XACS
Xiamen Atomistic Computing Suite
XACScloud.com

MLatom.com

XACS平台介绍(II)：基于XACS平台的计算化学（使用MLatom进行几何构型优化）

Pavlo O. Dral

Xiamen University, P.R. China

Visiting Professor in
Nicolaus Copernicus University, Poland

2 July 2024

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2 July 2024

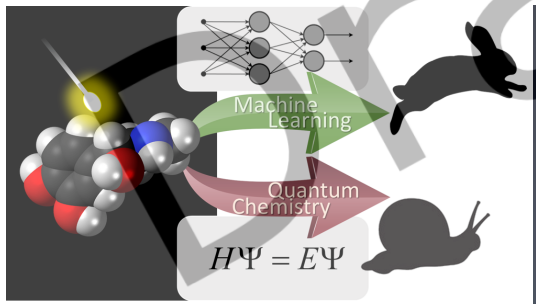
Pavlo O. Dral

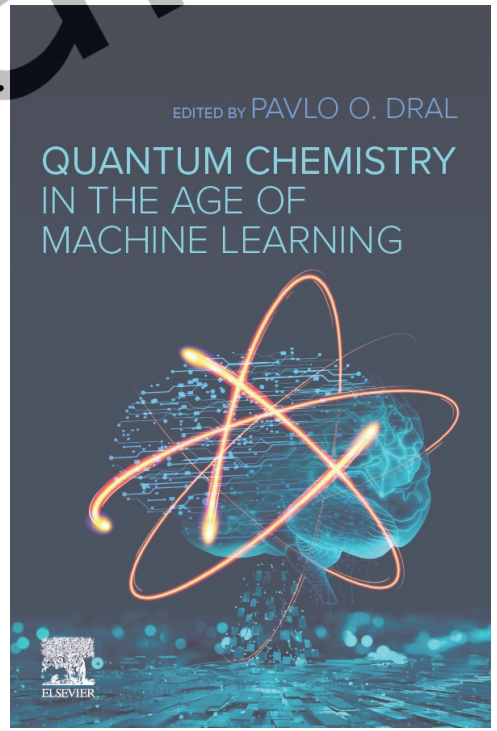
AI in computational chemistry

Professor | Outstanding Youth (Overseas)

Email: dral@xmu.edu.cn

Research Areas: artificial intelligence, quantum chemistry, dynamics, excited states, semi-empirical methods





MLatom.com

XACS
Xiamen Atomistic Computing Suite

nature communications
CHEMISTRY AND MATERIALS SCIENCES
TOP 25
READ ARTICLES OF 2021
OFFICIAL AUTHOR

2024-Present: Nicolaus Copernicus University, Visiting Professor
2021-Present: Xiamen University, Full Professor
2019-2021: Xiamen University, Associate Professor
2013-2019: Max-Planck-Institut für Kohlenforschung, Postdoc
2010-2013: University of Erlangen-Nürnberg, M.Sc. & Ph.D.
2008-2010: University of Erlangen-Nürnberg, M.Sc.
2004-2010: National Technical University of Ukraine "KPI", B.Sc. & M.Sc.

Research Interests:

Our research transforms chemical physics simulations by developing novel AI methods and providing software and cloud computing platforms.

✓Selected papers:

AI platform: *J. Chem. Theory Comput. 2024, 20, 1193*
AI-quantum dynamics: ***Nat. Commun.*** *2022, 13, 1930*
AI-quantum mechanics: ***Nat. Commun.*** *2021, 12, 7022*
AI-excited states: ***Nat. Rev. Chem.*** *2021, 5, 388*
AI force fields: ***Chem. Sci.*** *2021, 12: 14396*

Group website: dr-dral.com

Group & Acknowledgements

XACS
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XACScloud.com

MLatom.com

PCOSS

国家自然科学基金委员会
National Natural Science Foundation of China

嘉庚创新实验室
TAN KAH KEE INNOVATION LABORATORY

2023

2024

Learning materials

XACS
Xiamen Atomistic Computing Suite
XACScloud.com

MLatom.com

XACS Cloud

Cloud Computing

- Job Submitter
- Terminal
- File Manager
- Job Manager
- Jupyter Lab

Software

- Download

Learning

- Courses

Courses

Testimonials:

"Dr. Dral offers a fantastic introduction to the concepts around machine learning in chemistry!"

For teachers: Your course can be here!

计算化学与人工智能

计算化学和人工智能迷你课程
作者: Pavlo O.Dral
发布日期: 2024年6月14日

Go

Computational chemistry & AI

Hands-on course on computational chemistry and artificial intelligence (AI) by Pavlo O. Dral

Go

We open both courses for free for the workshop participants!

Recommend them further!

Learning materials

XACS
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MLatom.com

XACS Cloud

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- Job Submitter
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Software

- Download

Learning

- Courses

Courses

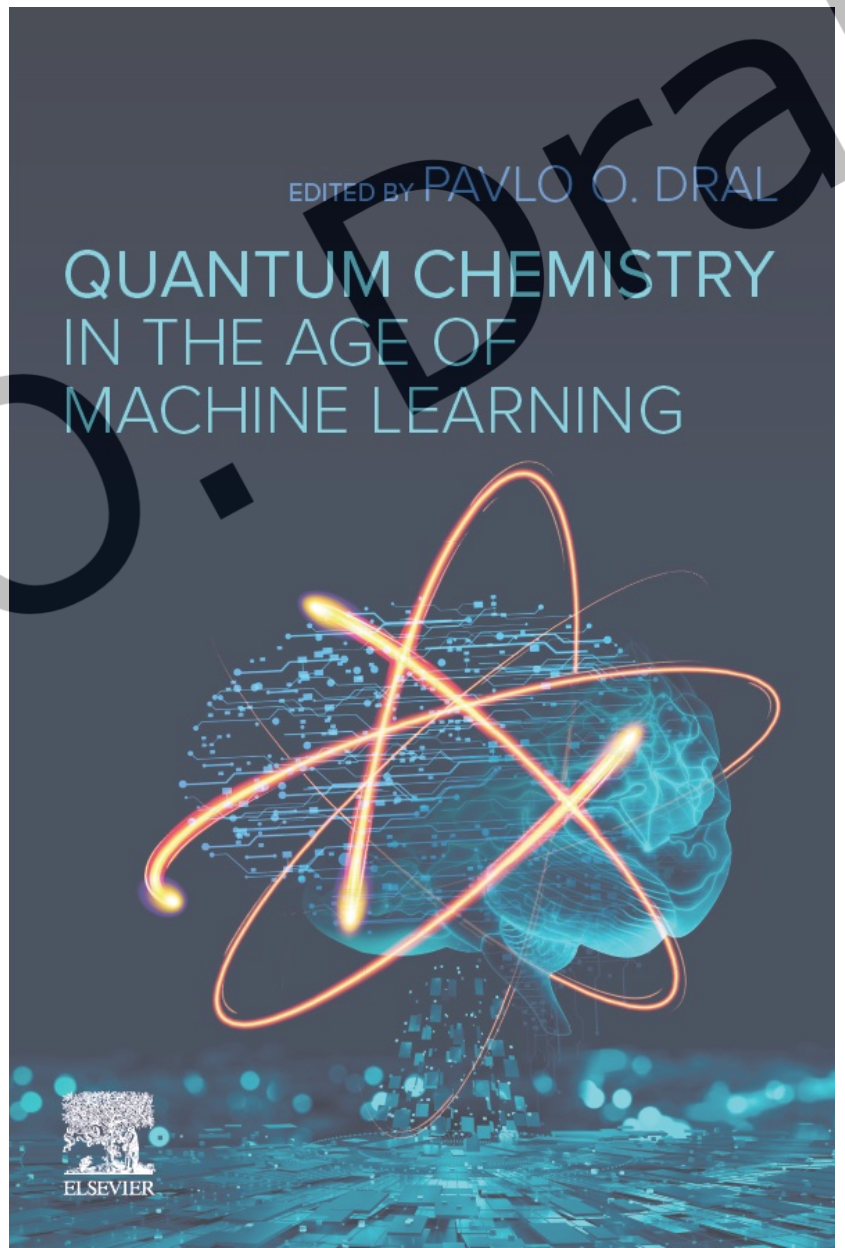
More valuable

Computational chemistry & AI

Hands-on course on computational chemistry and artificial intelligence (AI) by Pavlo O. Dral

Living + tutor (regularly updated)

Coming Soon



65 authors
27 chapters


Terminal


File Manager


Job Manager


Jupyter Lab

Software


Download

Learning


Courses


Workshops


Archive

Workshops

XACSW-2024

Course materials for
XACSW-2024
(第三届化学键与AI分子模拟
XACS研讨会课程资料)

Go

Open source (on github, pip install...); also run on XACScloud.com

Machine Learning

Simulations

MLatom

MLatom@GitHub
≠
MLatom@XACS

Quantum Chemistry

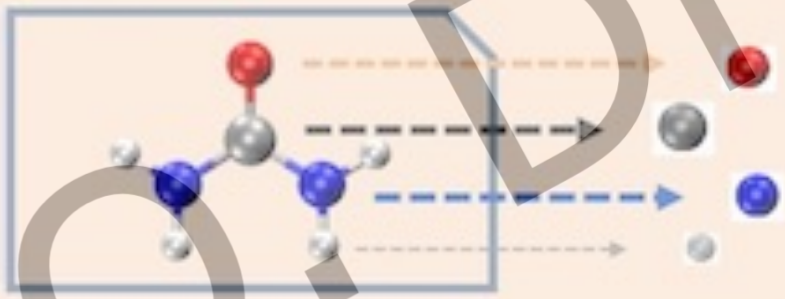
Data

Have it your way...

- Data in different formats and types **V3**

molecular_database

molecule



atom

- Python API **V3**

```
import mlatom as ml
```

- Input file

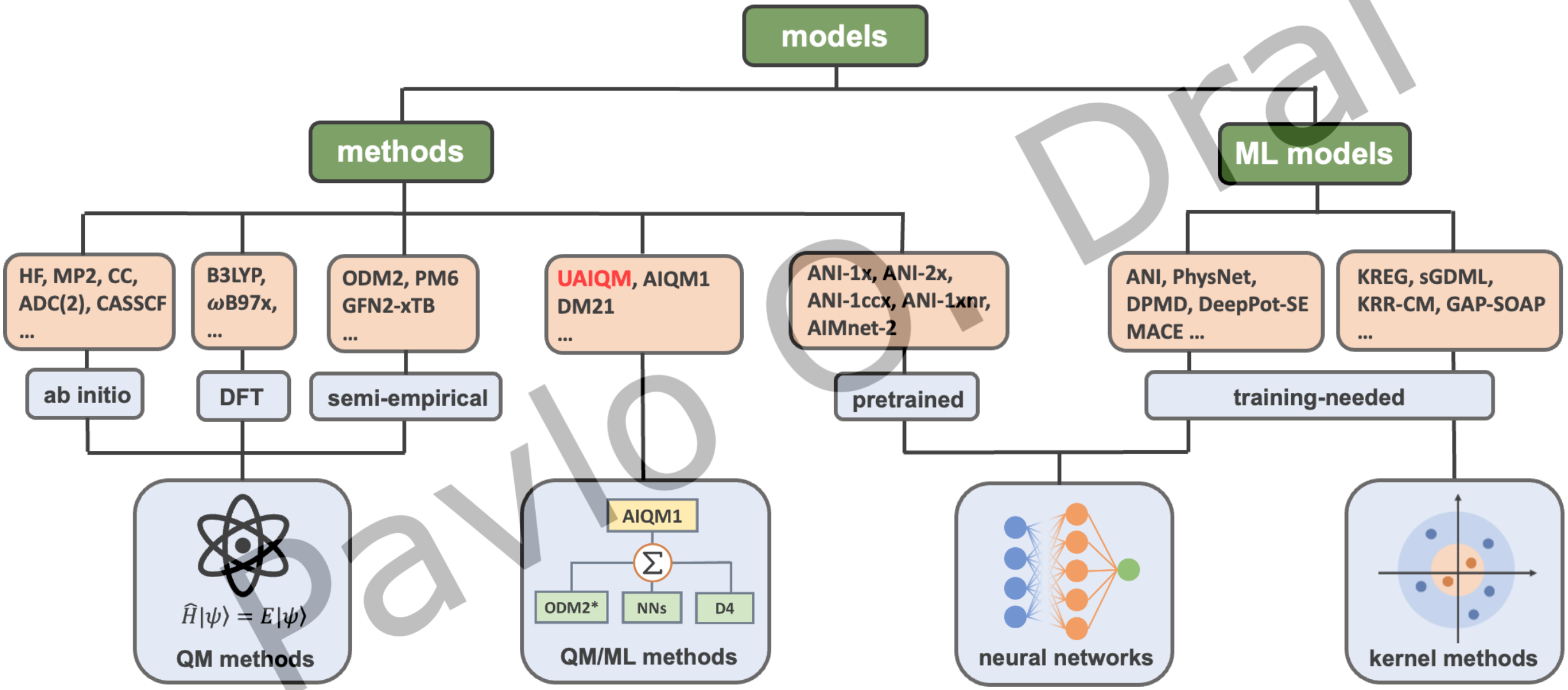
```
ANI-1ccx
geomopt
xyzfile=init.xyz
optxyz=opt.xyz
```

- Command line

```
> $mlatom ANI-1ccx geomopt xyzfile=init.xyz optxyz=opt.xyz
```


P. O. Dral, F. Ge, Y.-F. Hou, P. Zheng, Y. Chen, M. Barbatti, O. Isayev, C. Wang, B.-X. Xue, M. Pinheiro Jr, Y. Su, Y. Dai, Y. Chen, S. Zhang, L. Zhang, A. Ullah, Q. Zhang, Y. Ou. *J. Chem. Theory Comput.* **2024,** *20*, 1193

AI-enhanced computational chemistry

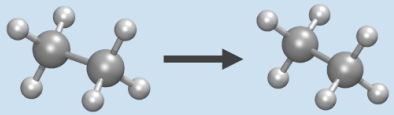


Updated based on: P. O. Dral, F. Ge, Y.-F. Hou, P. Zheng, Y. Chen, M. Barbatti, O. Isayev, C. Wang, B.-X. Xue, M. Pinheiro Jr, Y. Su, Y. Dai, Y. Chen, S. Zhang, L. Zhang, A. Ullah, Q. Zhang, Y. Ou. *JCTC* **2024,** *20*, 1193

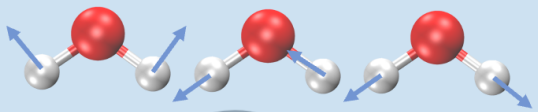
AI-enhanced computational chemistry

Single point calculations — Energies, forces, Hessian matrix...

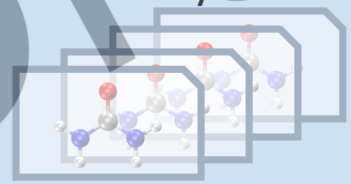
Geometry optimizations



Frequency calculations



Molecular dynamics



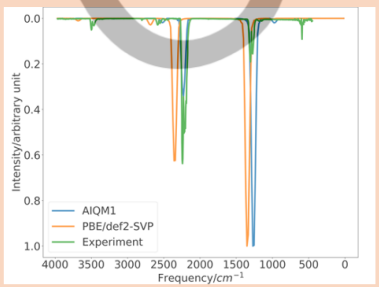
+PIMD coming soon...

Thermochemistry calculations

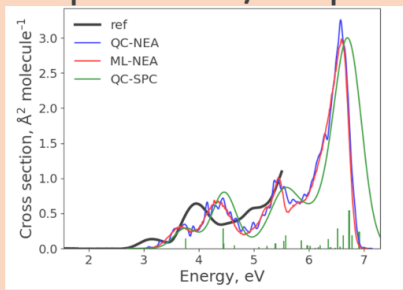
Heat of formation:

$$\Delta H_{\mathrm{at},T} = \left[\sum_A H_T(A)\right] - H_T$$

(Ro)vibrational spectra



One-photon UV/vis spectra



Properties & spectra

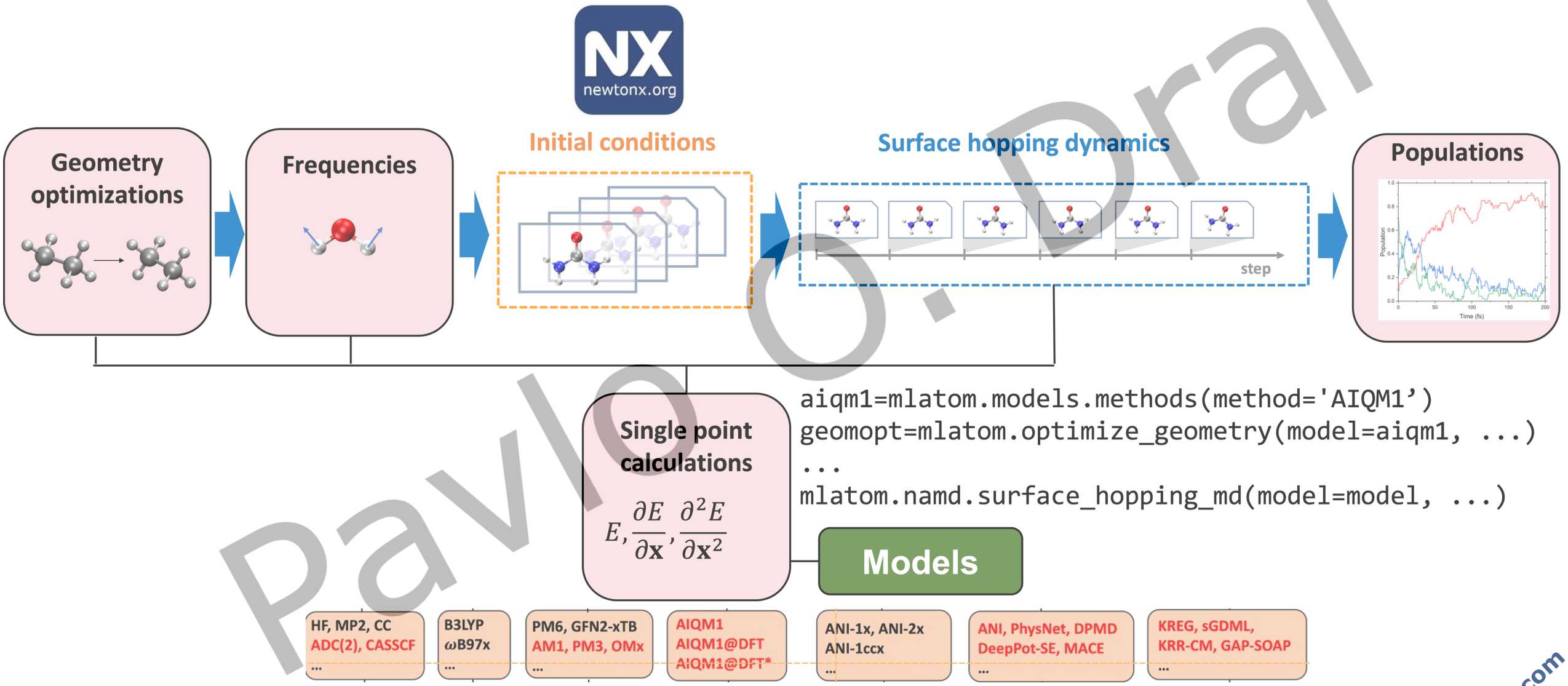
Simulations

Quantum dissipative dynamics

Two-photon absorption spectra

P. O. Dral, F. Ge, Y.-F. Hou, P. Zheng, Y. Chen, M. Barbatti, O. Isayev, C. Wang, B.-X. Xue, M. Pinheiro Jr, Y. Su, Y. Dai, Y. Chen, S. Zhang, L. Zhang, A. Ullah, Q. Zhang, Y. Ou. *J. Chem. Theory Comput.* **2024,** *20*, 1193

Surface-hopping dynamics



L. Zhang, M. Martyka, ..., J. Jankowska, M. Barbatti, P. O. Dral. *JCTC*, **2024**, *20*, 5043–5057

MLatom's interfaces

Extras!

MLQD

A Package for Quantum Dissipative Dynamics with Machine Learning
by Arif Ullah, Anhui University

[MLQD: A. Ullah, P. O. Dral. *Comput. Phys. Commun*. **2024**, *294*, 108940]

Wechat
Follow
XACS account

Slack
Answering your
questions in real time

Quantum chemical programs:

Gaussian, ORCA, PySCF, Turbomole, COLUMBUS

Semi-empirical quantum chemical programs:

xTB, SPARROW, MNDO

Machine learning programs:

PhysNet, GAP, TORCHANI, SGDML, hyperopt

Dynamics and other atomistic simulation:

ASE, NX newtonx.org

Not everything is available on the cloud...

Python API

对于KREG模型，我们可以使用简单的网格搜索优化

```
model = ml.models.kreg(model_file=f'kreg.npz')

sub, val = molDB.split(number_of_splits=2, fracti

model.hyperparameters['sigma'].minval = 2**-5 # A
model.optimize_hyperparameters(subtraining_molecu
                               optimization_algo
                               hyperparameters=
                               training_kwargs=
                               prediction_kwargs
lmbd = model.hyperparameters['lambda'].value ; si
valloss = model.validation_loss
print('Optimized sigma:', sigma)
print('Optimized lambda:', lmbd)
print('Optimized validation loss:', valloss)
# Train the model with the optimized hyperparamet
model.train(molecular_database=molDB, property_to
# Train the model with the optimized hyperparamet
model.train(molecular_database=molDB, property_to
```

输出如下所示（它可能随子训练集和验证集的随机子

```
Optimized sigma: 0.10511205190671434
Optimized lambda: 2.910383045673381e-11
Optimized validation loss: 3.1550365181164988e-0
```

其他参数也是可用的，例如SciPy(`Nelder-Mead`, `BFG`, `krylov`, `trust-exact`)和hyperopt库(`TPE`)。

Cloud Computing

- Job Submitter
- Terminal
- File Manager
- Job Manager
- Jupyter Lab

Software

- Download

Learning

- Courses
- Workshops

Statistics

Total CPU time used

4756h 1m

Job Information

* Job Name: 2024-05-30_0757

Job Location: from_job_submitter

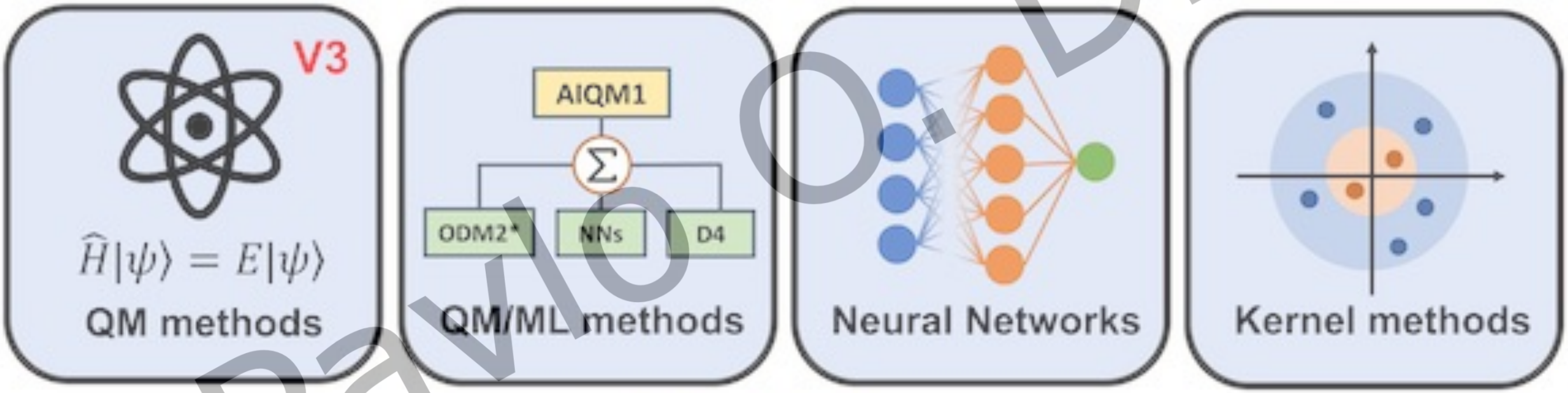
Job Type: XACS (auto detect) Gaussian Mlatom_d

Input File

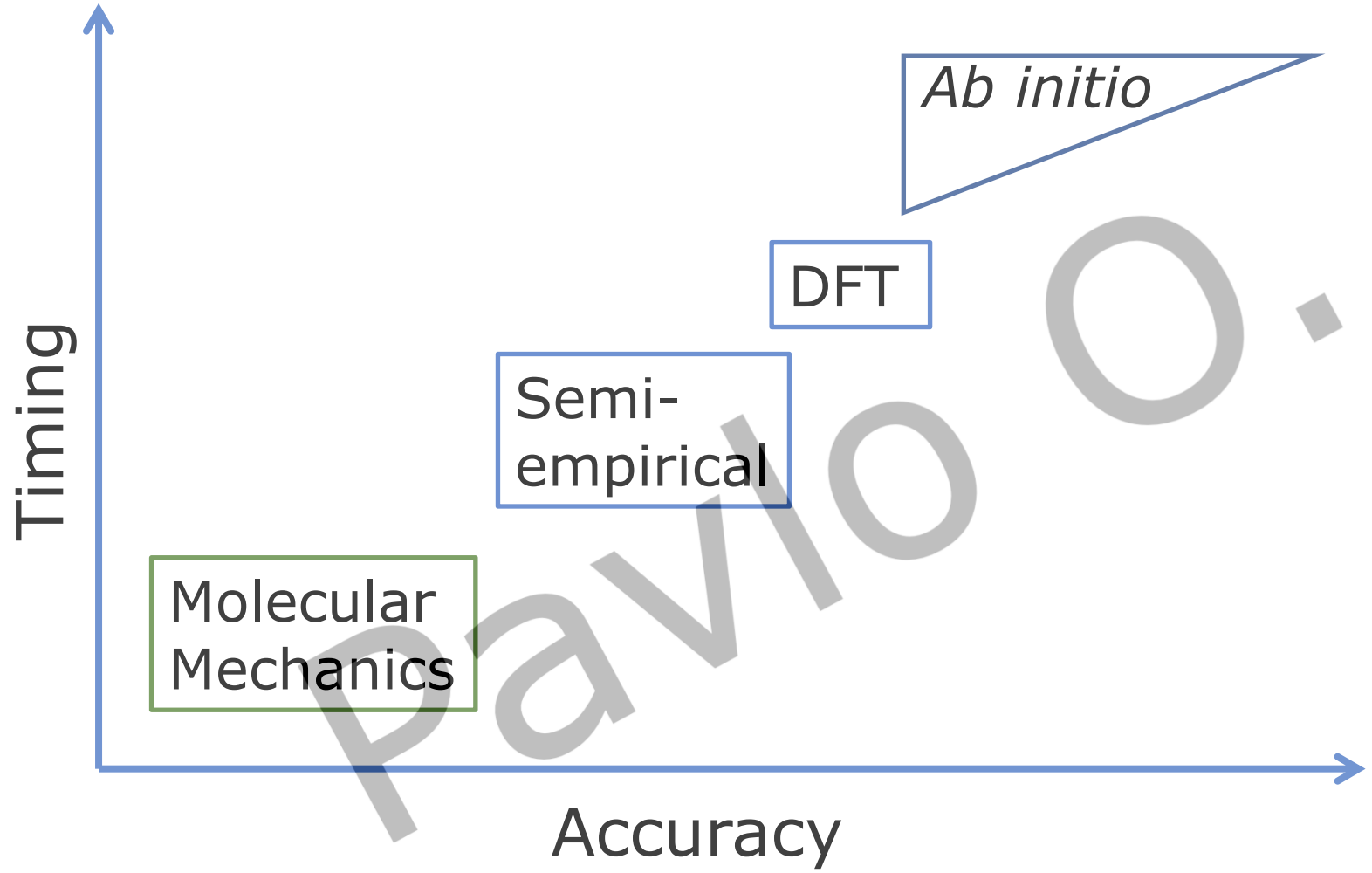
or edit XACS input file:

1

Models



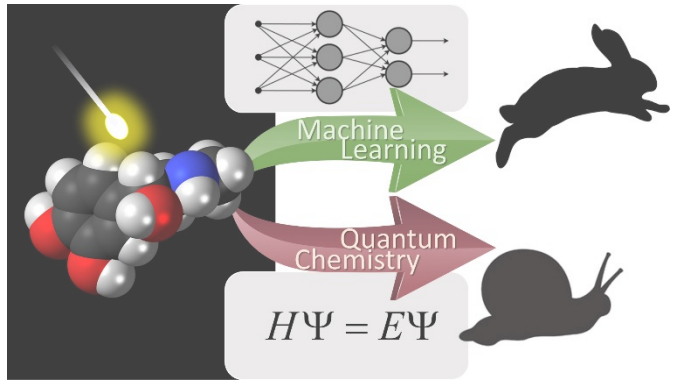
Quantum chemical perspective



P. O. Dral, *J. Phys. Chem. Lett.* **2020**, *11*, 2336

AI is a game changer

P. O. Dral, M. Barbatti, *Nat. Rev. Chem.* **2021,** *5*, 388



Ab initio

DFT

Semi-empirical

Machine Learning

Molecular Mechanics

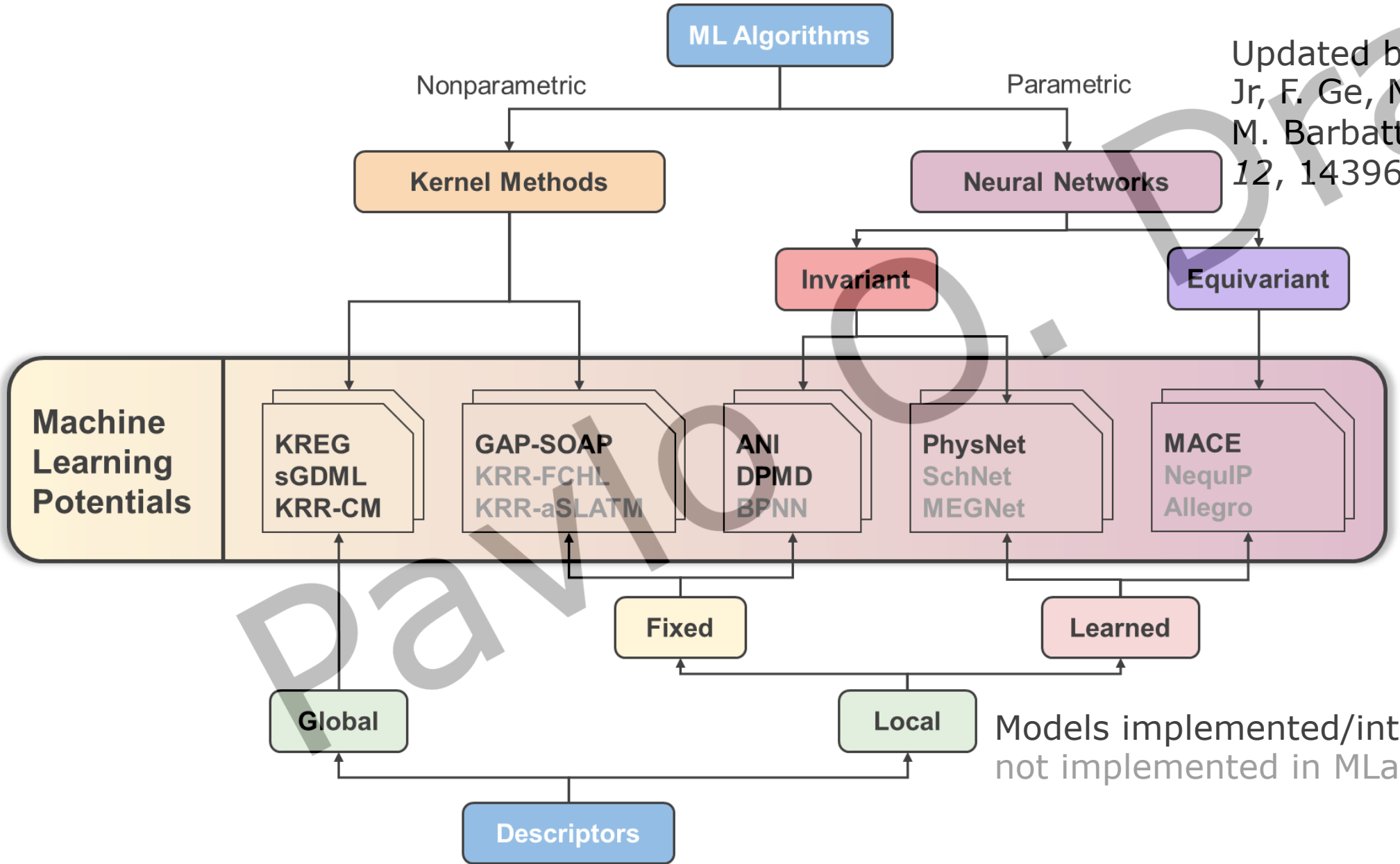
Timing

Accuracy

Figure: P. O. Dral, *J. Phys. Chem. Lett.* **2020**, *11*, 2336

Zoo of machine learning potentials

Categories of machine learning potentials

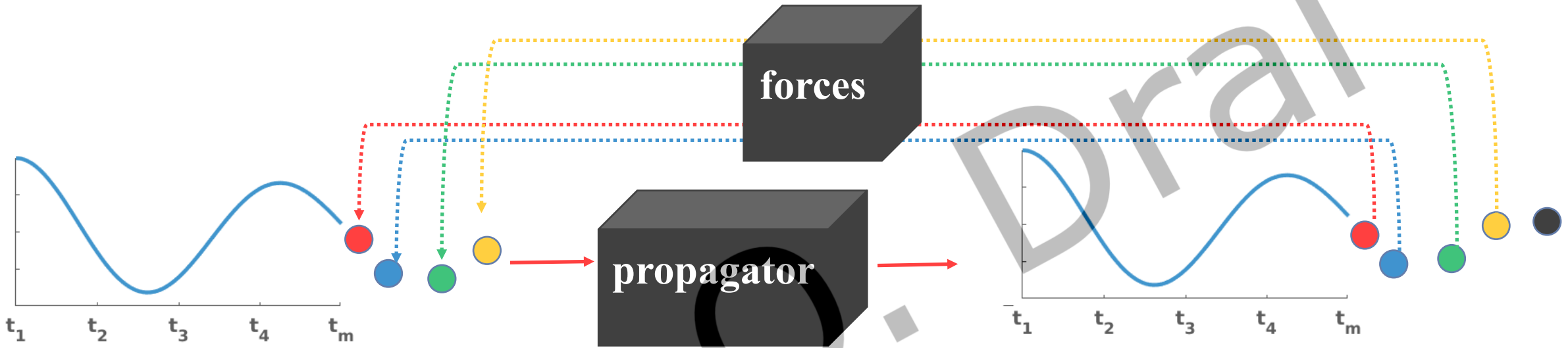


Updated based on M. Pinheiro Jr, F. Ge, N. Ferré, P. O. Dral, M. Barbatti. *Chem. Sci.* **2021**, *12*, 14396–14413

Models implemented/interfaced in MLatom

not implemented in MLatom

MD



$$F_{A,d} = -\frac{\partial E}{\partial x_{A,d}} = -\frac{\partial E^{\text{machine learning potential}}(\mathbf{x})}{\partial x_{A,d}}$$

Adapted from animation by Arif Ullah

Categories of machine learning potentials

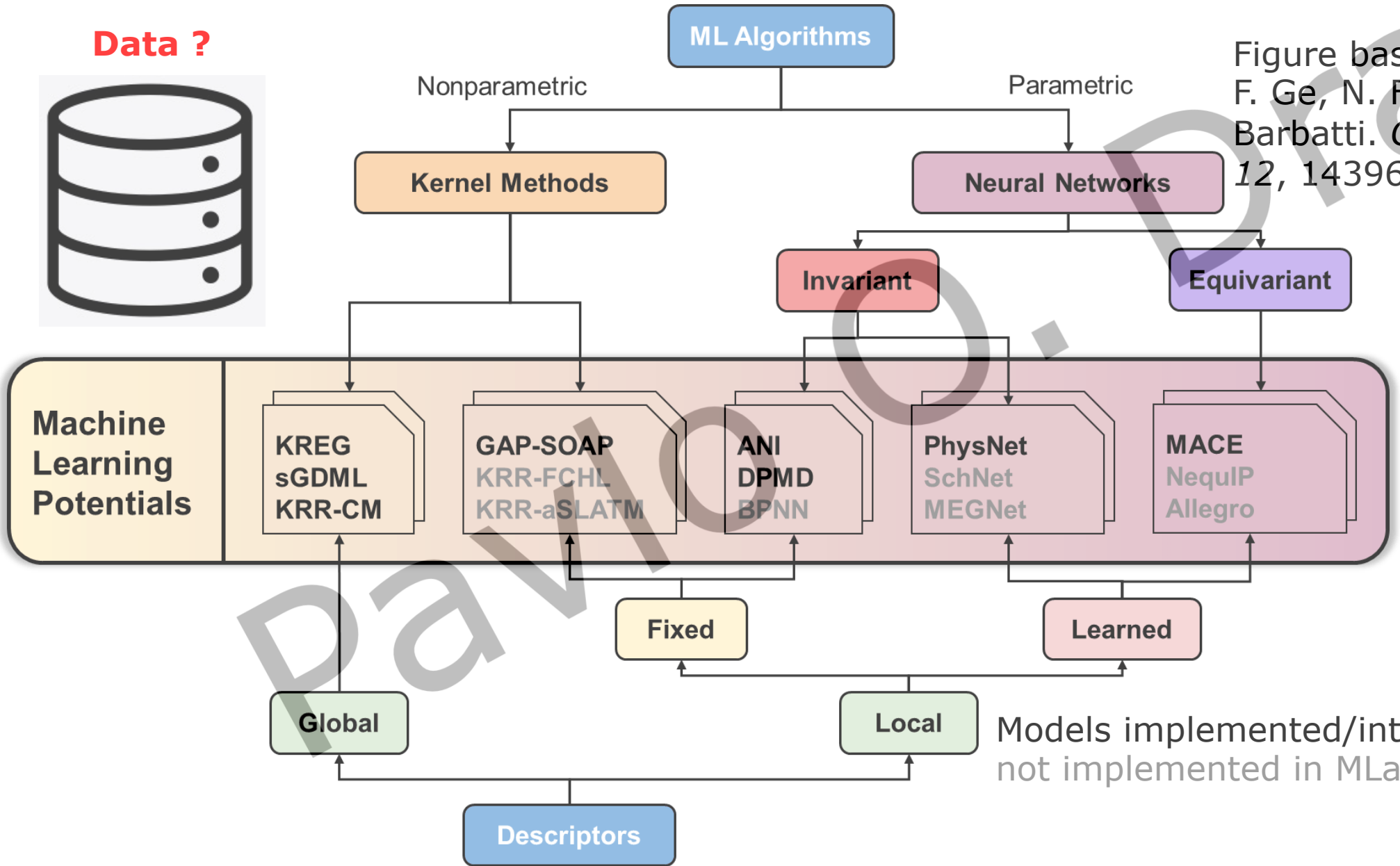
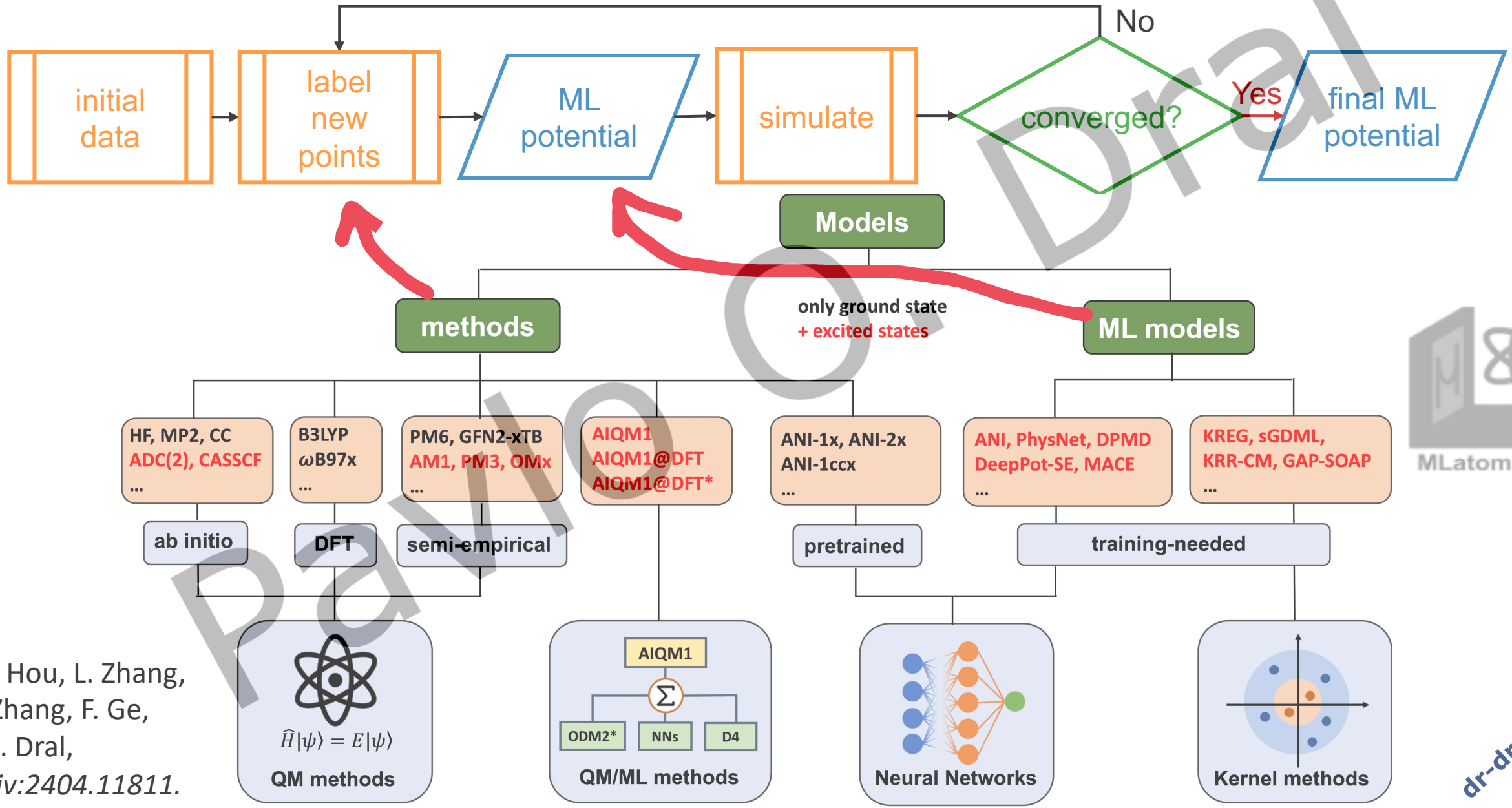


Figure based on M. Pinheiro Jr, F. Ge, N. Ferré, P. O. Dral, M. Barbatti. *Chem. Sci.* **2021**, *12*, 14396–14413

Models implemented/interfaced in MLatom
not implemented in MLatom

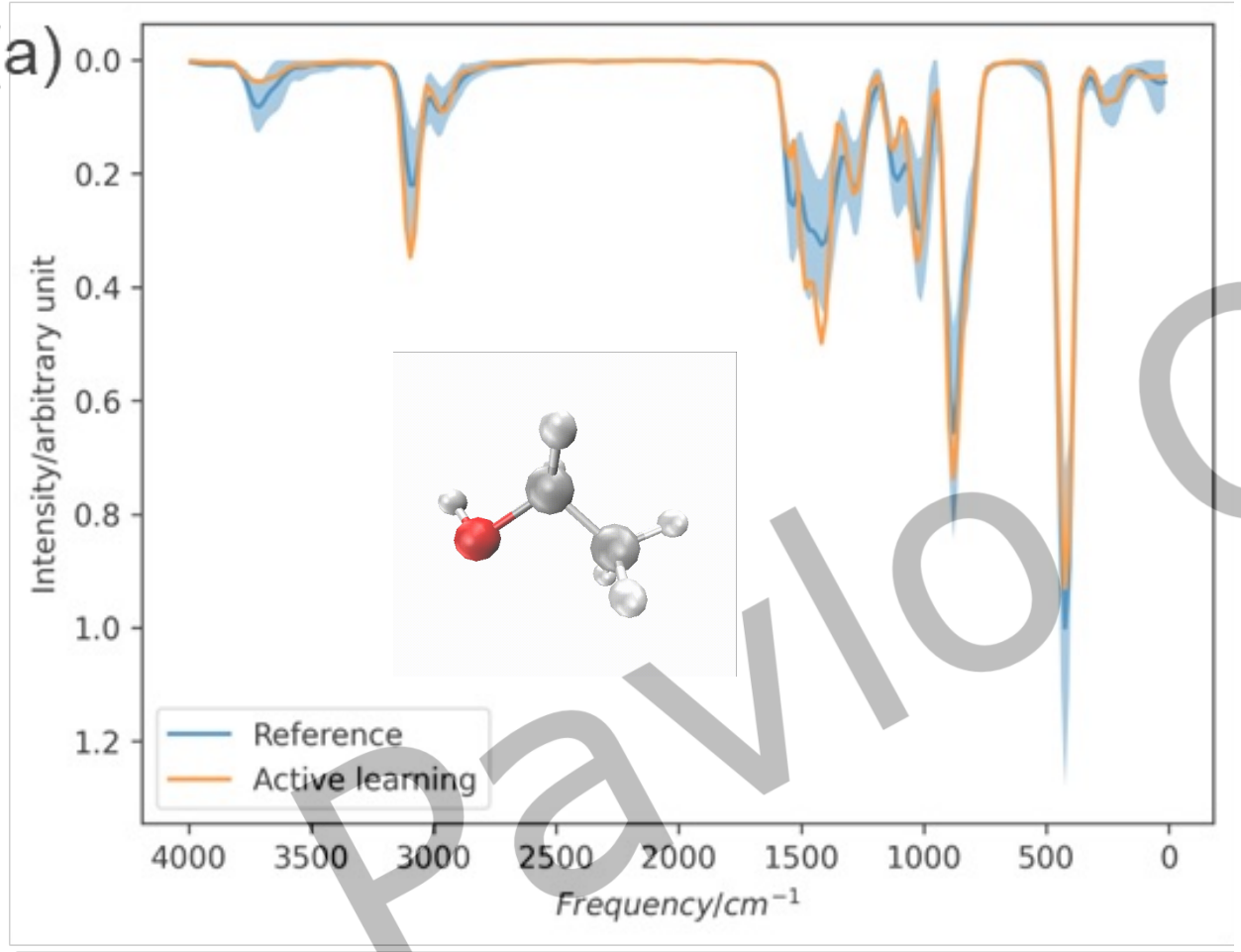
Physics-informed active learning

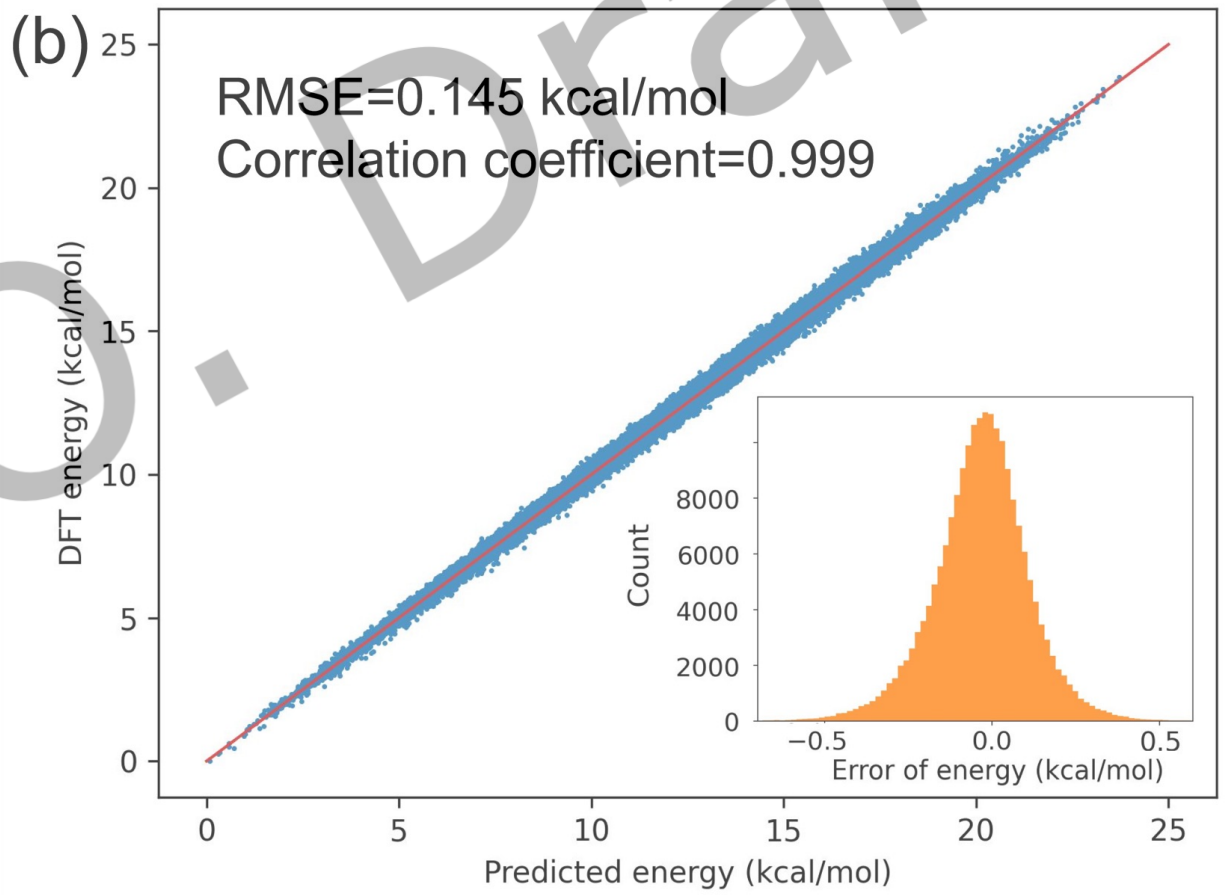


Y.-F. Hou, L. Zhang, Q. Zhang, F. Ge, P. O. Dral, *arXiv:2404.11811.*

Accurate vibrational spectra

< 1000 training points with ANI potential





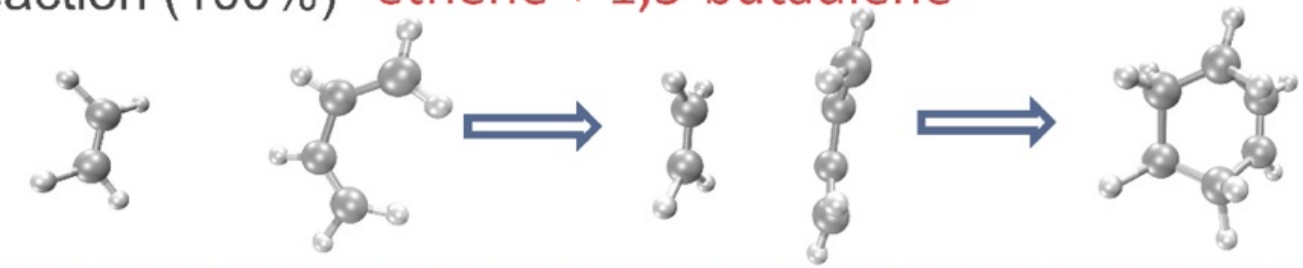
Ethanol spectra – 2 days of calculations on a 3080 RTX GPU

Y.-F. Hou, L. Zhang, Q. Zhang, F. Ge, P. O. Dral. *arXiv:2404.11811*.

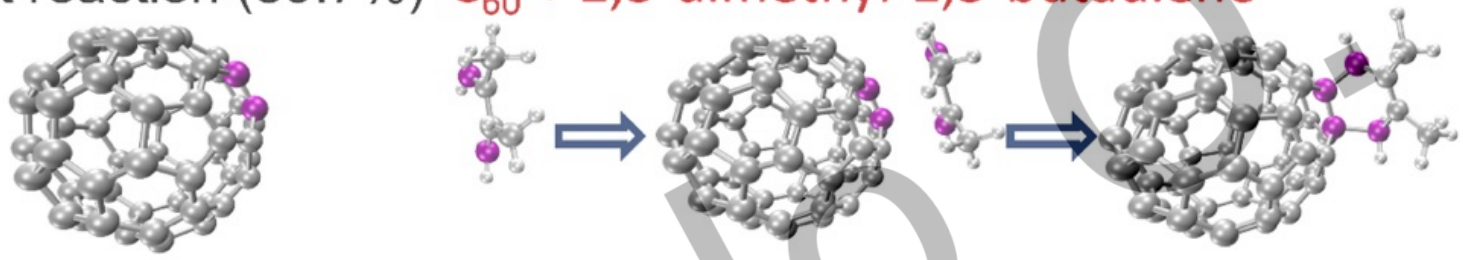
Time-resolved mechanisms

~3000 training points with ANI potential

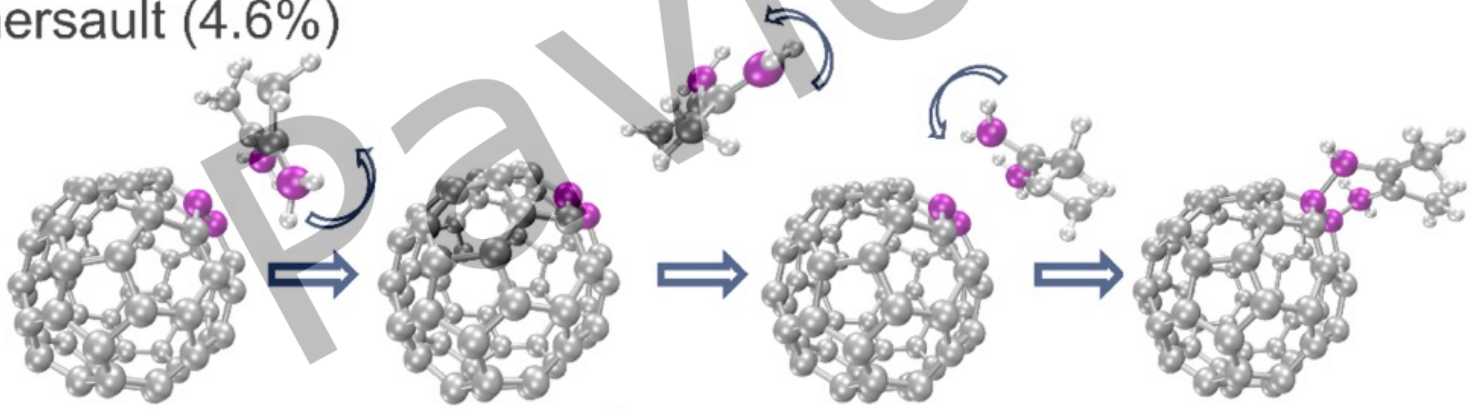
Direct reaction (100%) ethene + 1,3-butadiene

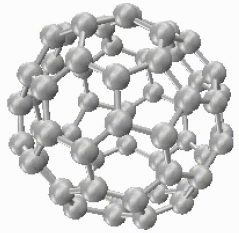


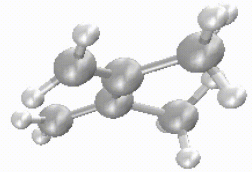
Direct reaction (89.7%) C_{60} + 2,3-dimethyl-1,3-butadiene



Somersault (4.6%)







Y.-F. Hou, Q. Zhang, P. O. Dral. https://doi.org/10.26434/chemrxiv-2024-hwsl4.

Categories of machine learning potentials

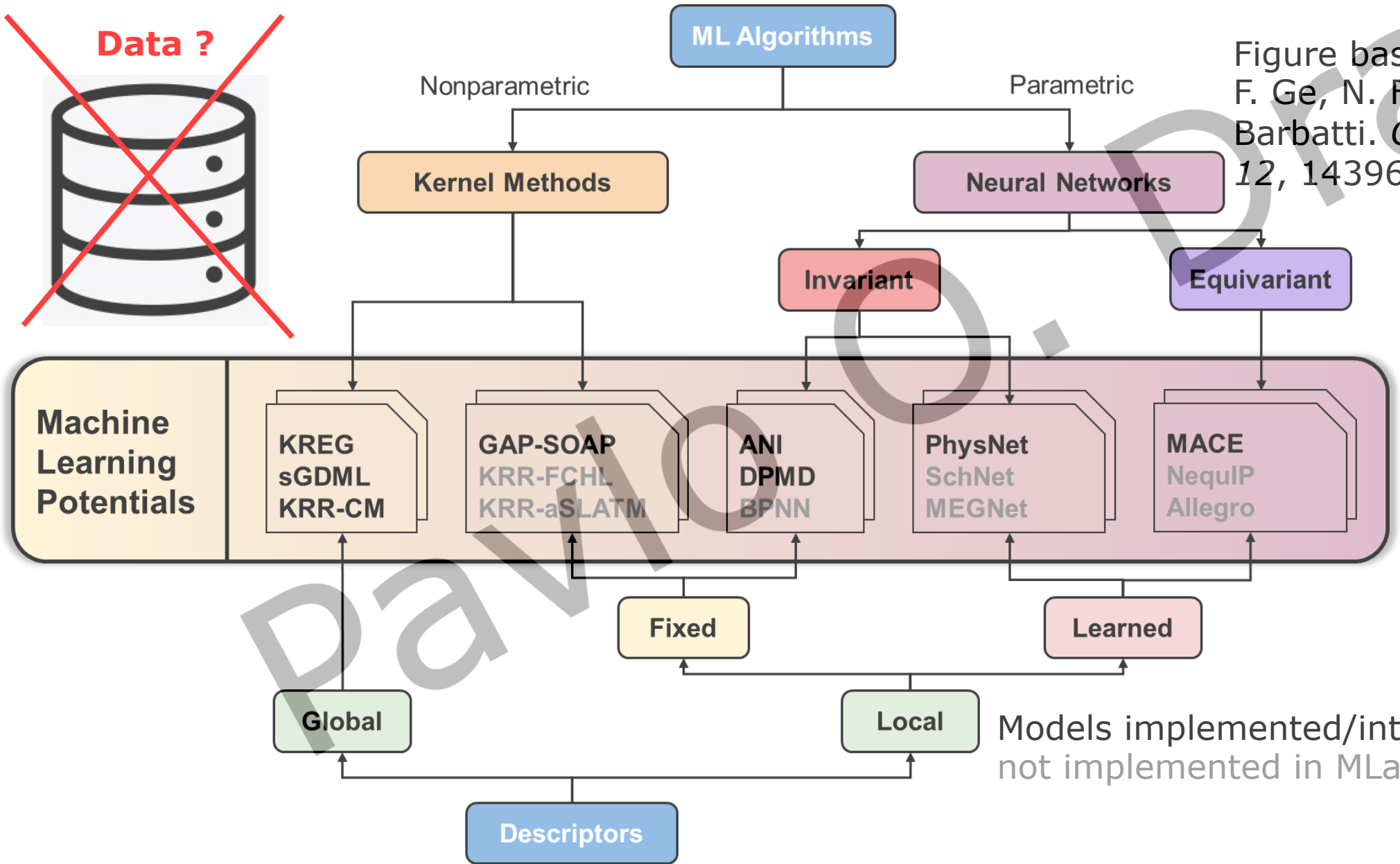


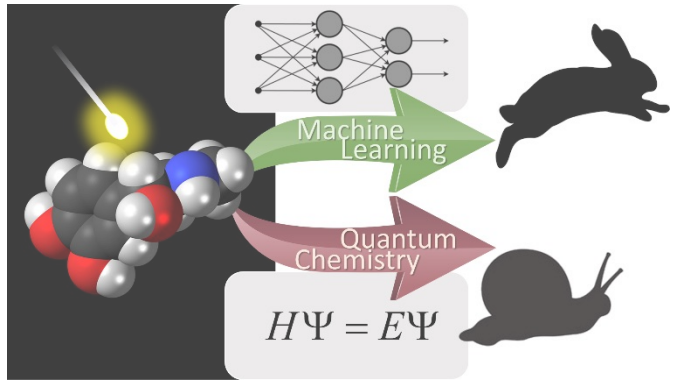
Figure based on M. Pinheiro Jr, F. Ge, N. Ferré, P. O. Dral, M. Barbatti. *Chem. Sci.* **2021**, *12*, 14396–14413

Models implemented/interfaced in MLatom

not implemented in MLatom

Universal models (no training needed)

P. O. Dral, M. Barbatti, *Nat. Rev. Chem.* **2021,** *5*, 388



Timing

Accuracy

Ab initio ML-ab initio

DFT ML-DFT DM21, CF22D, DENS24…

Semi-empirical ML-SQC **AIQM1**

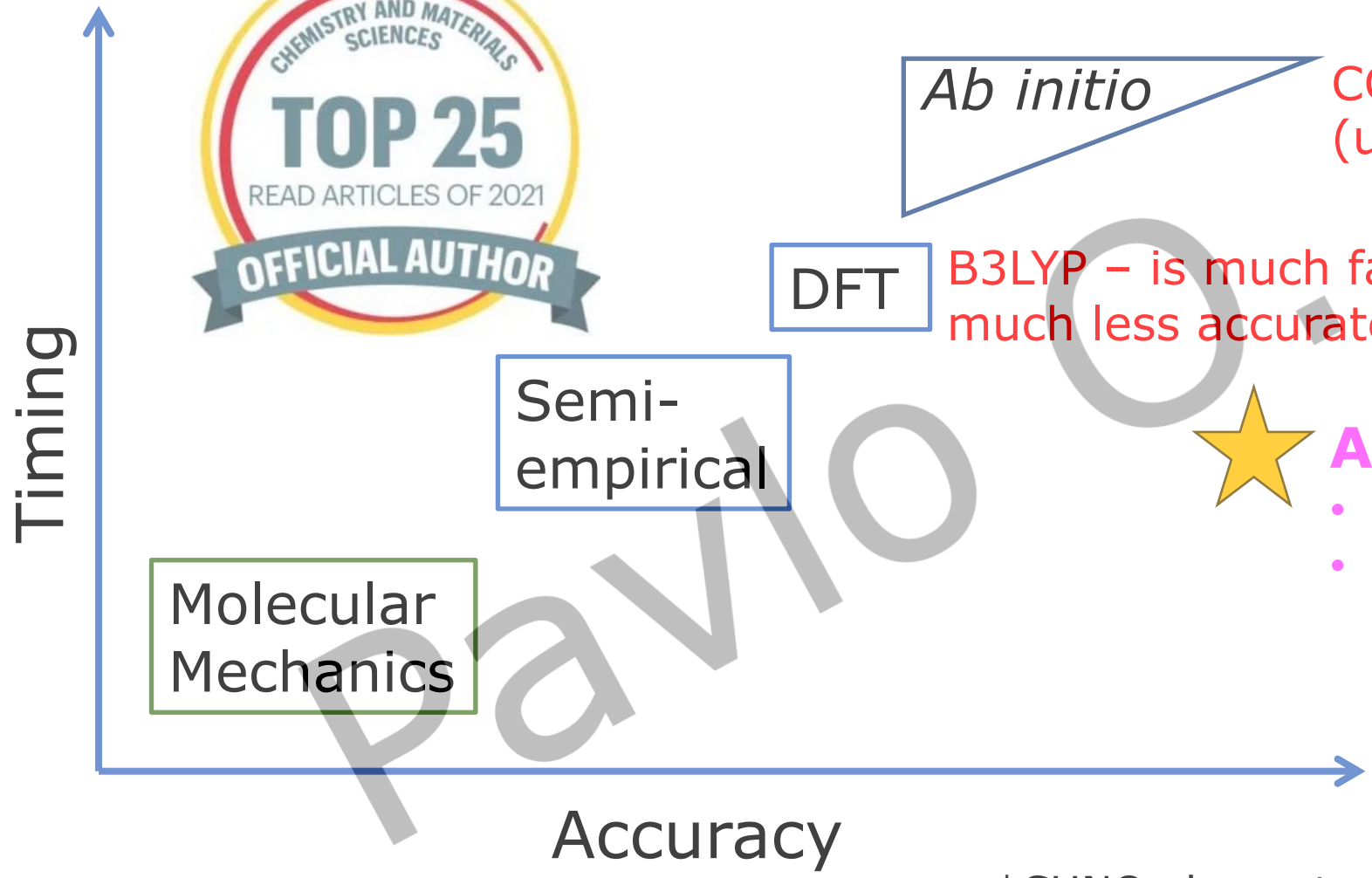
AIQM1: P. Zheng, R. Zubatyuk, W. Wu, O. Isayev, P. O. Dral, *Nat. Commun.* **2021**, *12*, 7022

Machine Learning ANI-1ccx, AIMnet-2, ANI-1xnr, …

Molecular Mechanics

Figure: P. O. Dral, *J. Phys. Chem. Lett.* **2020**, *11*, 2336

Quantum chemistry approximations



CCSD(T) – gold standard, very slow (use it if you can!)

B3LYP – is much faster than the CCSD(T) but is much less accurate

Do not use B3LYP if you can use AIQM1!

AIQM1*

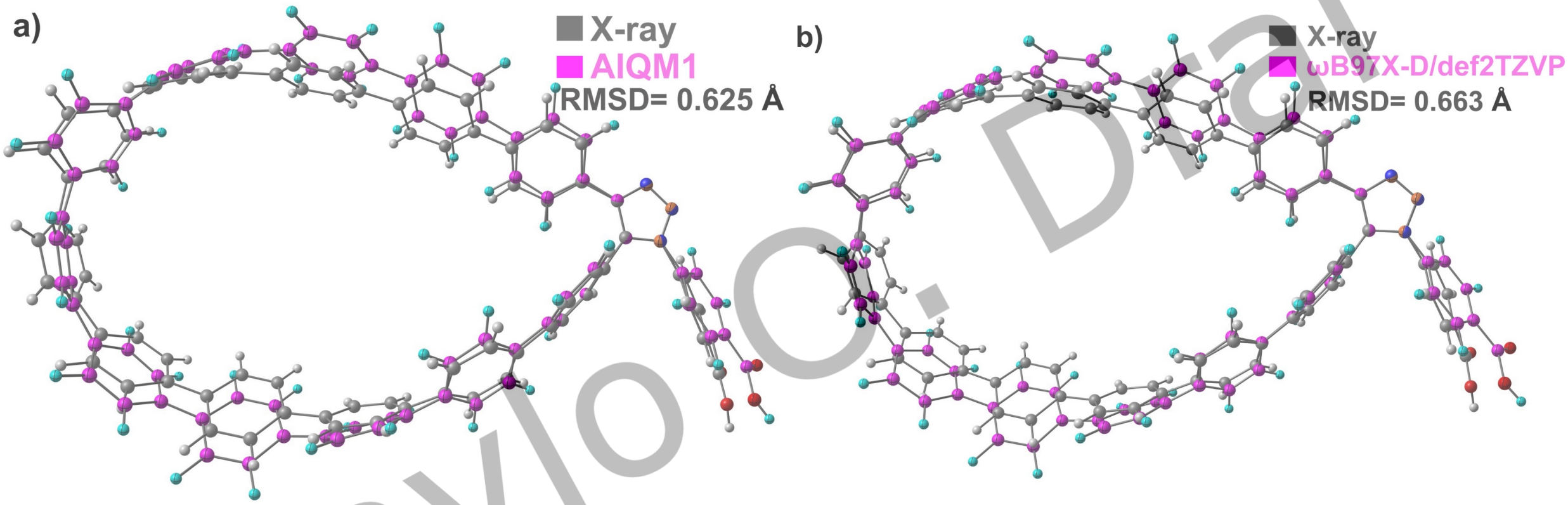
- **Accuracy of CCSD(T)**
- **Orders of magnitude faster than B3LYP**

AIQM1: P. Zheng, R. Zubatyuk, W. Wu, O. Isayev, P. O. Dral, *Nat. Commun.* **2021**, *12*, 7022

*CHNO elements only – extensions on the way

P. O. Dral, *J. Phys. Chem. Lett.* **2020**, *11*, 2336; *Chem. Commun.* **2024**, *60*, 3240

AIQM1 investigation of cycloparaphenylenes



2 CPU-minutes

1200 CPU-minutes

T. A. Schaub, A. Zieleniewska, R. Kaur, M. Minameyer, W. Yang, C. M. Schüßlbauer, L. Zhang, M. Freiberger, L. N. Zakharov, T. Drewello, P. O. Dral, D. Guldi, R. Jasti. Tunable Macrocyclic Polyparaphenylene Nanolassos via Copper-Free Click Chemistry. *Chem. Eur. J.* **2023**, *29*, e202300668

Revising experimental heats of formation

vinylacetylene

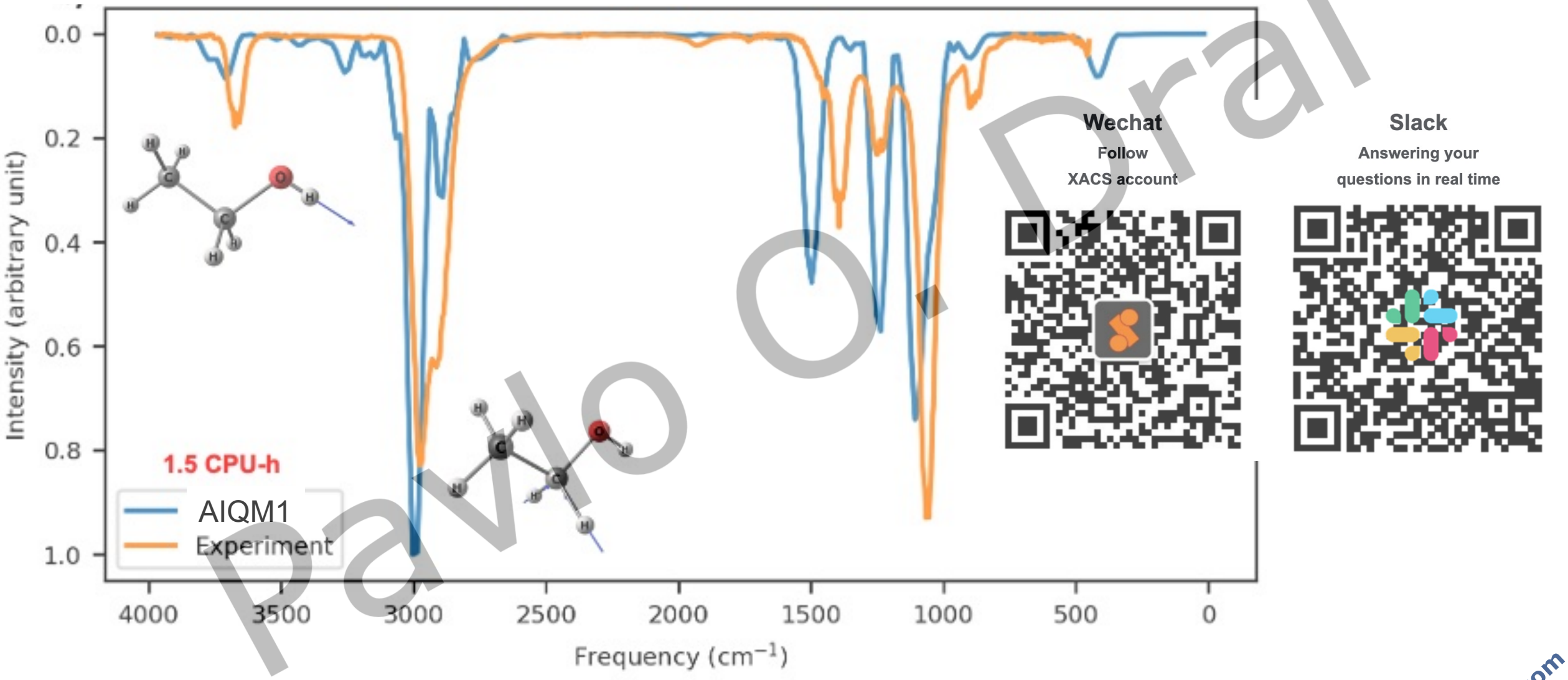
old experiment: 73
AIQM1: 69.1 (confident!)
G4: 69.1

Newer experimental data in NIST: **70.4**

Heats of formation in kcal/mol

P. Zheng, W. Yang, W. Wu, O. Isayev, P. O. Dral, *J. Phys. Chem. Lett.* **2022**, *13*, 3479

Path-integral MD



Y. Chen, Y.-F. Hou, O. Isayev, P. O. Dral. *Universal and Updatable Artificial Intelligence-Enhanced Quantum Chemical Foundational Models*. **2024**, *submitted*. https://doi.org/10.26434/chemrxiv-2024-604wb.

AIQM1 investigation of cycloparaphenylenes

AIQM1 also predicts fluorescence quenching

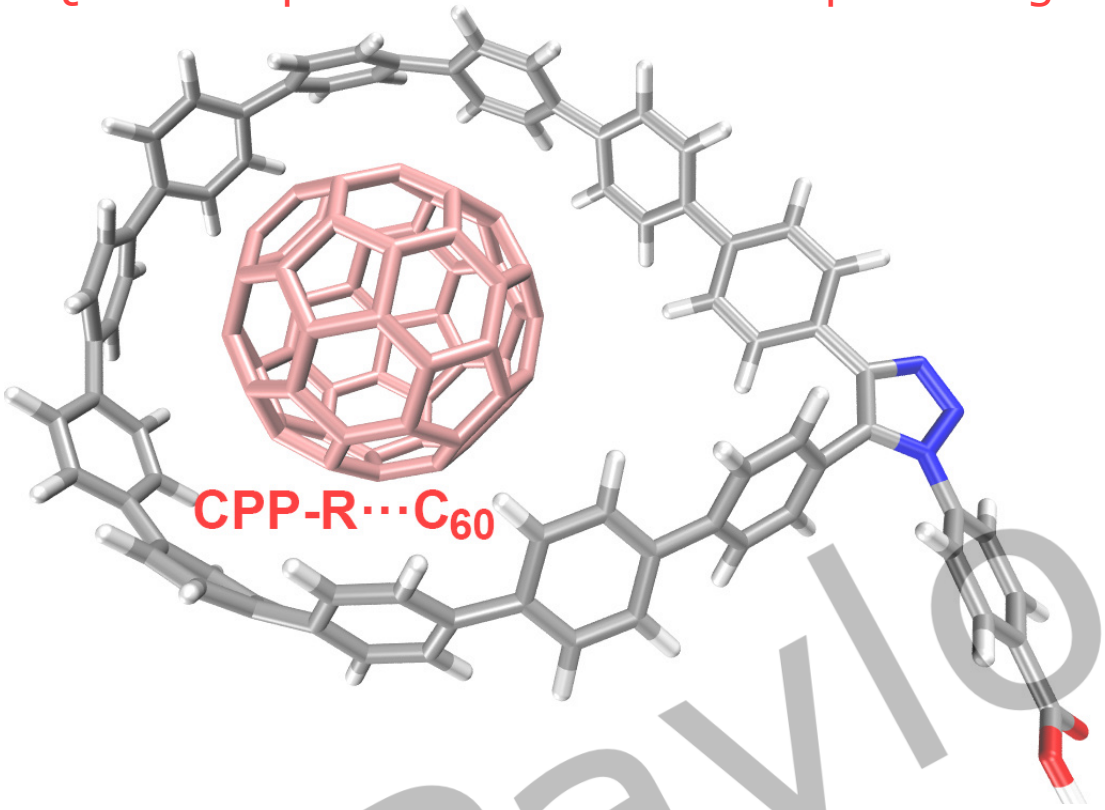


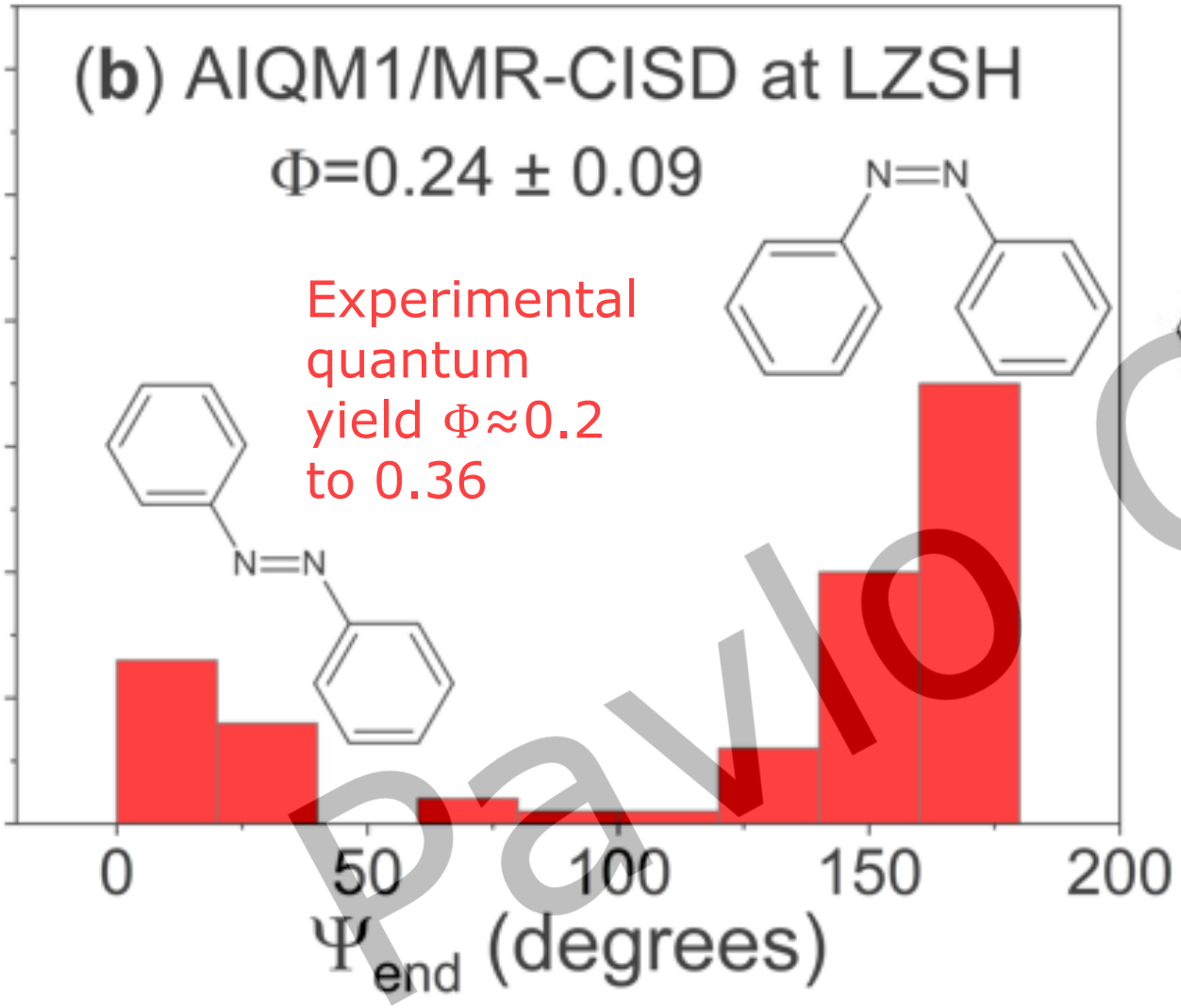
Table S9. Emission energy and oscillator strengths *f* of free molecules and their complexes with C_{60} and C_{70} at AIQM1/CIS in vacuum (S_1 to S_0 transition).

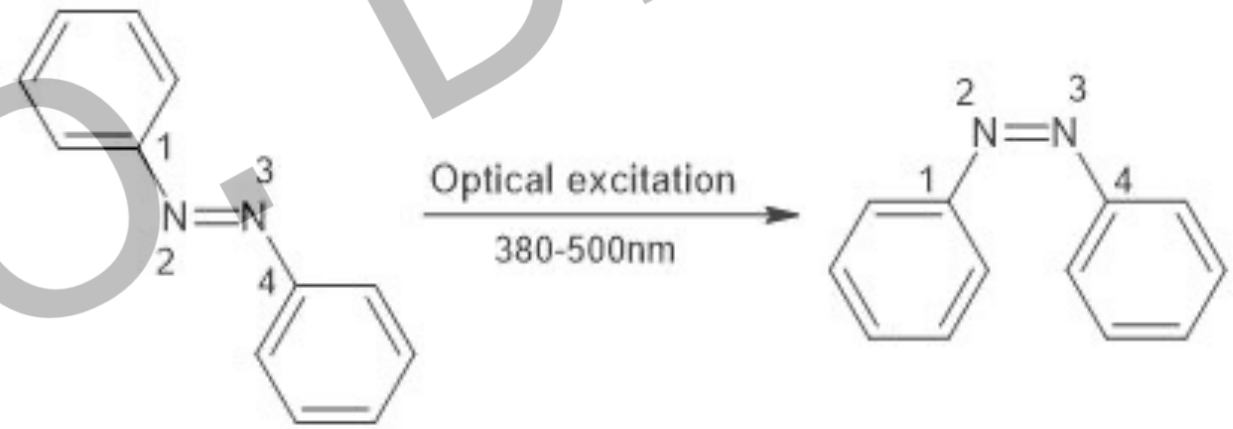
Species	*f*	Energy (eV)
3	0.750	3.11
4	0.751	3.12
5	0.750	3.12
6	0.750	3.12
7	0.748	3.12
3 ⊃ C_{60}	0.000	2.58
4 ⊃ C_{60}	0.000	2.58
5 ⊃ C_{60}	0.000	2.58
6 ⊃ C_{60}	0.000	2.58
7 ⊃ C_{60}	0.000	2.59
M-**3**⊃ C_{70}	0.000	2.10
M-**4** ⊃ C_{70}	0.000	2.09
M-**5** ⊃ C_{70}	0.000	2.10
M-**6** ⊃ C_{70}	0.000	2.10
M-**7** ⊃ C_{70}	0.000	2.10

AIQM1 can be useful for aggregation-induced emission, photocatalysis

T. A. Schaub, A. Zieleniewska, R. Kaur, M. Minameyer, W. Yang, C. M. Schüßlbauer, L. Zhang, M. Freiberger, L. N. Zakharov, T. Drewello, P. O. Dral, D. Guldi, R. Jasti. Tunable Macrocyclic Polyparaphenylene Nanolassos via Copper-Free Click Chemistry. *Chem. Eur. J.* **2023**, *29*, e202300668

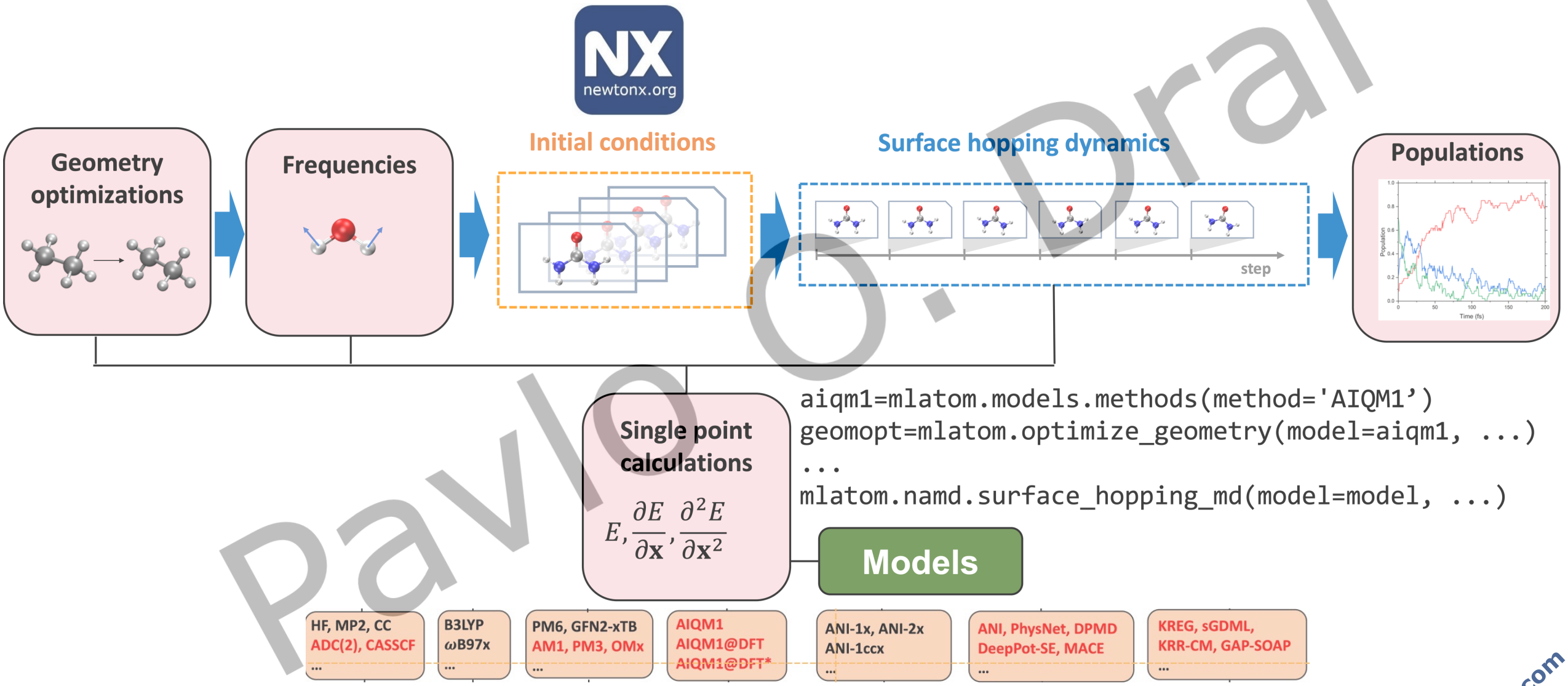
AIQM1 surface-hopping dynamics





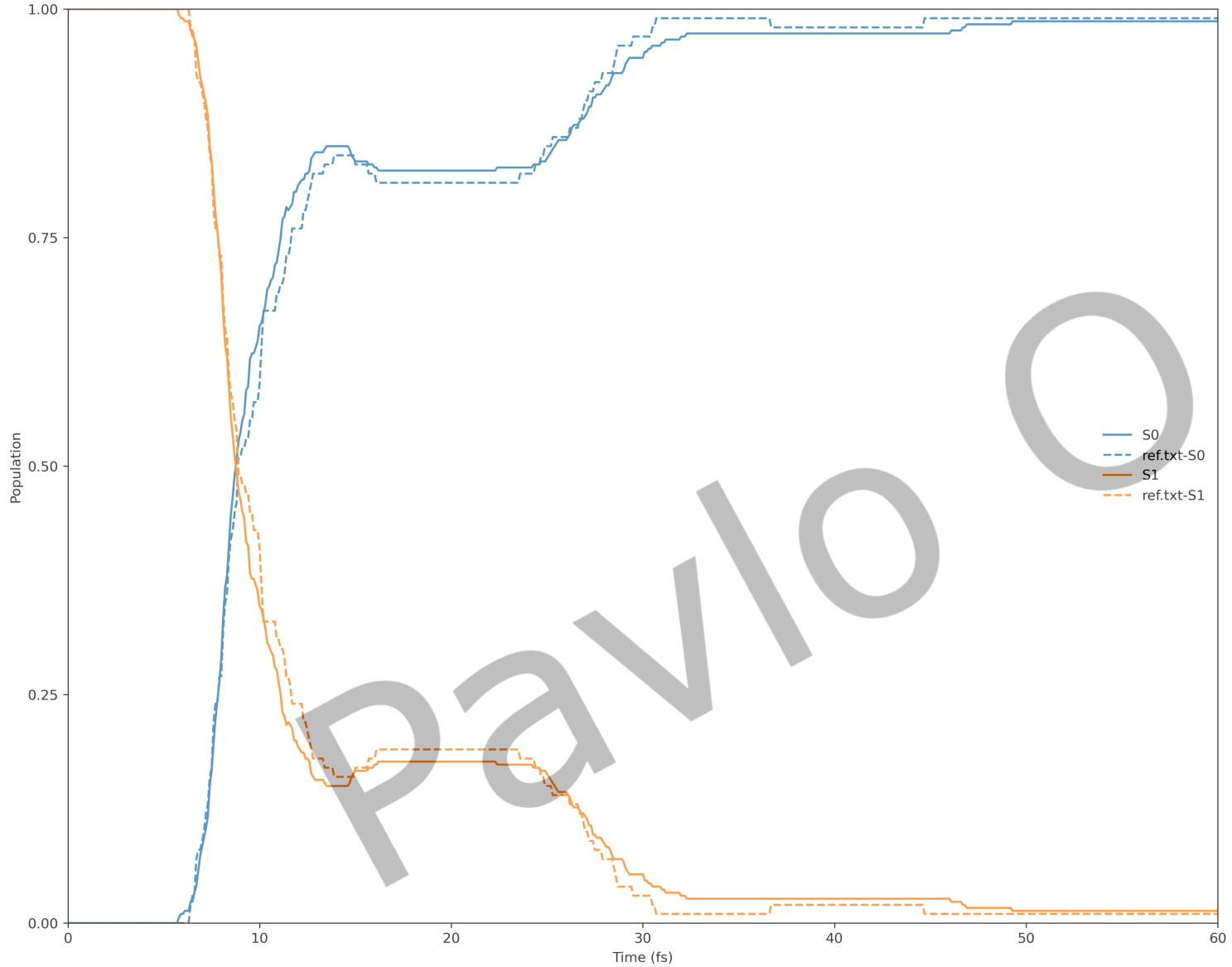
L. Zhang, M. Martyka, ..., J. Jankowska, M. Barbatti, P. O. Dral. *JCTC*, **2024**, *20*, 5043–5057

Surface-hopping dynamics

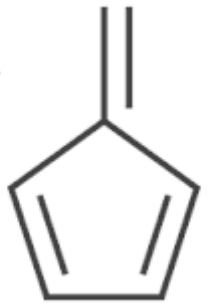


L. Zhang, M. Martyka, ..., J. Jankowska, M. Barbatti, P. O. Dral. *JCTC*, **2024**, *20*, 5043–5057

Physics-informed active learning



Fulvene



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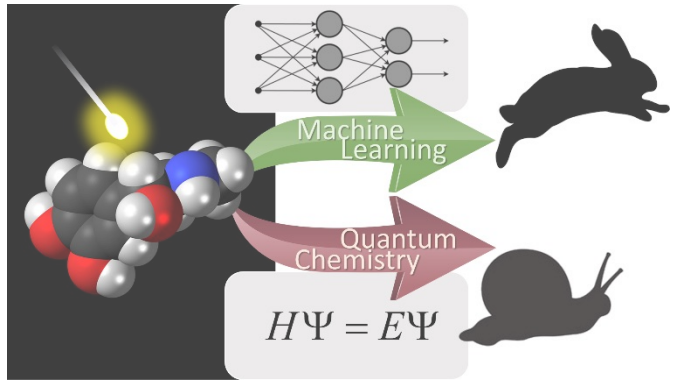
Answering your
questions in real time

M. Martyka, L. Zhang, Y.-F. Hou, M. Barbatti, P. O. Dral*, et al. *unpublished*

dr-dral.com

More and more models published faster and faster

P. O. Dral, M. Barbatti, *Nat. Rev. Chem.* **2021,** *5*, 388



Timing

Ab initio ML-ab initio

DFT ML-DFT DM21, CF22D, DENS24…

Semi-empirical ML-SQC AIQM1

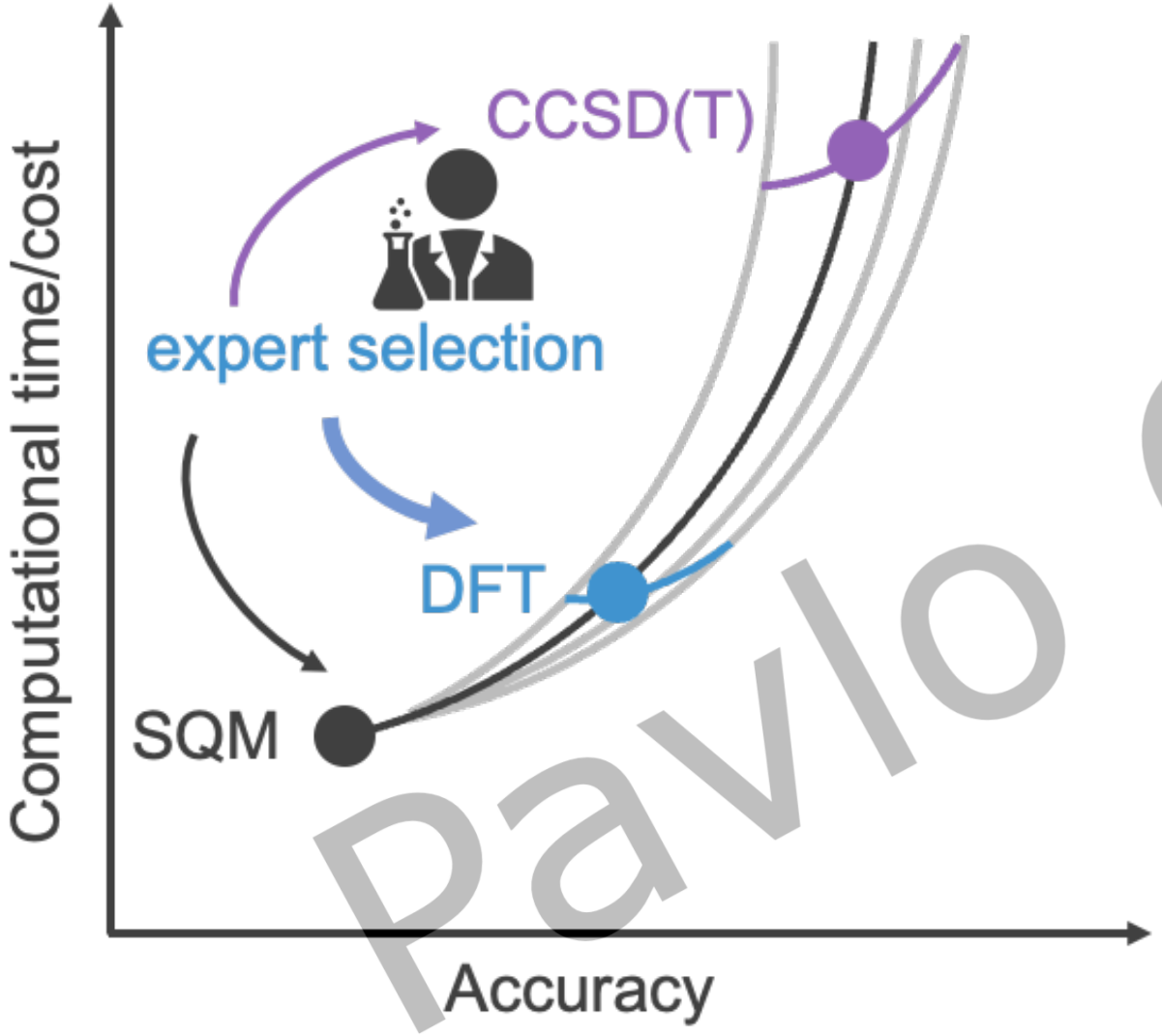
Machine Learning ANI-1ccx, AIMnet-2, ANI-1xnr, …

Molecular Mechanics

Accuracy

Figure: P. O. Dral, *J. Phys. Chem. Lett.* **2020**, *11*, 2336

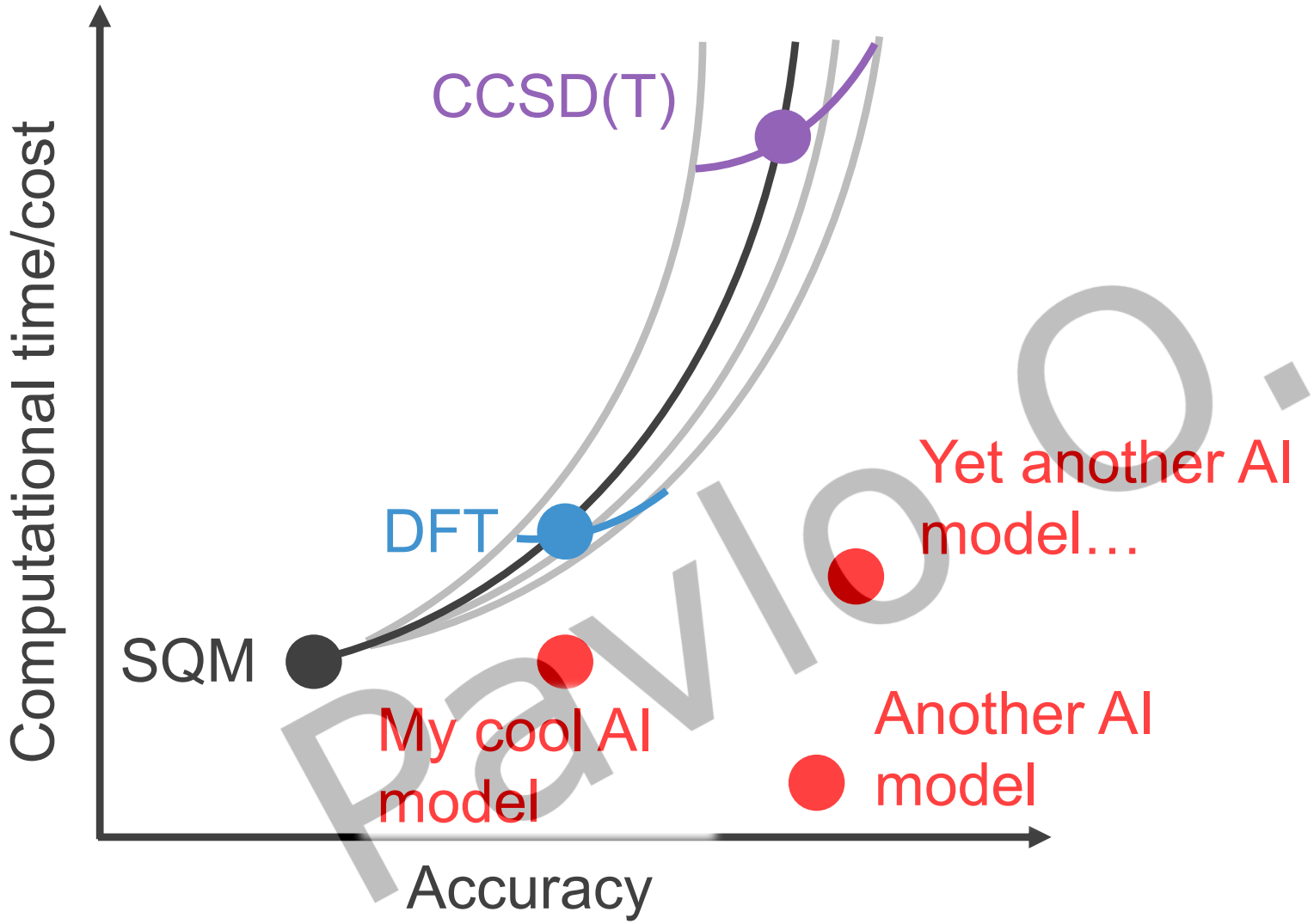
UAIQM: Universal and Updatable AI-QM models



We can use human expertise to select models

Y. Chen, Y.-F. Hou, O. Isayev, P. O. Dral. *Universal and Updatable Artificial Intelligence-Enhanced Quantum Chemical Foundational Models*. **2024**, *submitted*. https://doi.org/10.26434/chemrxiv-2024-604wb.

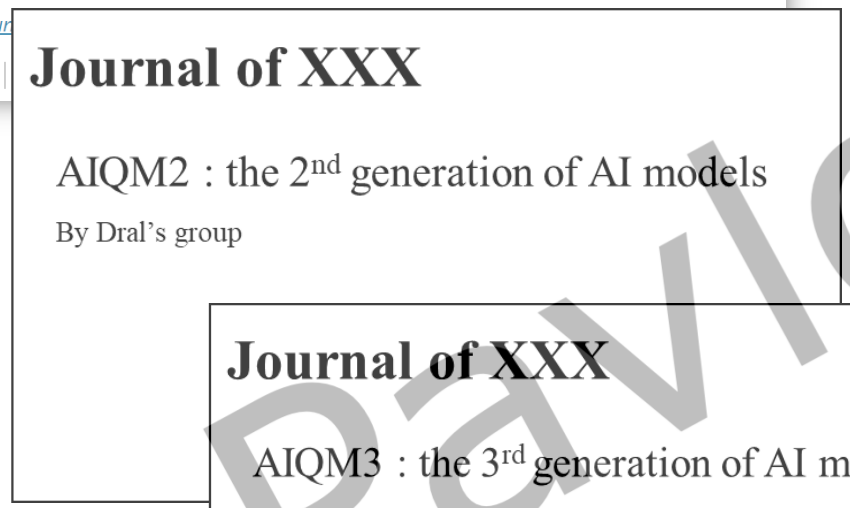
UAIQM: Universal and Updatable AI-QM models

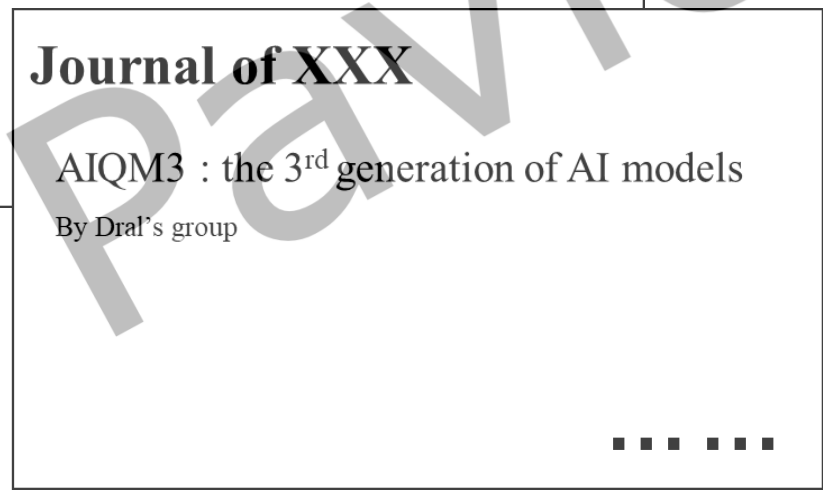


Try to create better models…

Y. Chen, Y.-F. Hou, O. Isayev, P. O. Dral. *Universal and Updatable Artificial Intelligence-Enhanced Quantum Chemical Foundational Models*. **2024**, *submitted*. https://doi.org/10.26434/chemrxiv-2024-604wb.

UAIQM: Universal and Updatable AI-QM models

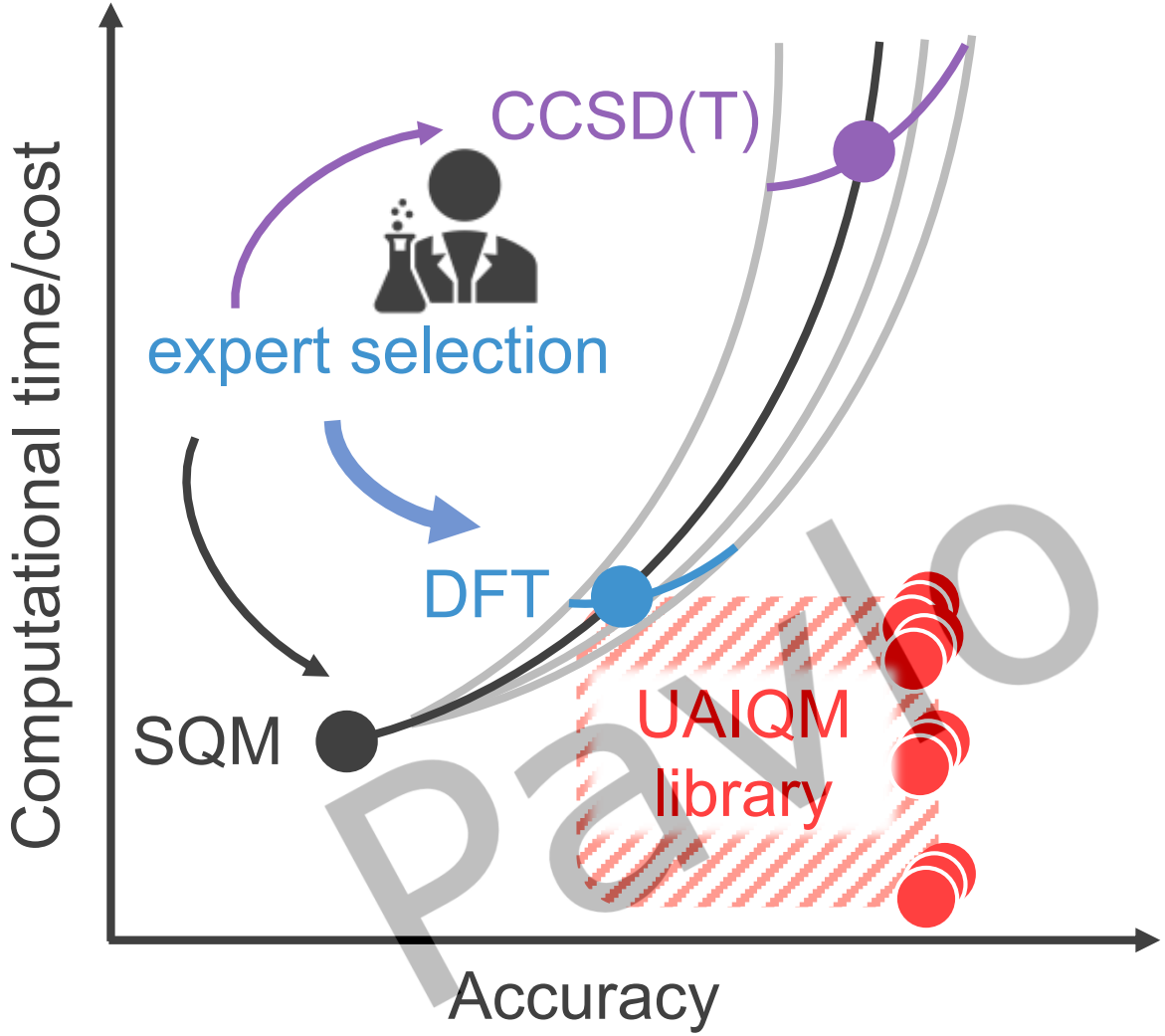




Reviewers 😐

* We might end up doing this...

UAIQM: Universal and Updatable AI-QM models

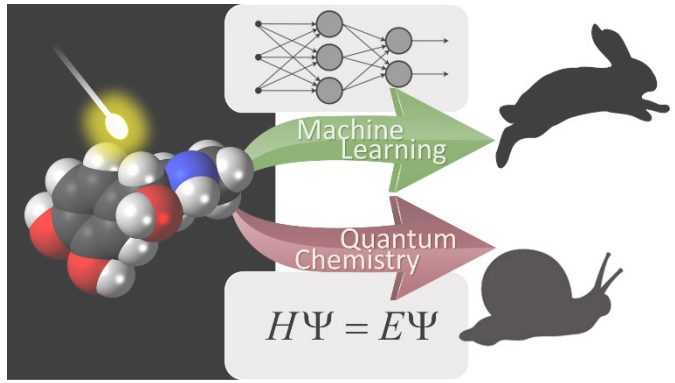


We put them together in a library and just give new models version numbers!

Y. Chen, Y.-F. Hou, O. Isayev, P. O. Dral. *Universal and Updatable Artificial Intelligence-Enhanced Quantum Chemical Foundational Models*. **2024**, *submitted*. https://doi.org/10.26434/chemrxiv-2024-604wb.

Can we do better?

P. O. Dral, M. Barbatti, *Nat. Rev. Chem.* **2021,** *5*, 388



Every model
(DFT or AI …)
has some problems!

Ab initio ML-ab initio

DFT ML-DFT DM21, CF22D, DENS24…

Semi-empirical ML-SQC AIQM1

Machine Learning ANI-1ccx, AIMnet-2, ANI-1xnr, …

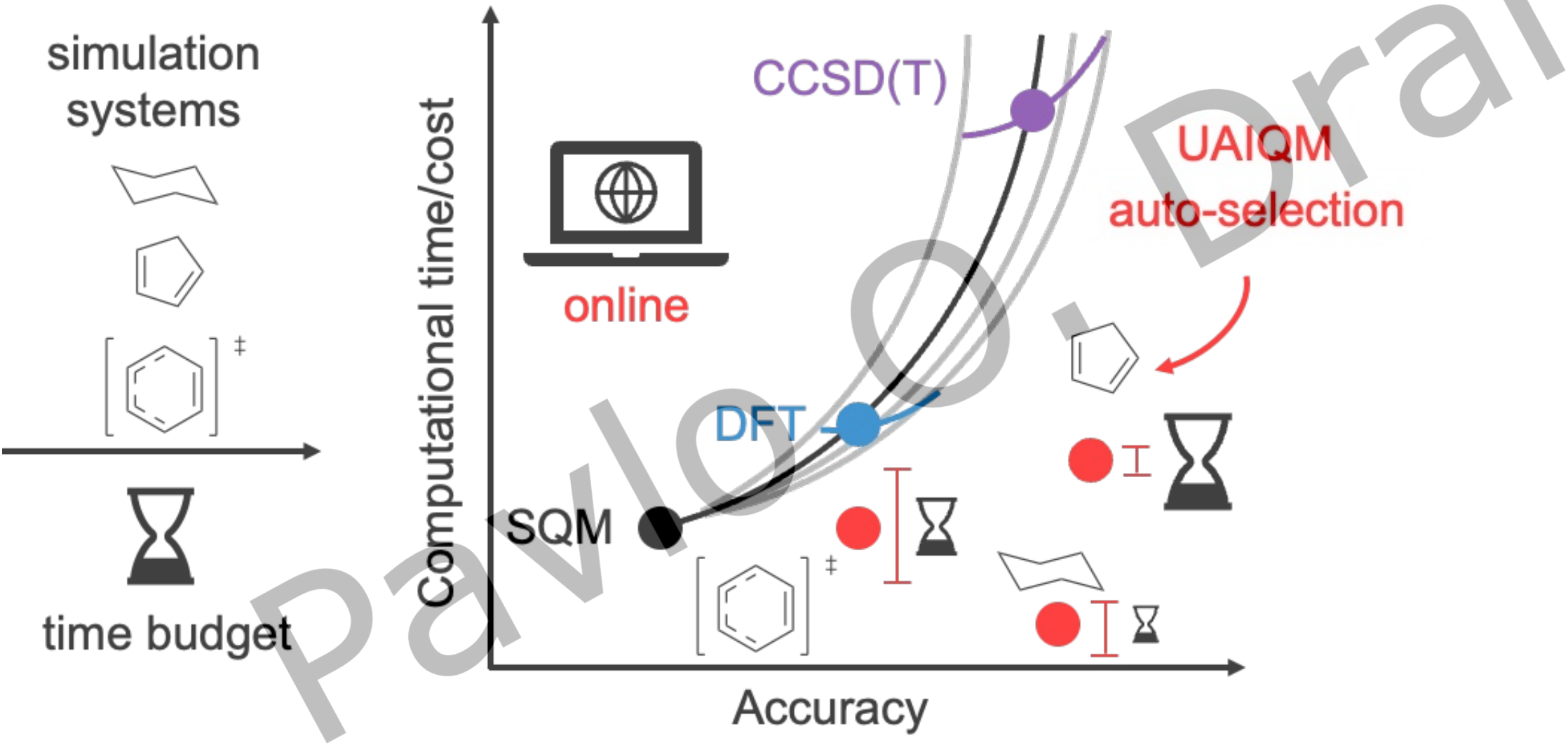
Molecular Mechanics

Timing

Accuracy

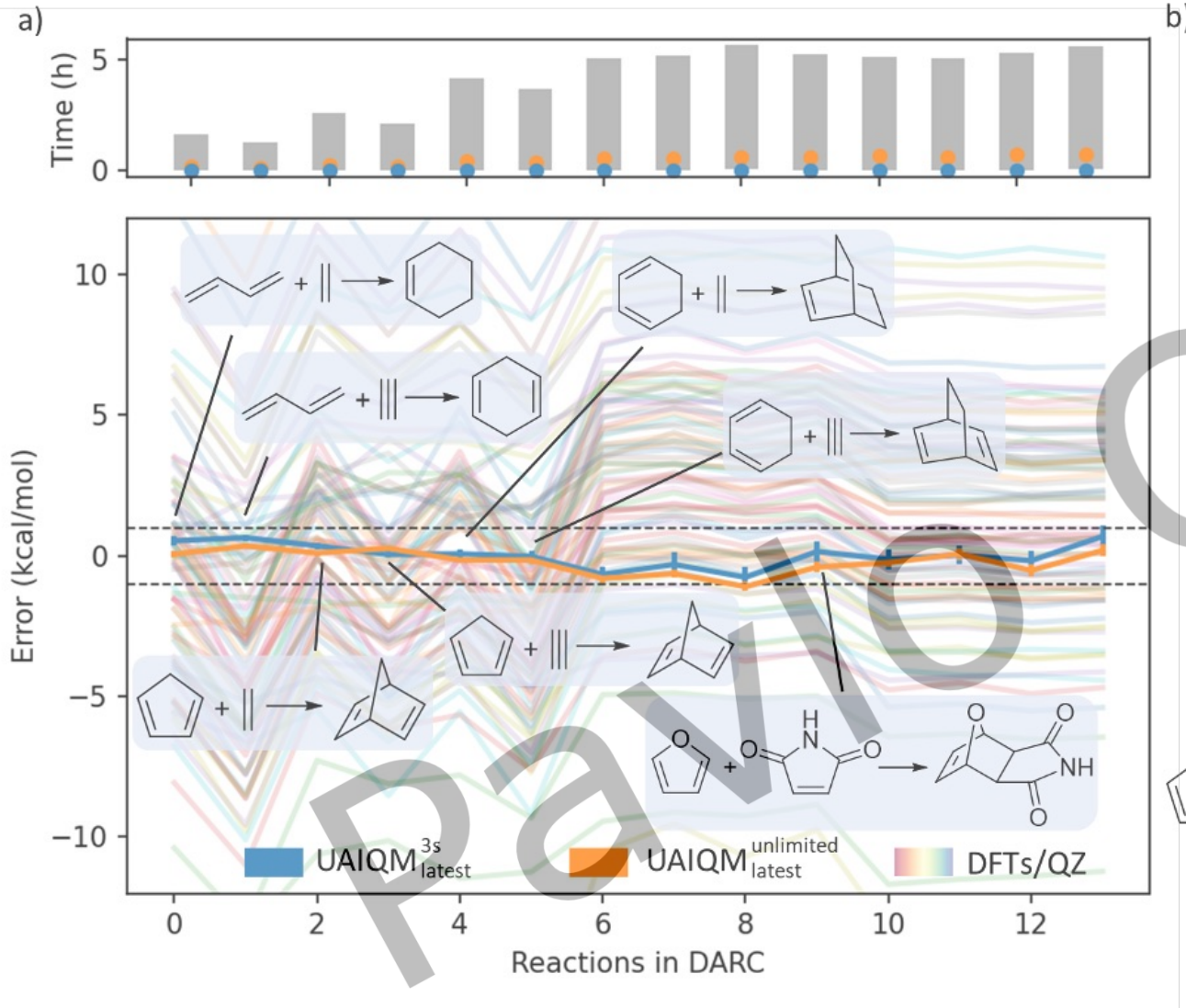
Figure: P. O. Dral, *J. Phys. Chem. Lett.* **2020**, *11*, 2336

UAIQM: Universal and Updatable AI-QM models



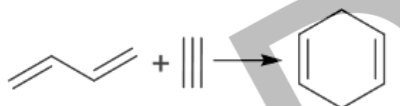
Y. Chen, Y.-F. Hou, O. Isayev, P. O. Dral. *Universal and Updatable Artificial Intelligence-Enhanced Quantum Chemical Foundational Models*. **2024**, *submitted*. https://doi.org/10.26434/chemrxiv-2024-604wb.

UAIQM: Universal and Updatable AI-QM models

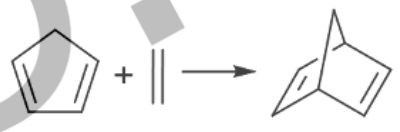


b)

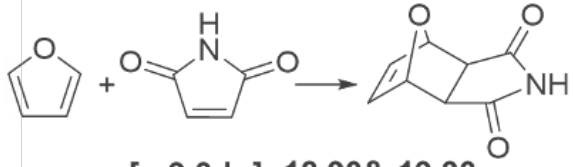
W1-F12 & CCSD(T)/CBS
DSD-BLYP-D3(BJ)/def2-QZVP
UAIQM (unlimited)
UAIQM (3 s time budget)



[~3.5 h] -60.80&-60.45
[~1.0 h] -59.67
[~0.1 h] -60.16±0.11
[~0.1 s] -60.44±0.10



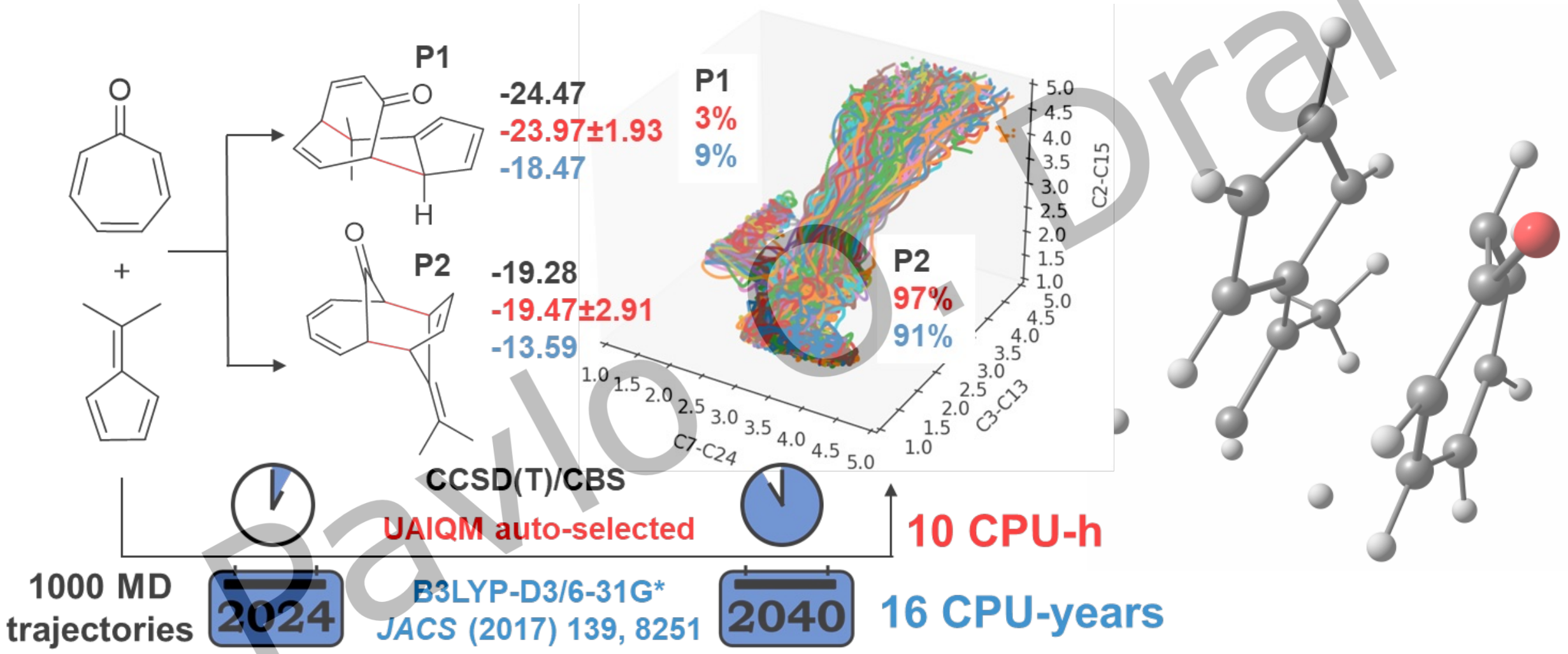
[~4.5 h] -29.9&-29.69
[~2.5 h] -27.93
[~0.3 h] -29.81±0.09
[~0.1 s] -29.55±0.13



[~9.0 h] -18.90&-19.30
[~5.0 h] -15.18
[~0.6 h] -19.31±0.19
[~0.1 s] -18.75±0.37

Y. Chen, Y.-F. Hou, O. Isayev, P. O. Dral. *Universal and Updatable Artificial Intelligence-Enhanced Quantum Chemical Foundational Models*. **2024**, *submitted*. https://doi.org/10.26434/chemrxiv-2024-604wb.

UAIQM: Universal and Updatable AI-QM models



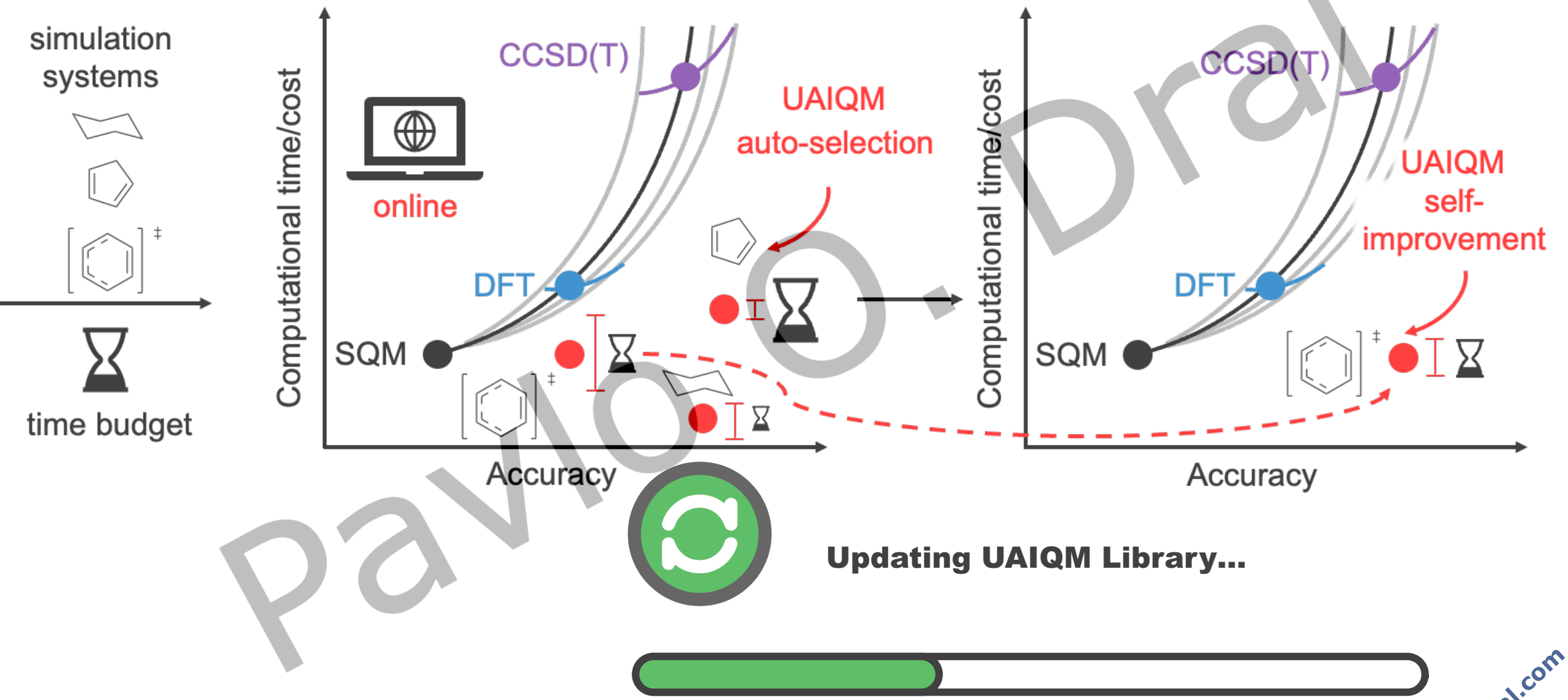
Y. Chen, Y.-F. Hou, O. Isayev, P. O. Dral. *Universal and Updatable Artificial Intelligence-Enhanced Quantum Chemical Foundational Models*. **2024**, *submitted*. https://doi.org/10.26434/chemrxiv-2024-604wb.

UAIQM: Universal and Updatable AI-QM models

```
================================================================================
WARNING: Uncertainty is too high for selected UAIQM method



Properties of molecule 1

Selected UAIQM method: uaiqm_gfn2xtbstar@cc
Selected version: 20240106

Standard deviation of ML contribution    :      0.00546625 Hartree      3.43012 kcal/mol
Baseline contribution                    :     -2.73848388 Hartree
NN contribution                          :     -0.27210359 Hartree
D4 contribution                          :     -0.00007046 Hartree
Total energy                             :     -3.01065793 Hartree

================================================================================
```

Y. Chen, Y.-F. Hou, O. Isayev, P. O. Dral. *Universal and Updatable Artificial Intelligence-Enhanced Quantum Chemical Foundational Models*. **2024**, *submitted*. https://doi.org/10.26434/chemrxiv-2024-604wb.

UAIQM: Universal and Updatable AI-QM models



Y. Chen, Y.-F. Hou, O. Isayev, P. O. Dral. *Universal and Updatable Artificial Intelligence-Enhanced Quantum Chemical Foundational Models*. **2024**, *submitted*. https://doi.org/10.26434/chemrxiv-2024-604wb.

XACS
Xiamen Atomistic Computing Suite
XACScloud.com

MLatom.com

XACS平台介绍(II)：基于XACS平台的计算化学（使用MLatom进行几何构型优化）

Pavlo O. Dral

Xiamen University, P.R. China

Visiting Professor in
Nicolaus Copernicus University, Poland

2 July 2024

CONTENTS:

```
B3LYP/6-31G*
geomopt
xyzfile='5
```

number of atoms

blank line

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C          0.0000000000        0.0000000000        0.0000000000
H          1.0870000000        0.0000000000        0.0000000000
H         -0
H         -0
H         -0
'
```

```
B3LYP/6-31G*
geomopt
xyzfile='5

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H          1.0870000000        0.0000000000        0.0000000000
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H         -0.3623333220        0.5124167161       -0.8875317869
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2

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H 0 0 0.7
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geomopt
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geomopt
xyz
```

```
GFN2-xTB
geomopt
xyz
```

```
MP2/cc-pVDZ
geomopt
xyzfi
```

```
ANI-1ccx
geomopt
xyzfile='5
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geomopt
xyz
```

```
UAIQM
geomopt
xyzfile='5

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H          1.0870000000          0.0000000000          0.0000000000
H         -0.3623333220         -1.0248334322         -0.0000000000
H         -0.3623333220          0.5124167161         -0.8875317869
H         -0.3623333220          0.5124167161          0.8875317869
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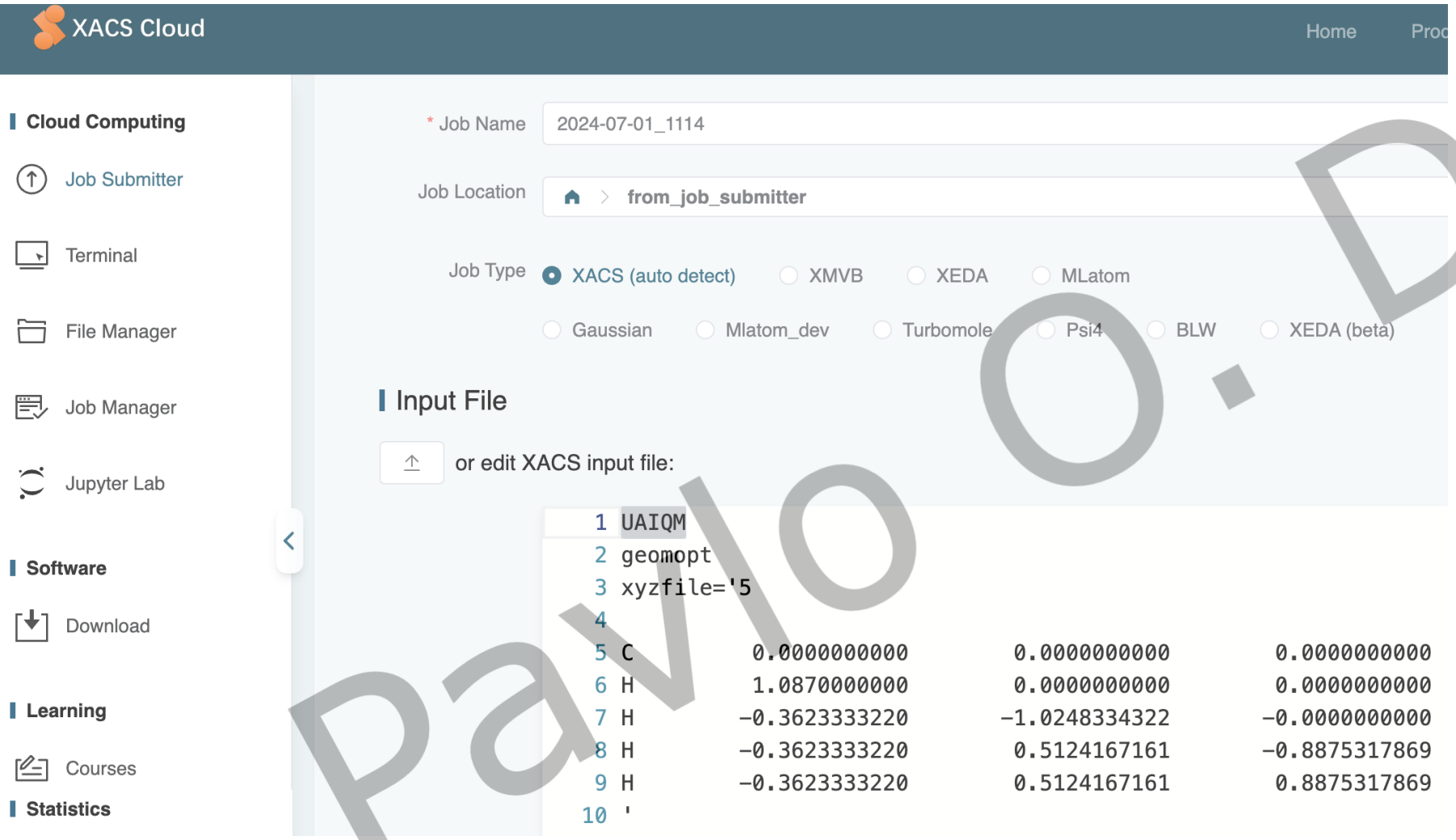
XACS Cloud
Home
Proc
Cloud Computing
Job Submitter
Terminal
File Manager
Job Manager
Jupyter Lab
Software
Download
Learning
Courses
Statistics
* Job Name
2024-07-01_1114
Job Location
from_job_submitter
Job Type
XACS (auto detect)
XMVB
XEDA
MLatom
Gaussian
Mlatom_dev
Turbomole
Psi4
BLW
XEDA (beta)
Input File
or edit XACS input file:
1 UAIQM
2 geomopt
3 xyzfile='5
4
5 C 0.0000000000 0.0000000000 0.0000000000
6 H 1.0870000000 0.0000000000 0.0000000000
7 H -0.3623333220 -1.0248334322 -0.0000000000
8 H -0.3623333220 0.5124167161 -0.8875317869
9 H -0.3623333220 0.5124167161 0.8875317869
10 '
Submit

Job Name | input search content | Submission Time: 2024-04-01 - 2024-07-01 | all state

Auto Refresh: On

Job Name	Id	CPU cores	Node	Partition	Submission time	Start time	State	Action
2024-07-01_1849	1724581	8	w009	6226r	2024-07-01 18:49:54	2024-07-01 18:49:55	RUNNING	

Job Name | input search content | Submission Time: 2024-04-01 - 2024-07-01 | all state

Auto Refresh: On

Job Name	Id	CPU cores	Node	Partition	Submission time	Start time	State	Action
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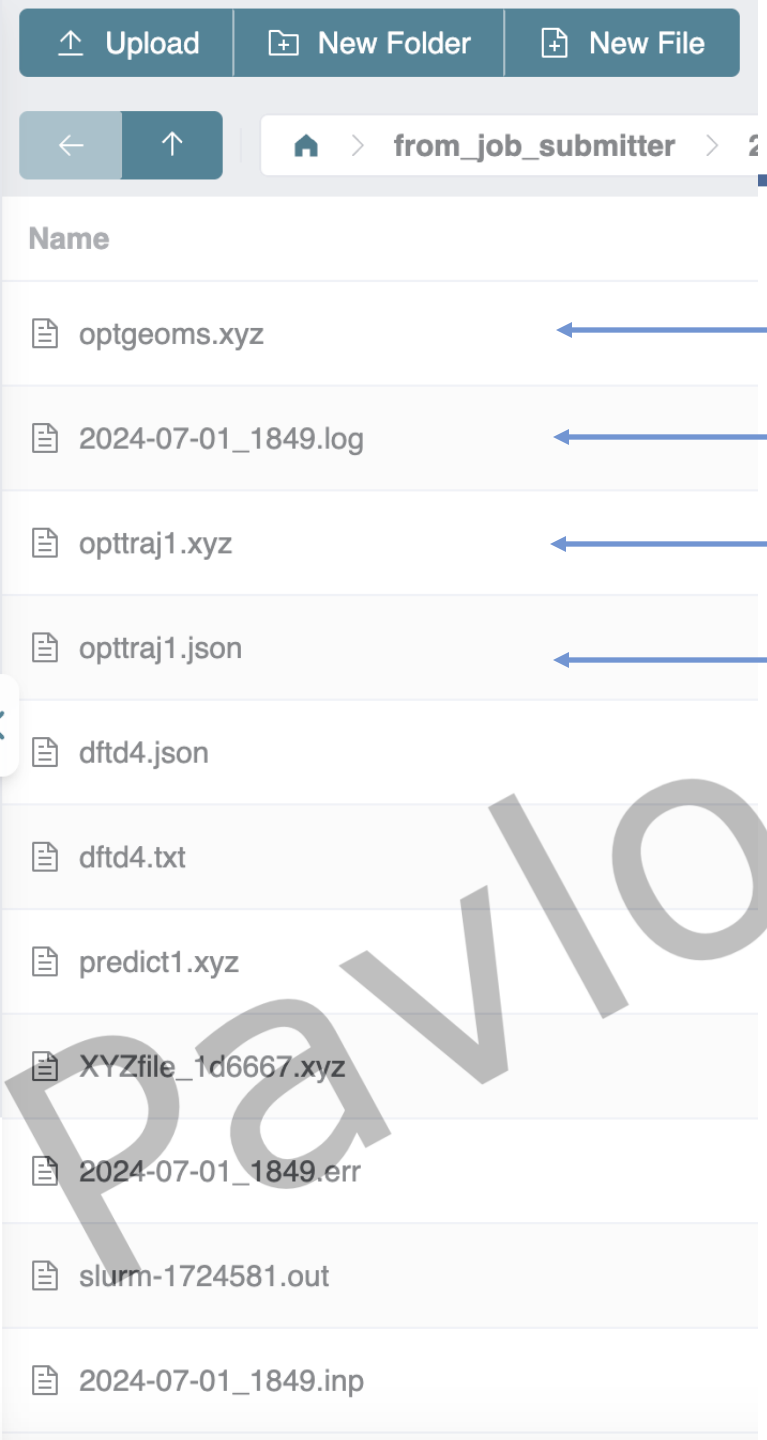

file with optimized geometries

output file

optimization trajectory in xyz format

optimization trajectory in json format

```
Energy gradients norm:              0.000005 Hartree/Angstrom



  Iteration          Energy (Hartree)
      |      1            -40.4648603269632
      |      2            -40.4648603825890


Final properties of molecule 1

Selected UAIQM method: uaiqm_gfn2xtbstar@cc
Selected version: 20240106

Standard deviation of ML contribution    :      0.00009751 Hartree          0.06119 kcal/mol
Baseline contribution                    :     -4.17449301 Hartree
NN contribution                          :    -36.29026544 Hartree
D4 contribution                          :     -0.00010194 Hartree
Total energy                             :    -40.46486038 Hartree
```