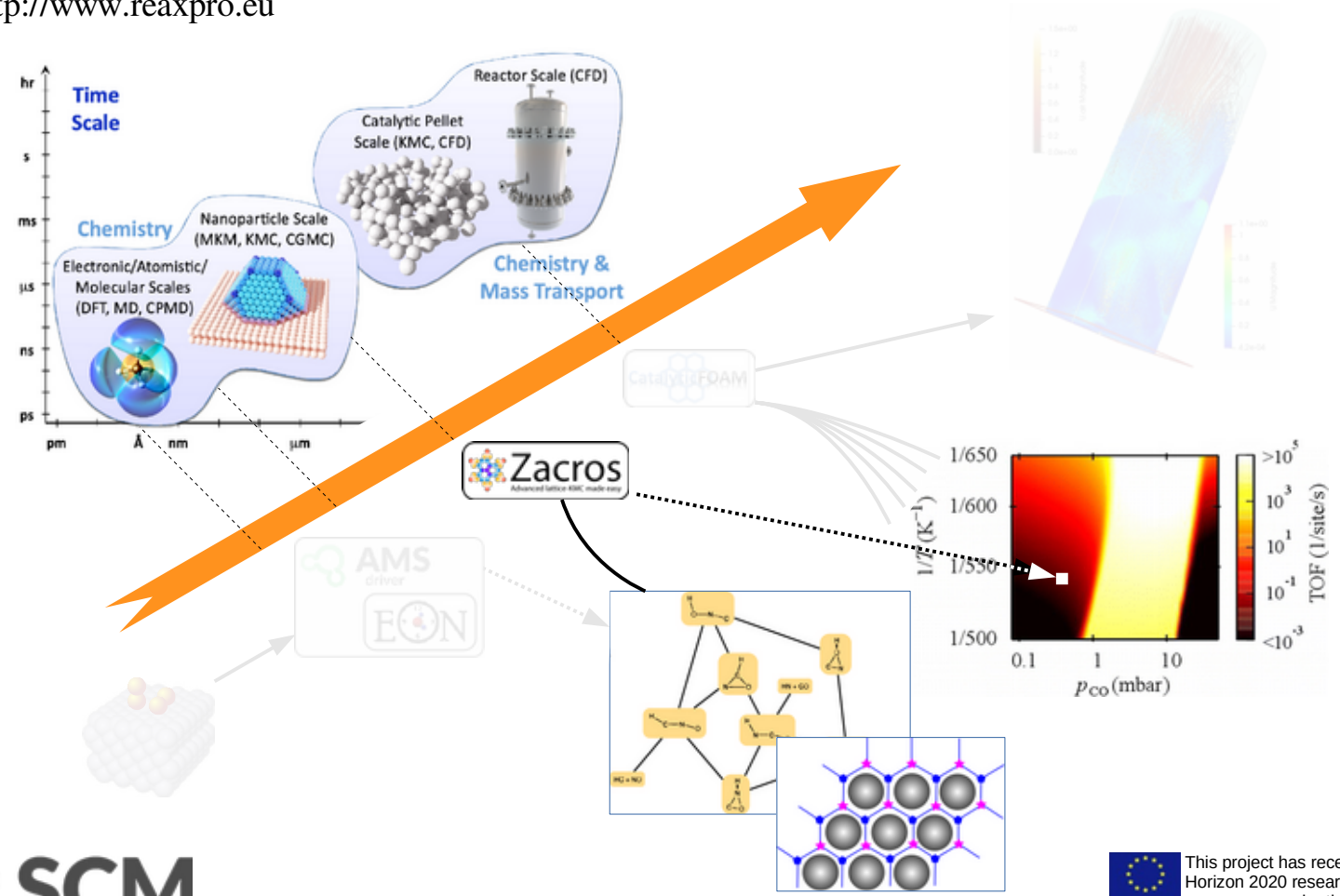
The ReaxPro Project

http://www.reaxpro.eu



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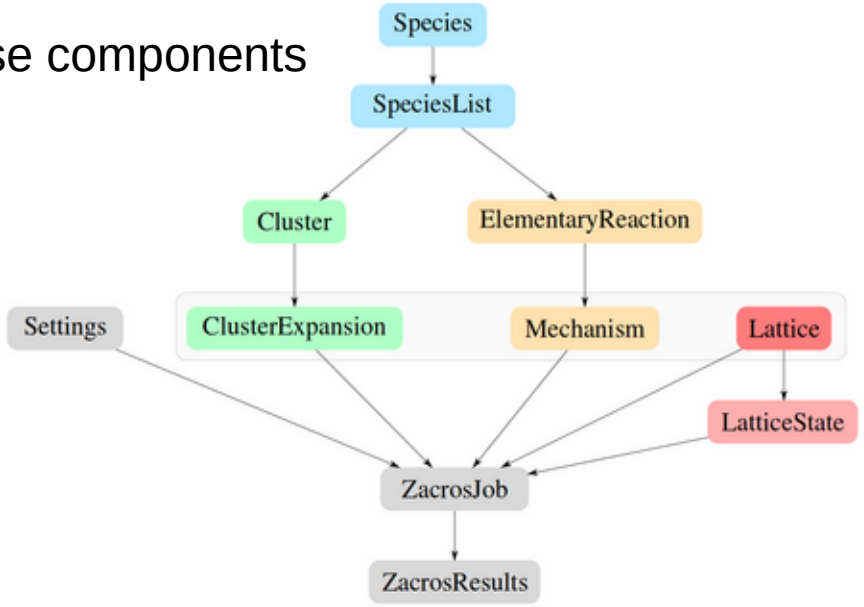
PyZacros

https://github.com/SCM-NV/pyZacros

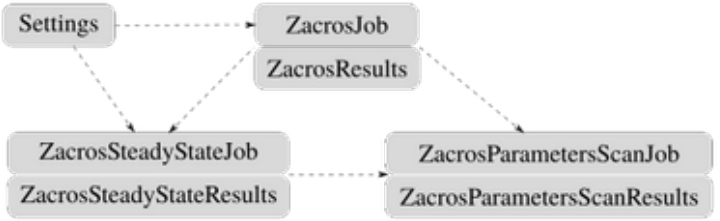
pyZacros is a collection of tools that aims to provide a powerful, flexible, and easily extendable Python interface to Zacros. It is designed as an extension of the python library PLAMS.

pyZacros inherits from PLAMS the robust way of managing the inputs file preparation, job execution, file management, and output file processing. Above and above that, it also offers the possibility of postprocessing the results and building very advanced data workflows.

Base components



Extended components



pyZacros: Zacros python interface

https://github.com/SCM-NV/pyZacros

```
loader = scm.pyzacros.RKFLoader( results_ads )
loader.lattice.set_repeat_cell( (10,10) )

settings = scm.pyzacros.Settings()
settings.temperature = 273.15
settings.pressure = 1.01325
settings.molar_fraction.CO = 0.1

dt = 1e-8
settings.max_time = 1000*dt
settings.snapshots = ('logtime', dt, 3.5)
settings.species_numbers = ('time', dt)

job = scm.pyzacros.ZacrosJob( lattice=loader.lattice, mechanism=loader.mechanism,
                              cluster_expansion=loader.clusterExpansion, settings=settings )
results_pz = job.run()
results_pz.plot_lattice_states( results_pz.lattice_states() )
```

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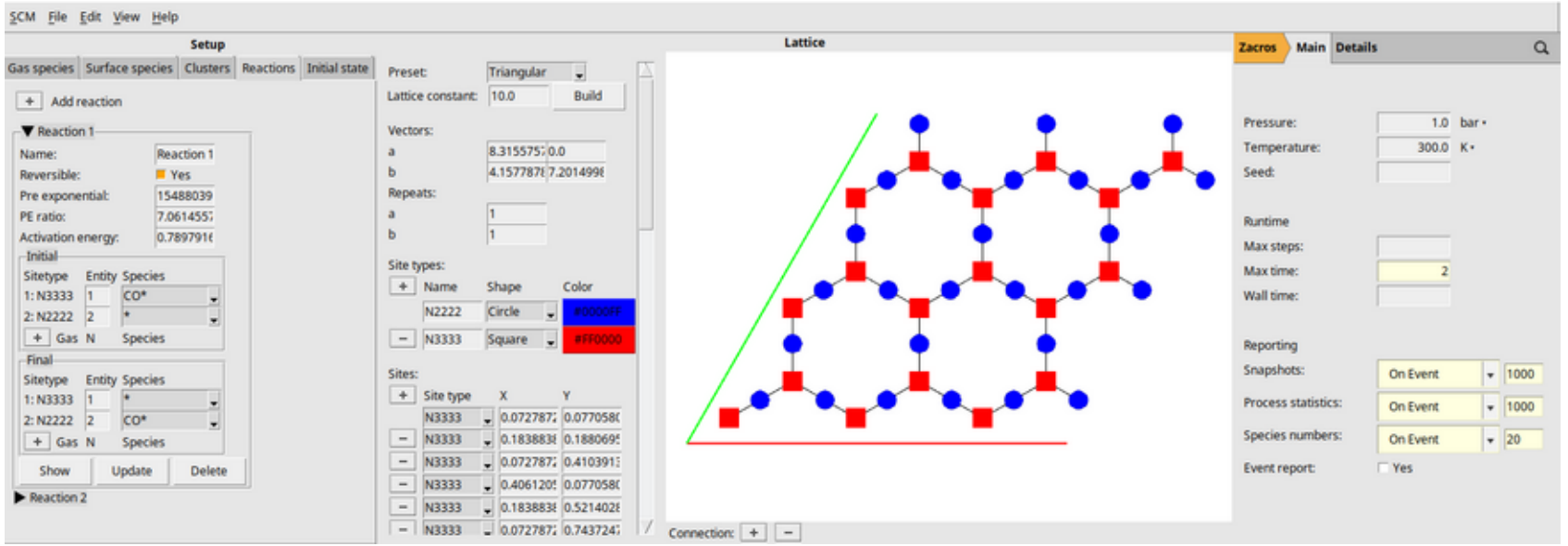
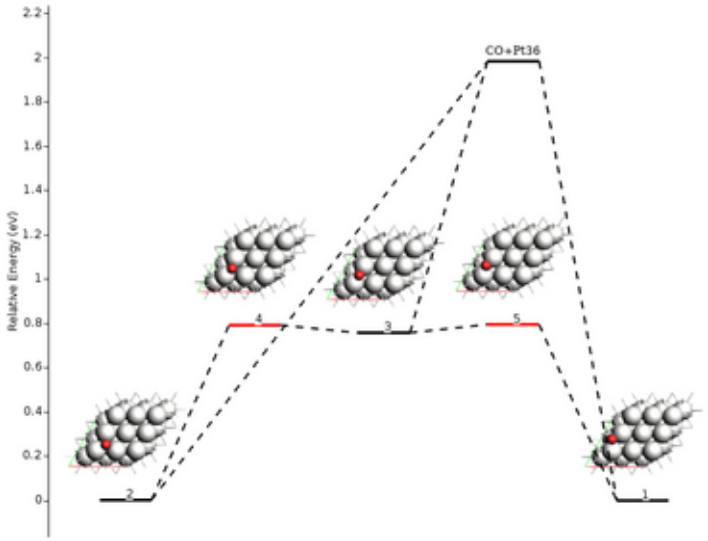
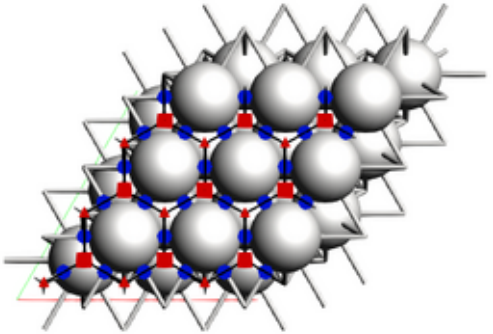
PyZacros: Graphical User Interface

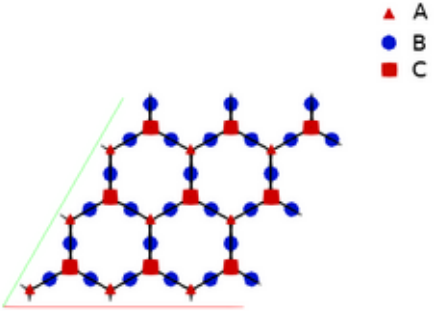


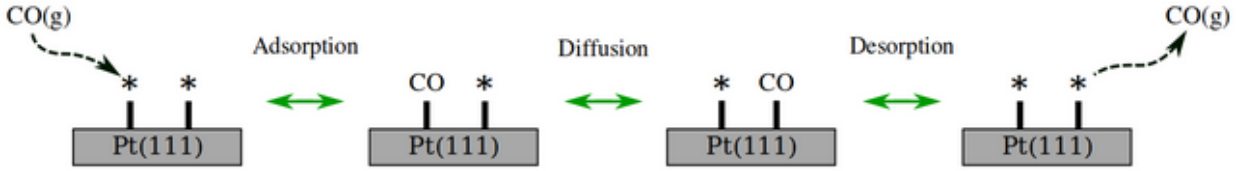
Poisoning of Pt(111) by CO

https://www.scm.com/doc/pyzacros/examples/COPt111.html





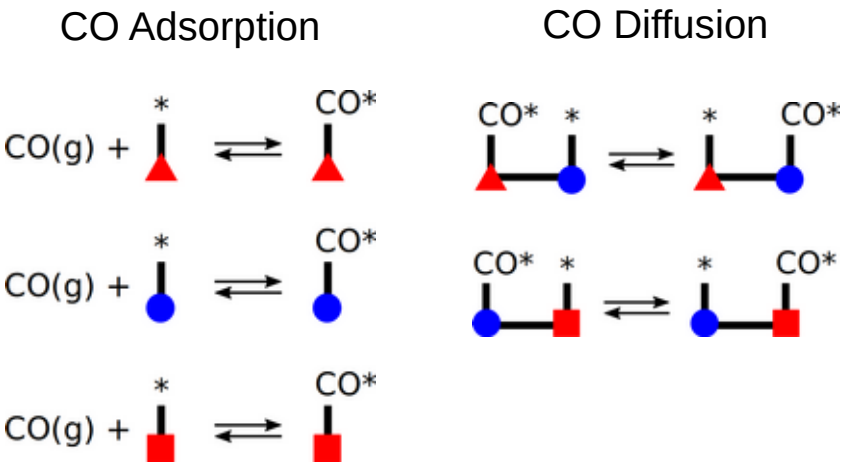


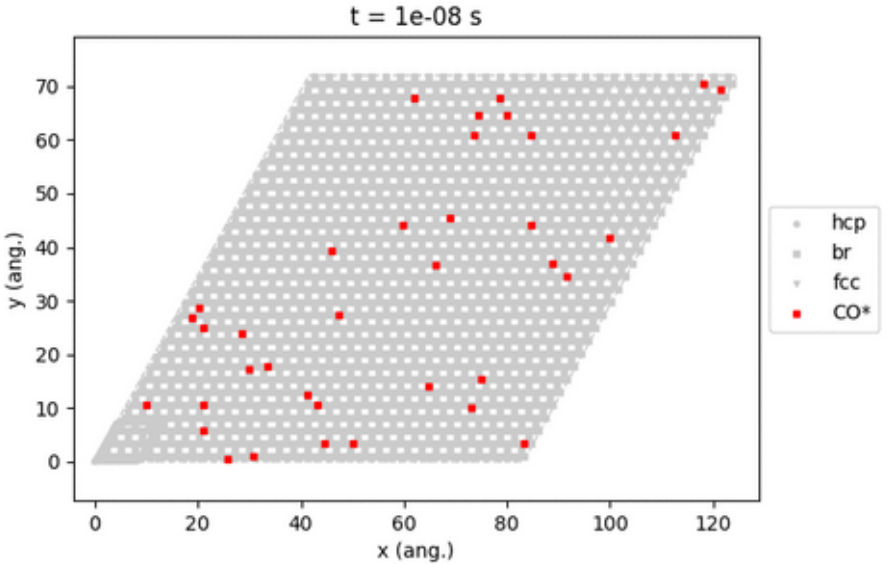


Engine: ReaxFF (CHONSFPtClNi.fff)

Poisoning of Pt(111) by CO

https://www.scm.com/doc/pyzacros/examples/COPt111.html



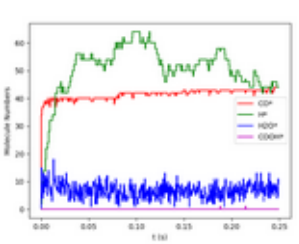


Engine: ReaxFF (CHONSFPtClNi.fff)

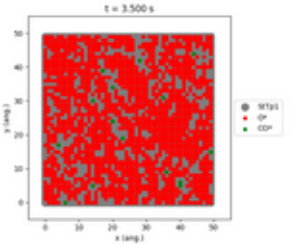
PyZacros Examples

https://github.com/SCM-NV/pyZacros

Simple examples

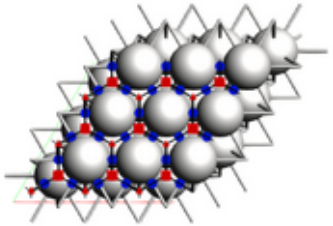


Water-gas shift reaction on Pt(111)

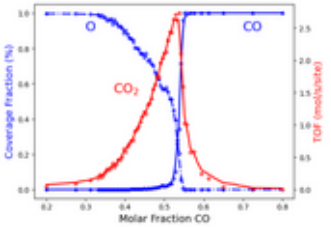


Ziff-Gulari-Barshad model

Advanced examples

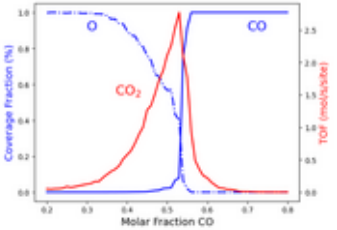


Poisoning of Pt(111) by CO: From atomistic to mesoscopic modeling

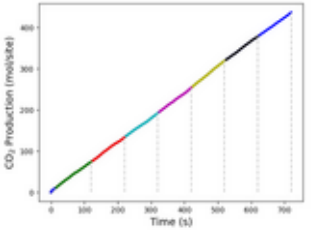


Ziff-Gulari-Barshad model: Phase Transitions and ML-based Surrogate Model

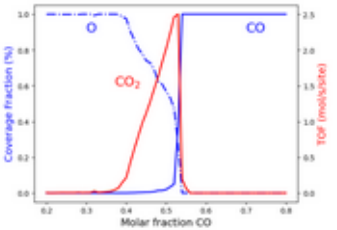
Intermediate examples



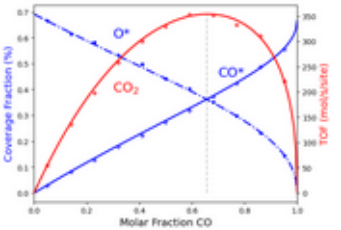
Ziff-Gulari-Barshad model: Phase Transitions



Ziff-Gulari-Barshad model: Steady State Conditions



Ziff-Gulari-Barshad model: Phase Transitions under Steady State Conditions

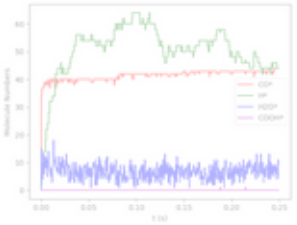


Langmuir-Hinshelwood model: Acceleration by Automated Rescaling of the Rate Constants

PyZacros Examples

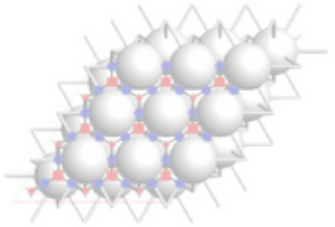
https://github.com/SCM-NV/pyZacros

Simple examples

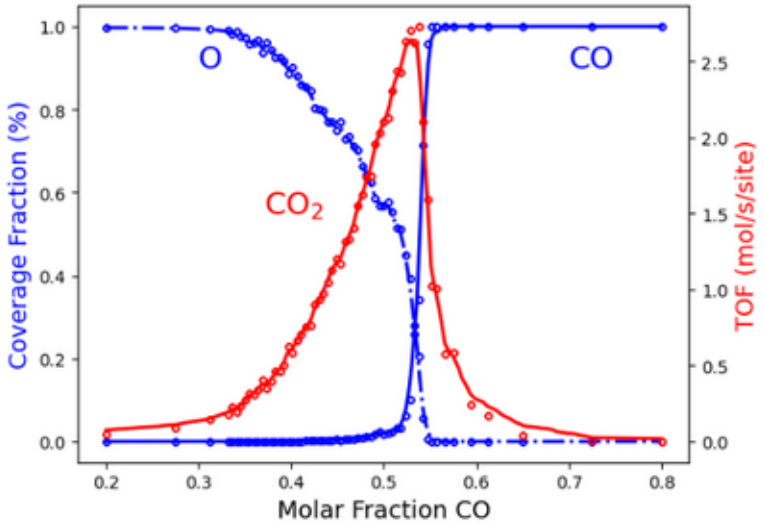


Water-gas shift reaction on Pt(111)

Advanced examples

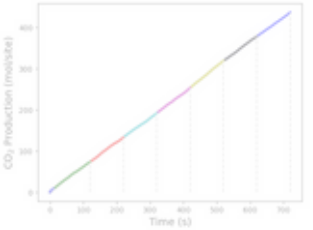


Poisoning of Pt(111) by CO:
From atomistic to mesoscopic modeling

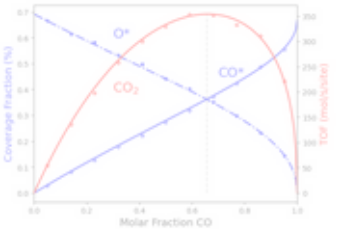


Ziff-Gulari-Barshad model:
Phase Transitions and ML-based Surrogate Model

es



Ziff-Gulari-Barshad model:
Steady State Conditions



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Acceleration by Automated Rescaling of the Rate Constants

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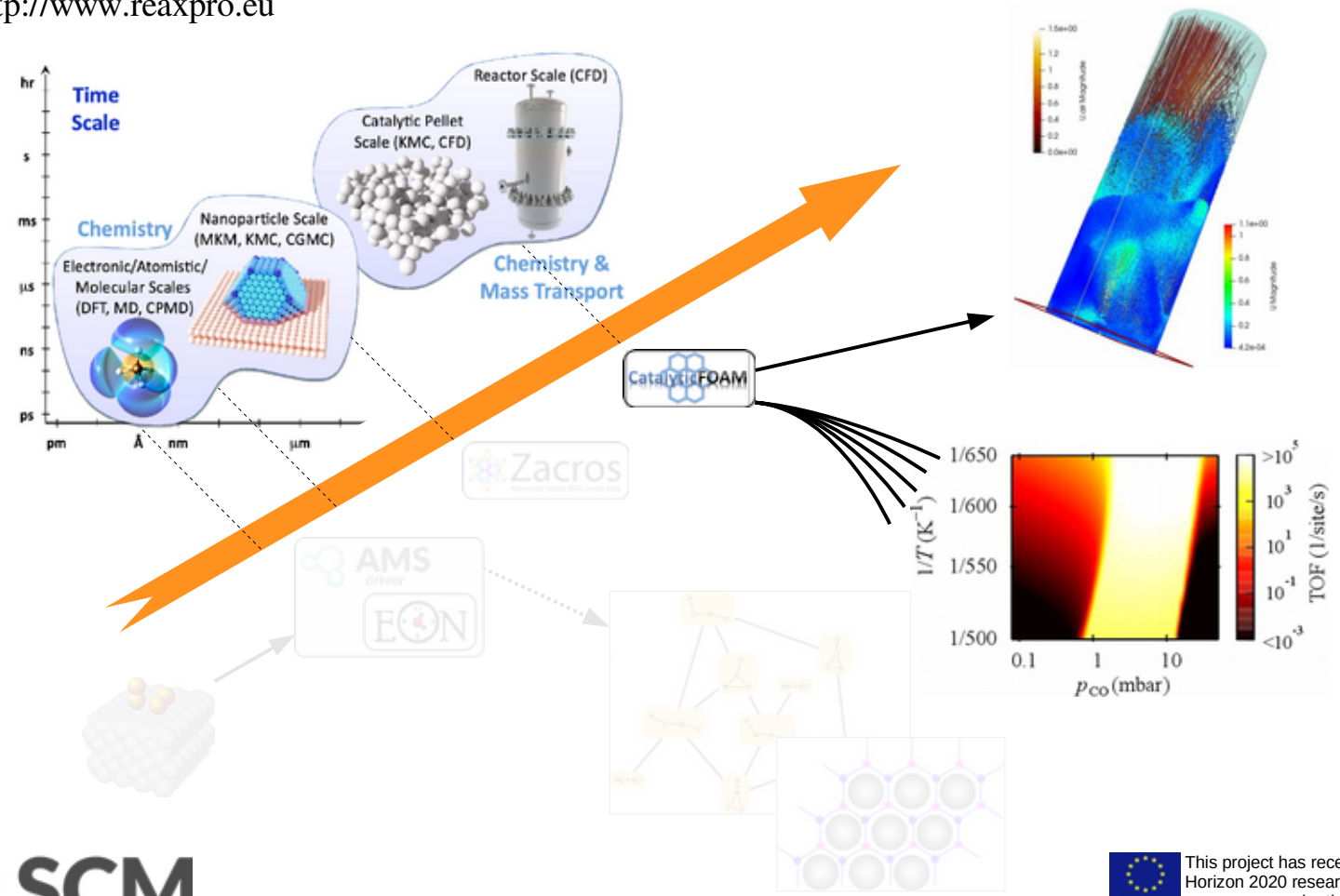
http://www.reaxpro.eu



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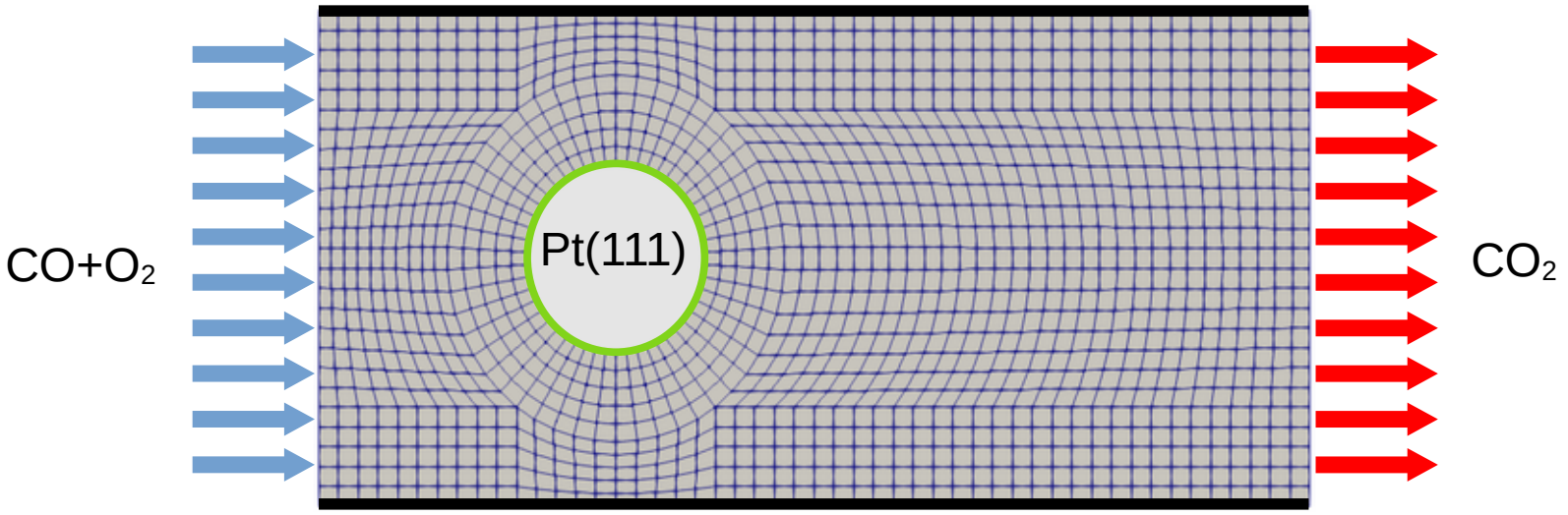
CO oxidation on Pt(111)

CatalyticFOAM allows for the solution of Navier-Stokes equations for complex and general geometries for reacting flows at surfaces, based on microkinetic descriptions of the surface reactivity.

T = 673.15 K, P = 1 atm, gas-velocity 0.1 m/s



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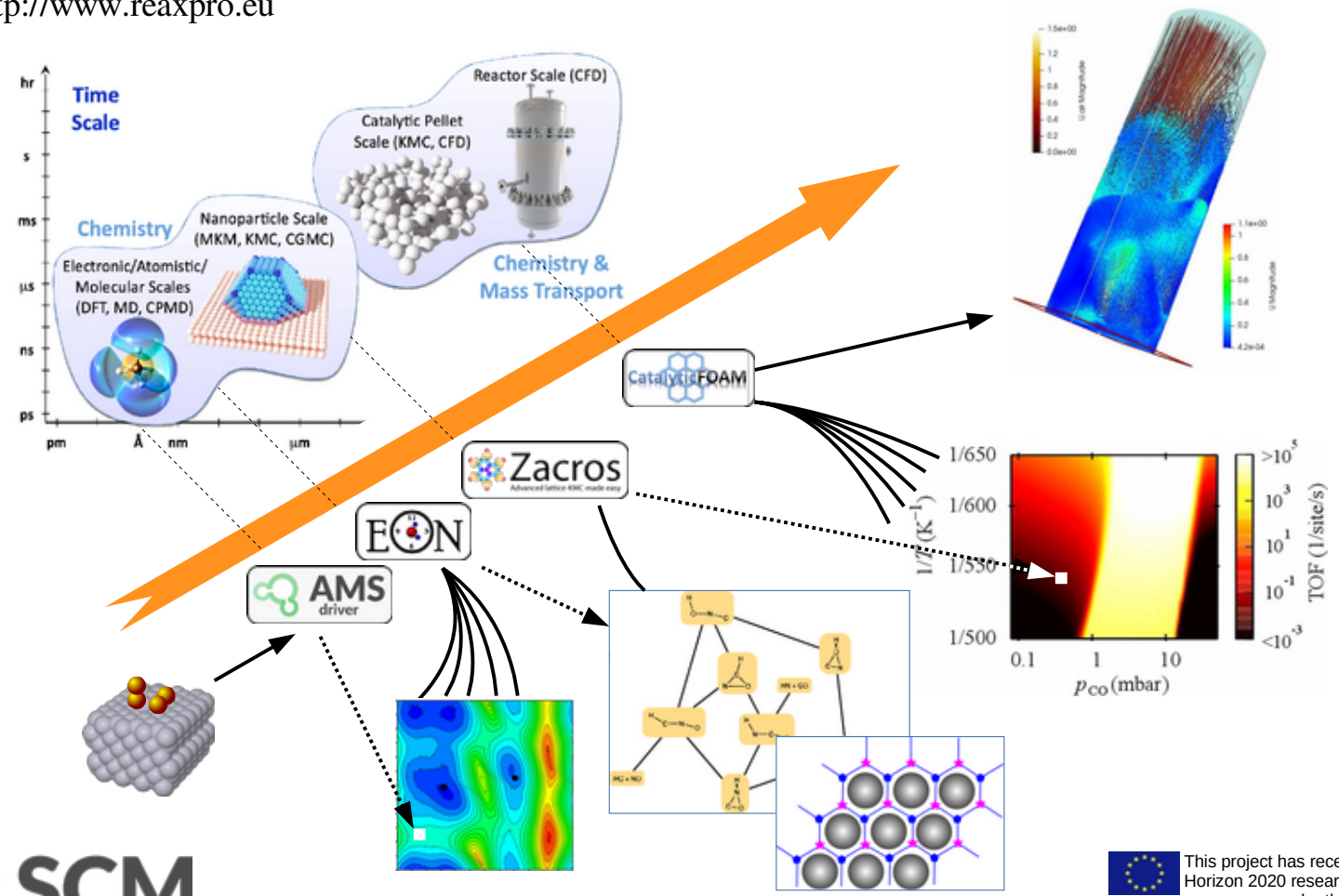

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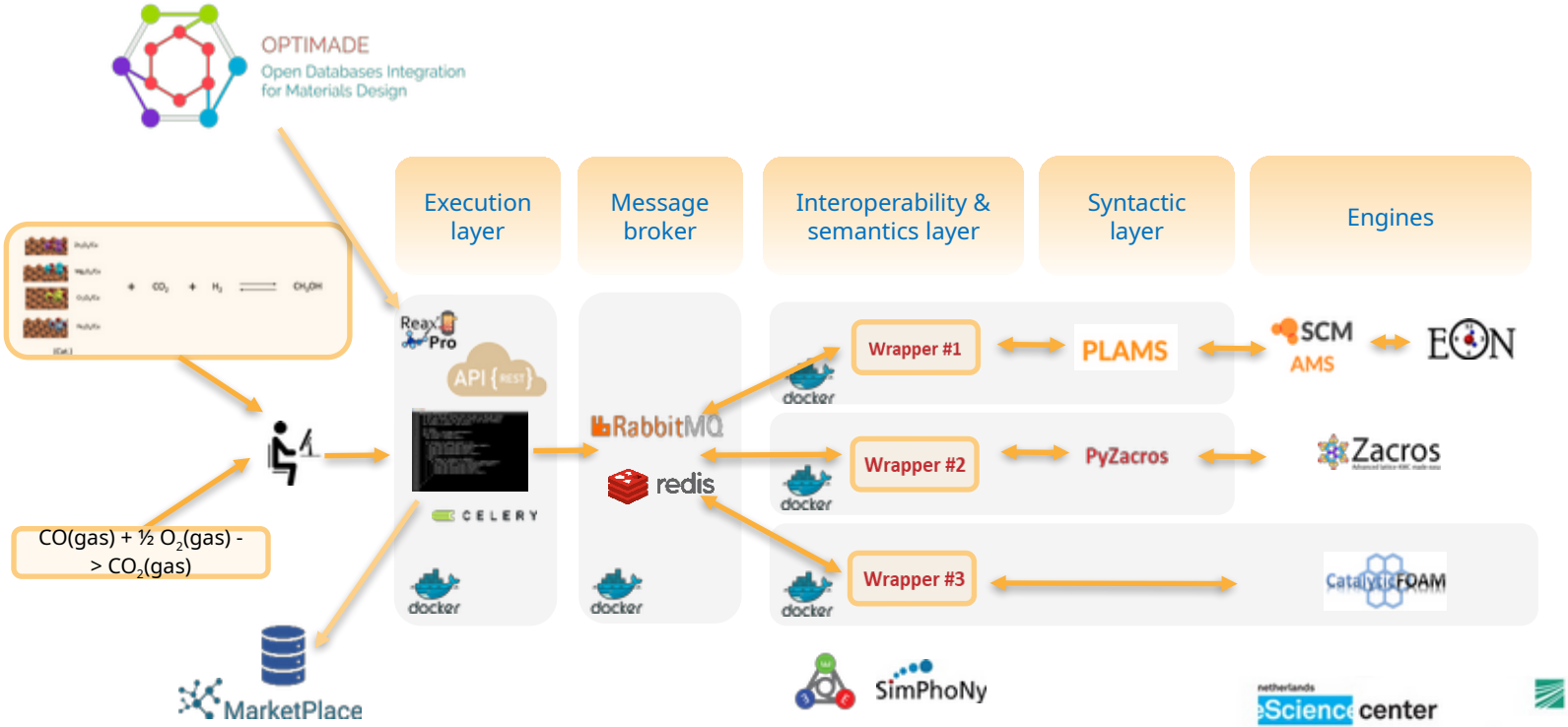
ReaxPro Platform



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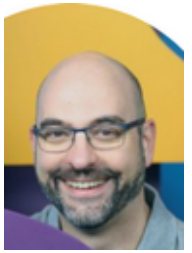
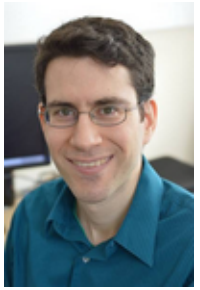
Matthias Büschelberger
Joana Francisco Morgado



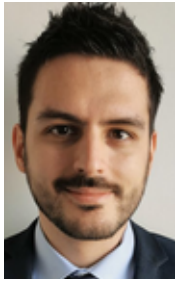
Acknowledgements

Alejandro Peña-Torres

Hannes Jonsson



Michail Stamatakis



Mauro Bracconi

Matteo Maestri

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Thanks!