

Universal ML models

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4 July 2024

2. Computing of F_2
3. Resonance in C_6H_6
4. Computing of O_2
5. Computing of post-VBSCF methods
6. Computing of diabatic states with VB theory
7. Menshutkin Reaction $NH_3 + CH_3Cl \rightarrow [NH_3CH_3]^+ + Cl^-$
8. Charge-shift bonding in propellane

MACHINE LEARNING

1. Machine learning basics
2. ML for PES
3. Universal machine learning models
 - 3.1. What are the universal ML models?
 - 3.2. Frequencies and thermochemistry
 - 3.3. Uncertainty quantification
 - 3.4. Qualitative problems with PES shape
4. Spectroscopy

[Home](#) / 3. Universal machine learning models

3. Universal machine learning models

- What are the universal ML models?
- Frequencies and thermochemistry
- Uncertainty quantification

3.1. What are the universal ML models?

Computational cost

SQM

DFT (N^3)

CCSD(T) (N^7)

DM21

MLatom 3: A Platform for Mac Computational Chemistry Simulations

MLATOM@XACS FOR AI-ENHANCED COMPUTATIONAL CHEMISTRY

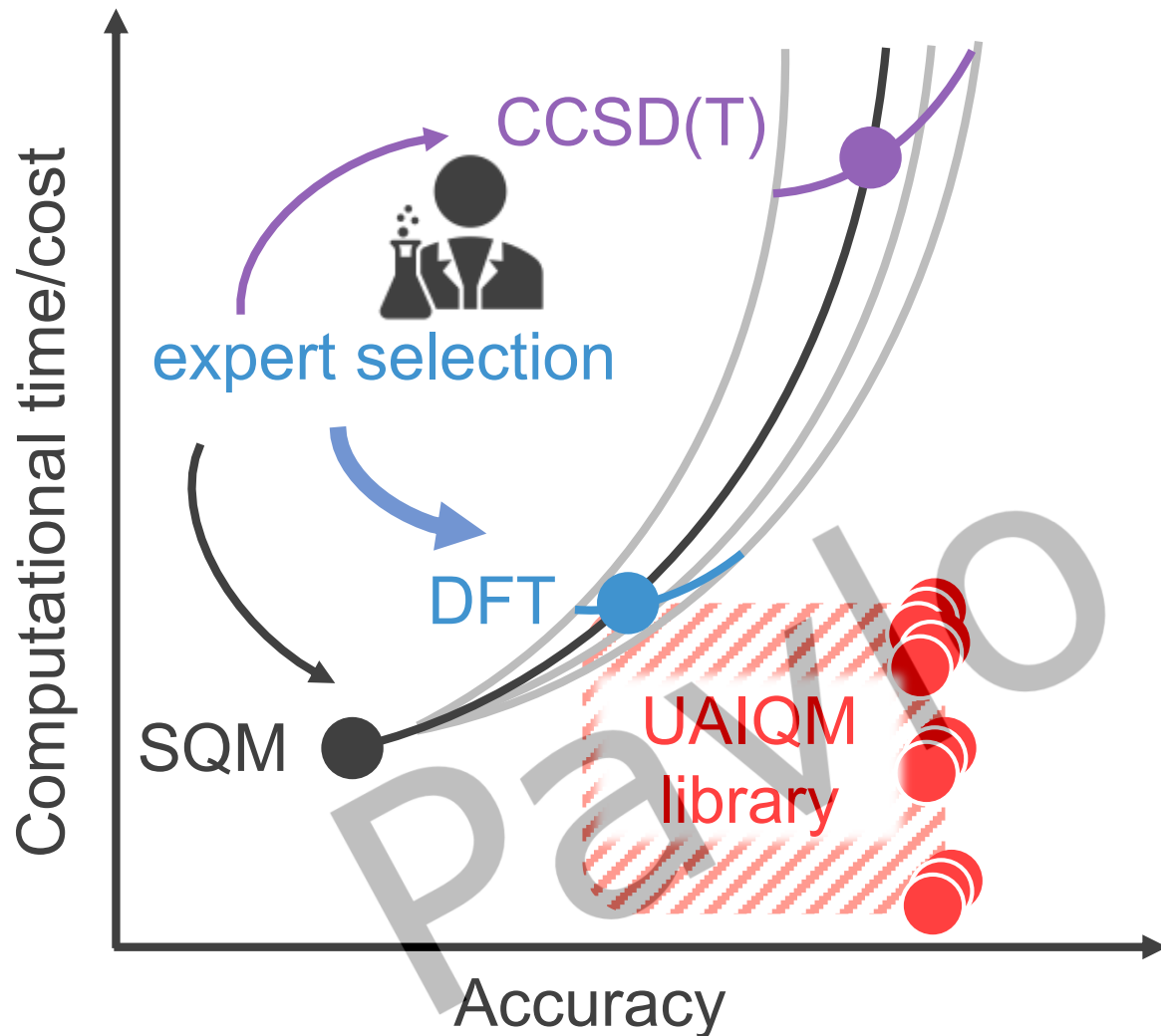
Density Functional Theory (DFT)

00:31

21:38

01:55

00:28



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

Can we do better?

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

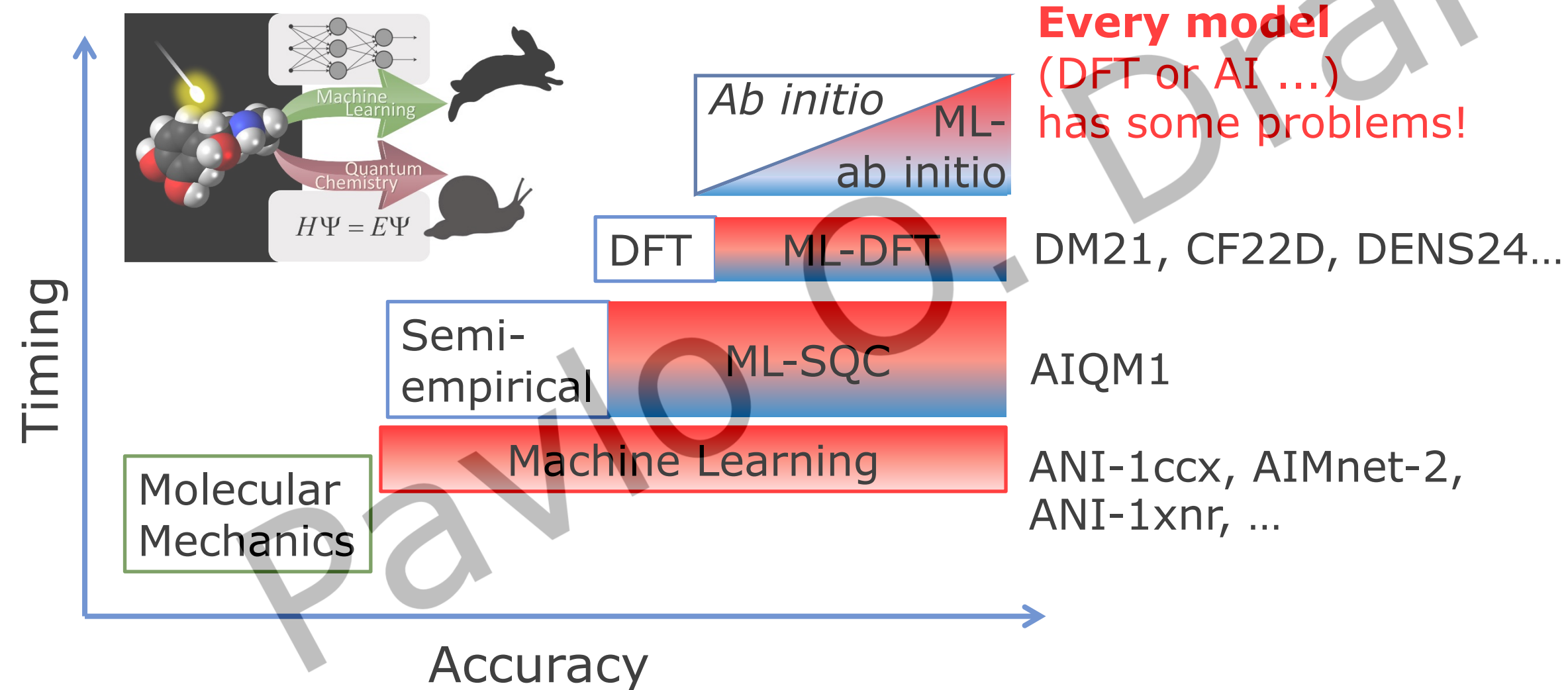
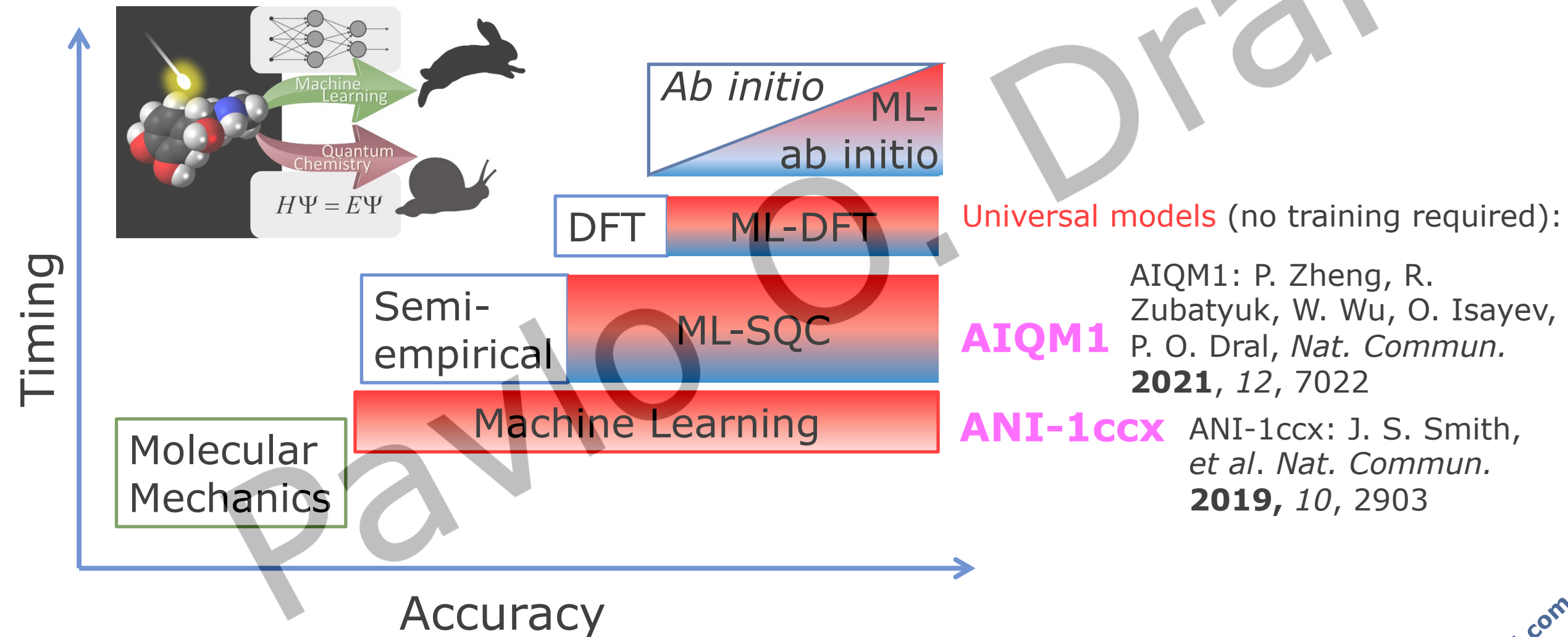
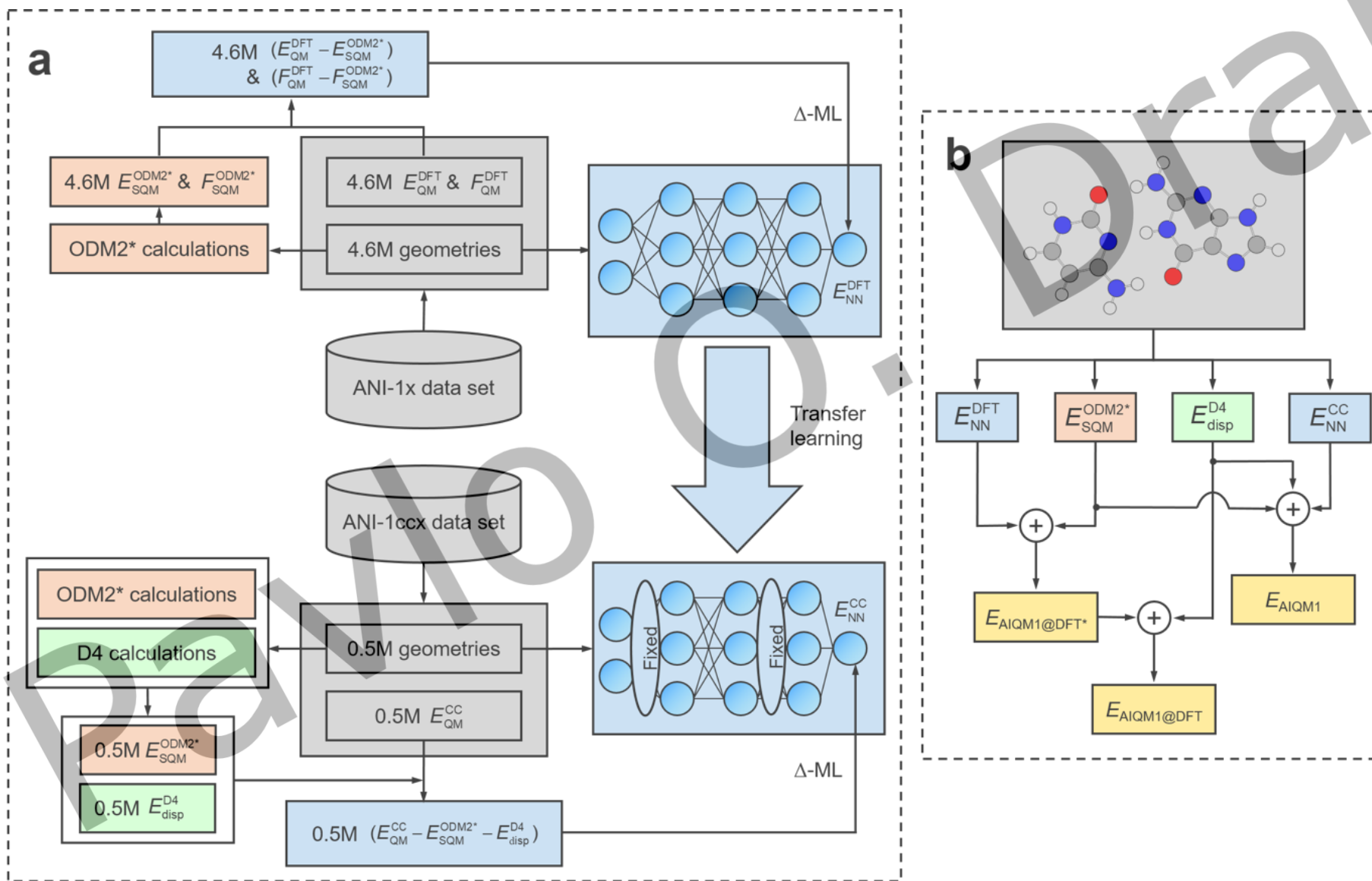


Figure: P. O. Dral, *J. Phys. Chem. Lett.* **2020**, 11, 2336

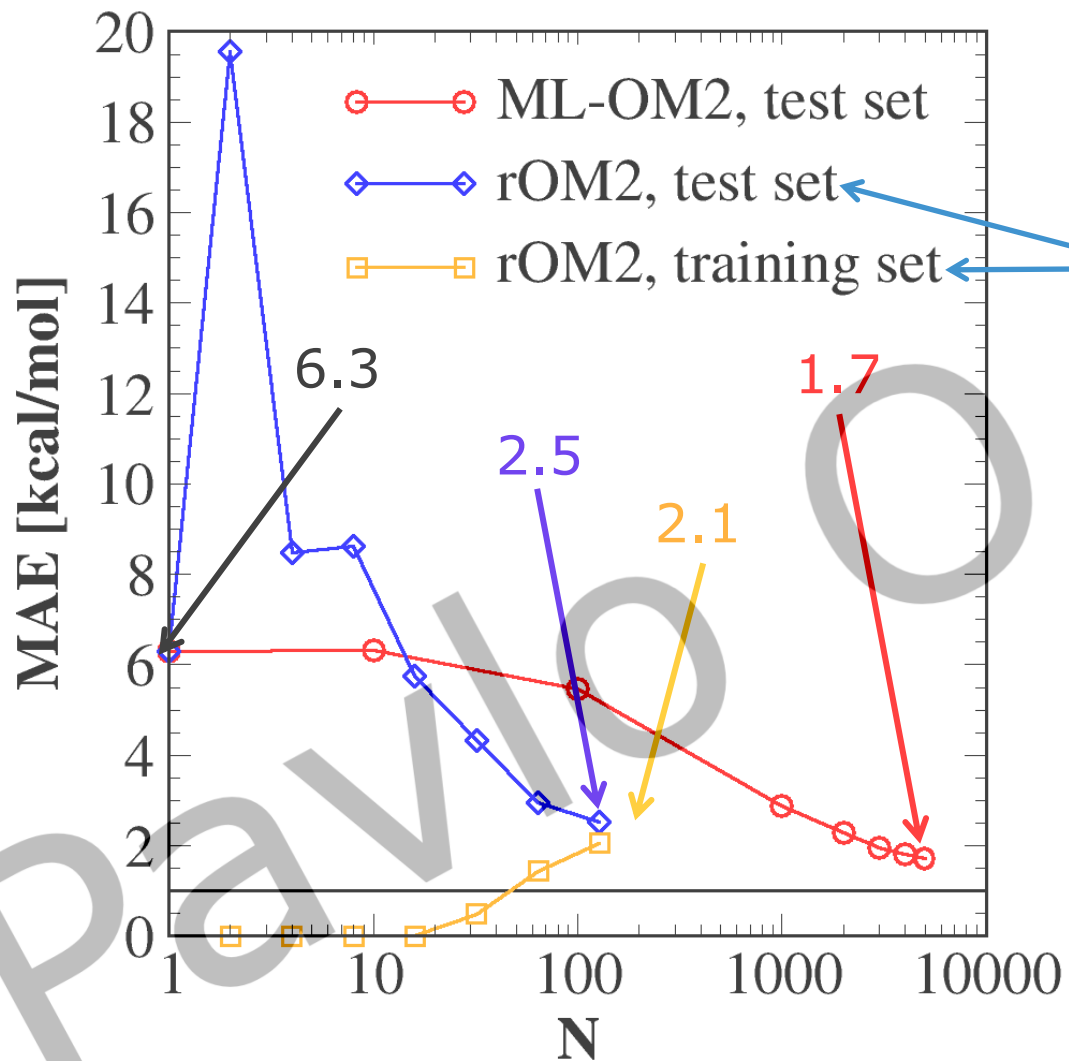
P. O. Dral, M. Barbatti, *Nat. Rev. Chem.* **2021**, 5, 388



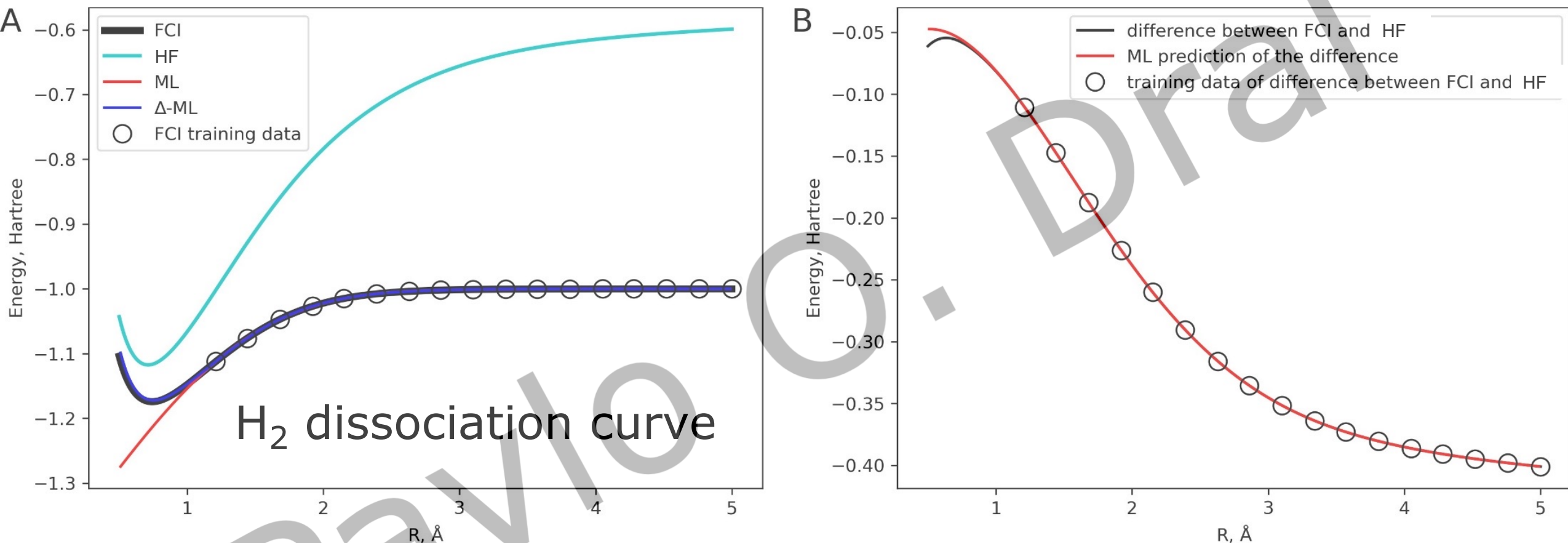
Perspective: P. O. Dral, *J. Phys. Chem. Lett.* **2020**, 11, 2336



Improving Hamiltonian



Traditional reparametrization (molecule-specific orbital exponents in the basis set)



Δ -learning: R. Ramakrishnan, P. O. Dral, M. Rupp, O. A. von Lilienfeld,
J. Chem. Theory Comput. **2015**, *11*, 2087

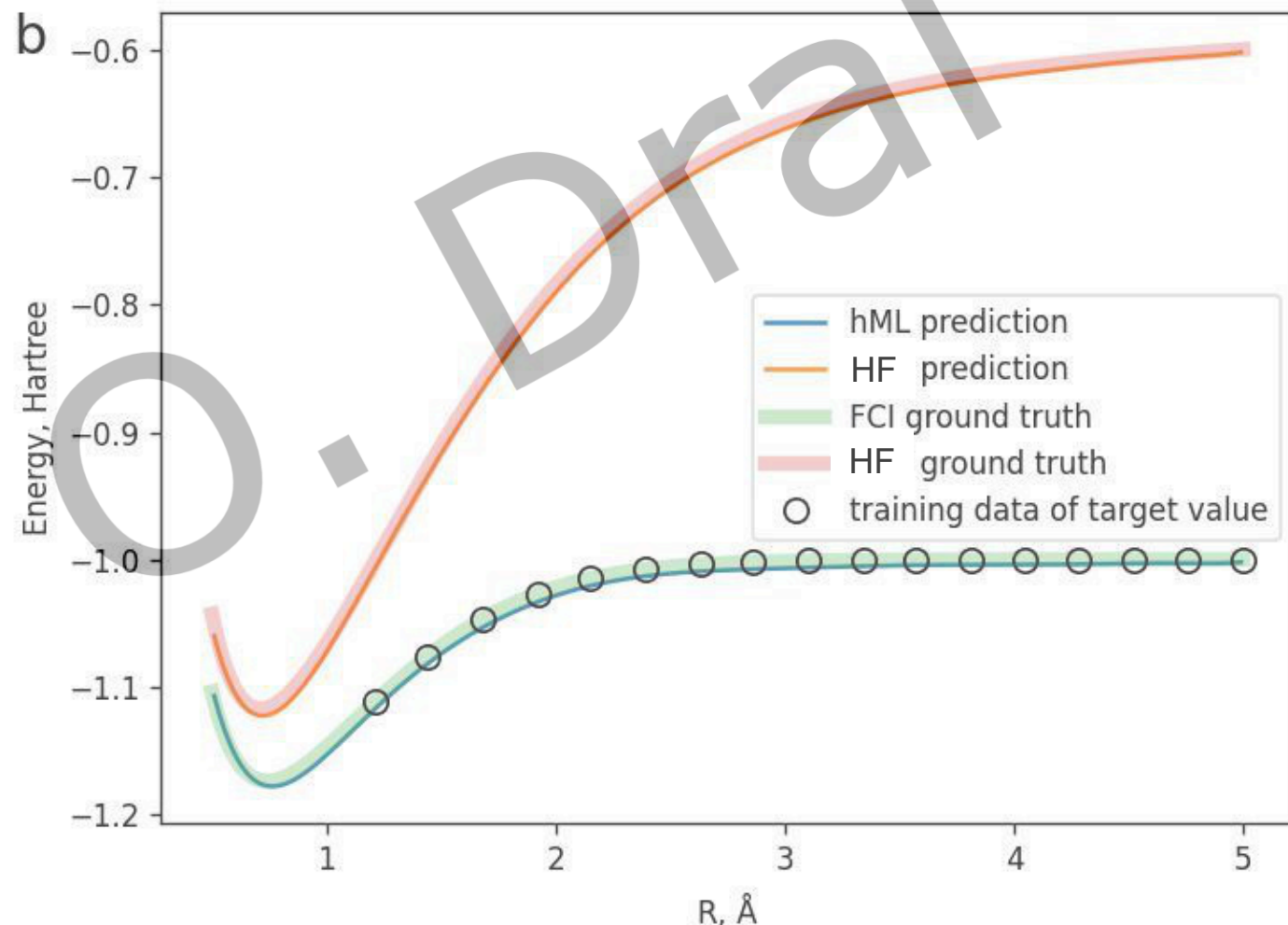
Figure: Pavlo O. Dral, Tetiana Zubatiuk, Bao-Xin Xue, Learning from multiple quantum chemical methods: Δ -learning, transfer learning, co-kriging, and beyond. In *Quantum Chemistry in the Age of Machine Learning*, Pavlo O. Dral, Ed. Elsevier: **2023**. Paperback ISBN: 9780323900492

Automatic procedure to find optimal training points for each delta-model

$$\hat{y}_{\Sigma,i} = \sum_M \hat{y}_{M,i}(N_{\text{tr},M})$$

hML for H_2

$$\text{hML} = \Delta_0^{\text{HF}} + \Delta_{\text{HF}}^{\text{FCI}}$$



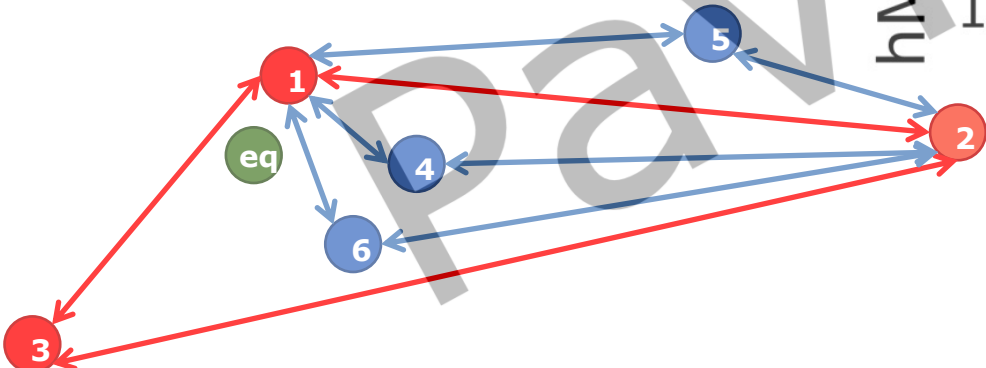
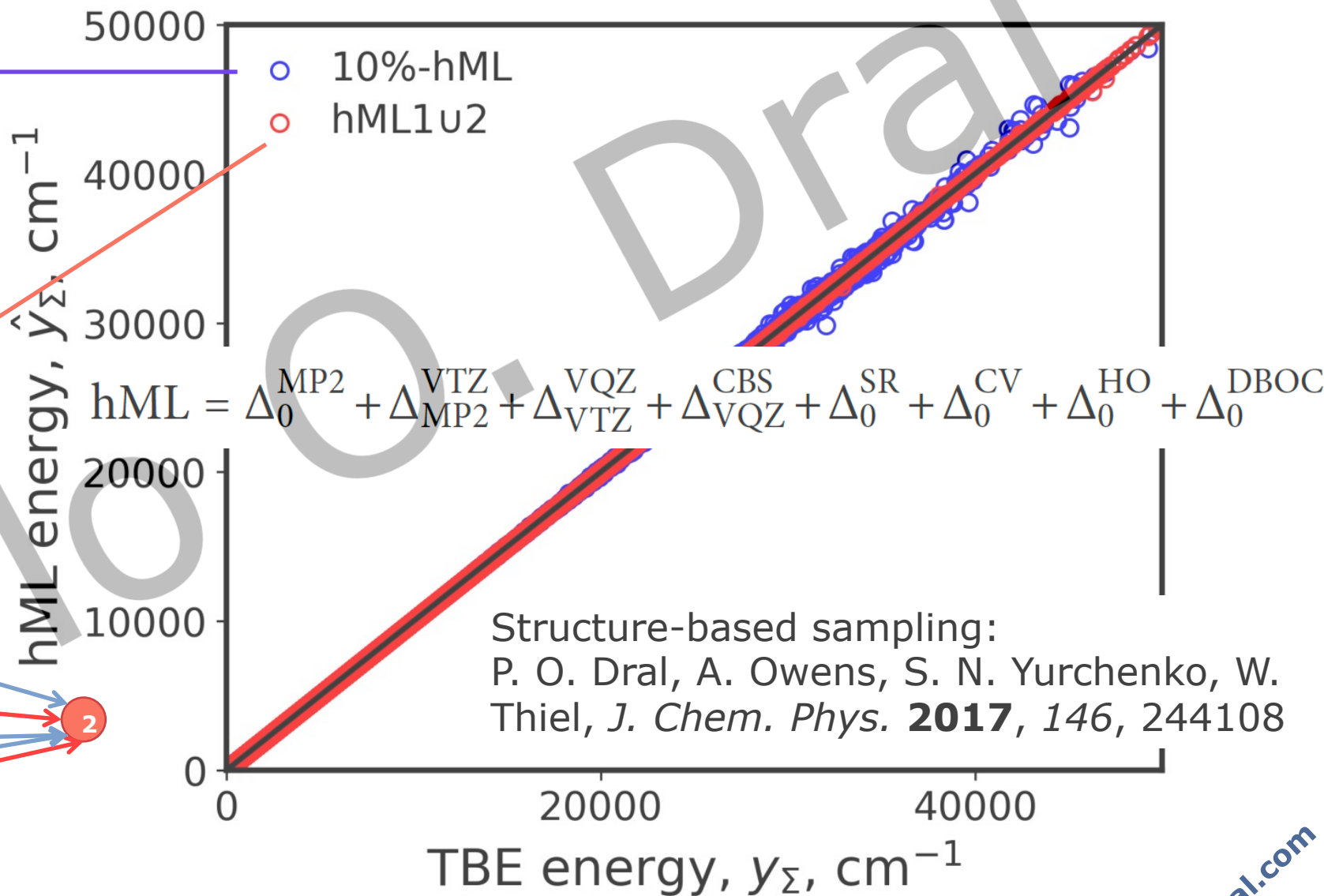
Hierarchical ML: P. O. Dral, A. Owens, A. Dral, G. Csányi, *J. Chem. Phys.* **2020**, *152*, 204110

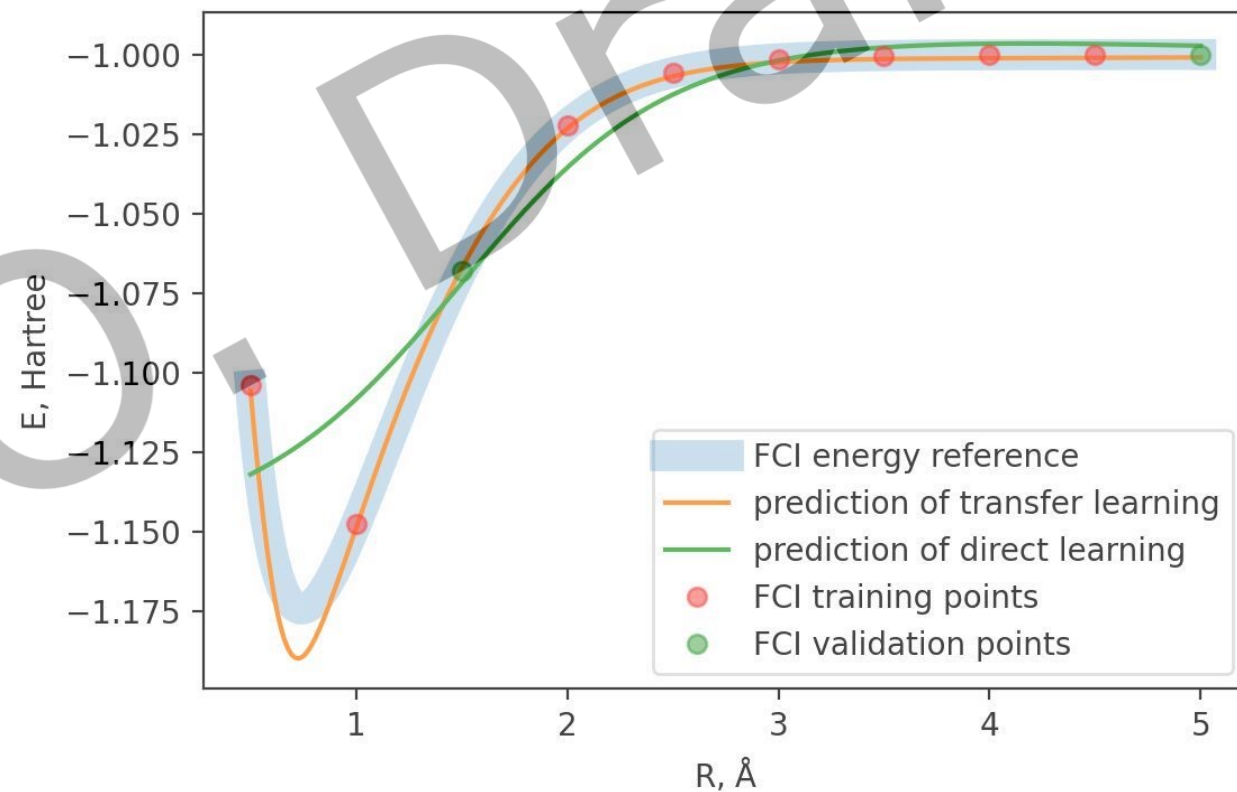
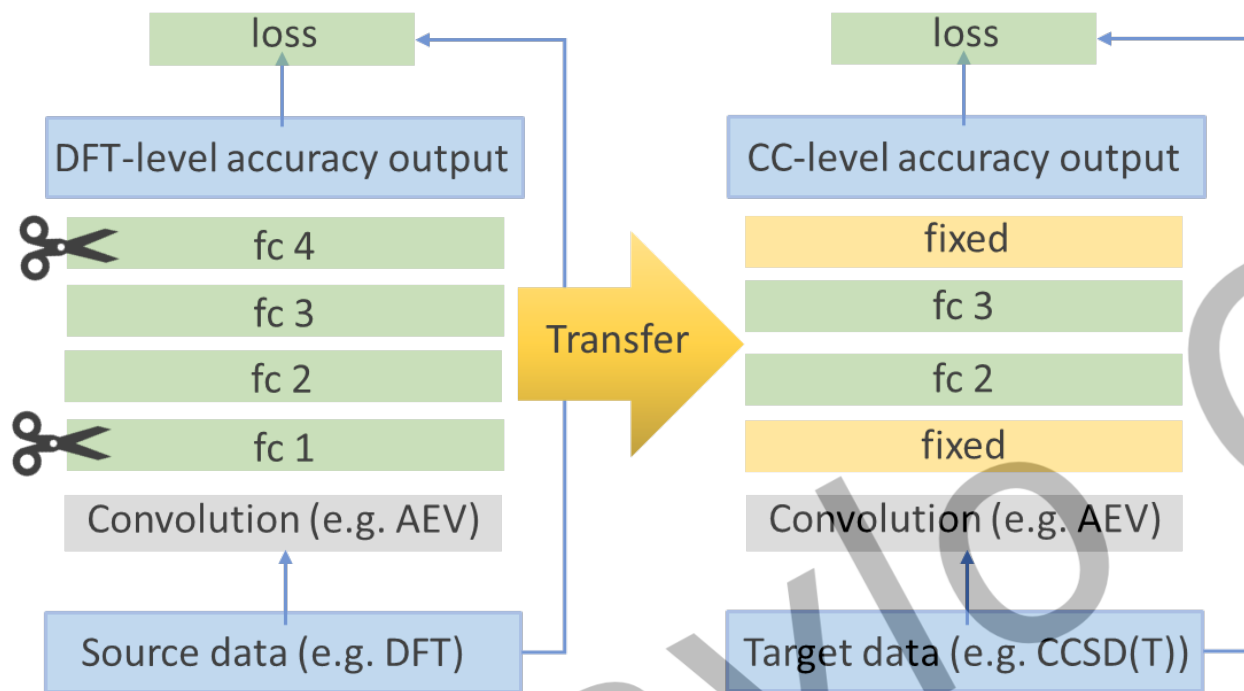
Figure: Pavlo O. Dral, Tetiana Zubatiuk, Bao-Xin Xue, Learning from multiple quantum chemical methods: Δ -learning, transfer learning, co-kriging, and beyond. In *Quantum Chemistry in the Age of Machine Learning*, Pavlo O. Dral, Ed. Elsevier: **2023**. Paperback ISBN: 9780323900492

Pure ML-model trained on **saved 90% of CPU-time**

Weighted RMSE:
 $3.49 \text{ cm}^{-1} = 0.01 \text{ kcal/mol}$

Δ -ML models:
saved 99% of CPU-time
Weighted RMSE:
 $1.12 \text{ cm}^{-1} = 0.003 \text{ kcal/mol}$

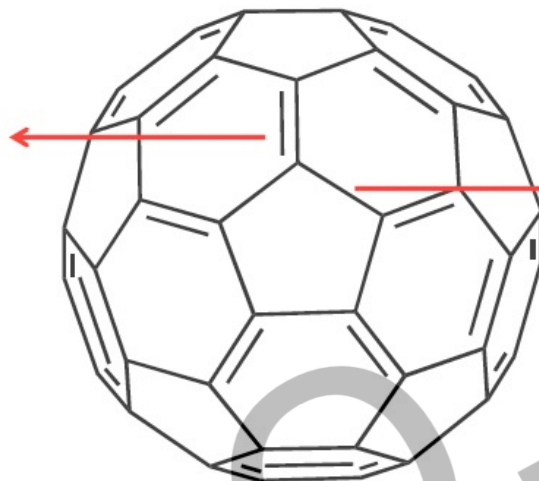




Figures: Pavlo O. Dral, Tetiana Zubatiuk, Bao-Xin Xue, Learning from multiple quantum chemical methods: Δ -learning, transfer learning, co-kriging, and beyond. In *Quantum Chemistry in the Age of Machine Learning*, Pavlo O. Dral, Ed. Elsevier: **2023**. Paperback ISBN: 9780323900492

a

1.355–1.401 (experiment)
1.393 (AIQM1)
1.388 (AIQM1@DFT(*))
1.379 (ω B97X(-D4)/
def2-TZVPP)
1.451 (ANI-1ccx)



1.432–1.467 (experiment)
1.467 (AIQM1)
1.464 (AIQM1@DFT(*))
1.448 (ω B97X(-D4)/
def2-TZVPP)
1.451 (ANI-1ccx)

c MGHBL9 and MGNHBL11 benchmark

$\text{H}_3\text{C}-\text{H}$
1.086
1.086

$\text{H}-\text{H}$
0.741
0.726

$\text{HO}-\text{H}$
0.957
0.958

$\text{HC}\equiv\text{C}-\text{H}$
1.203 1.063
1.205 1.064

$\text{N}\equiv\text{C}-\text{H}$
1.153 1.065
1.152 1.065

$\cdot\text{O}-\text{H}$
0.970
0.959

$^-\text{N}=\text{N}^+=\text{O}$
1.128 1.184
1.120 1.186

$\text{OC}=\text{O}$
1.160
1.160

$\text{O}=\text{C}(\text{H})-\text{H}$
1.203 1.101
1.205 1.101

$\text{H}_2\text{N}-\text{H}$
1.012
1.012

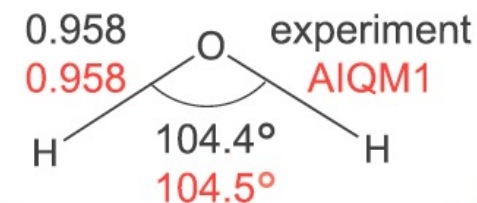
experiment
AIQM1

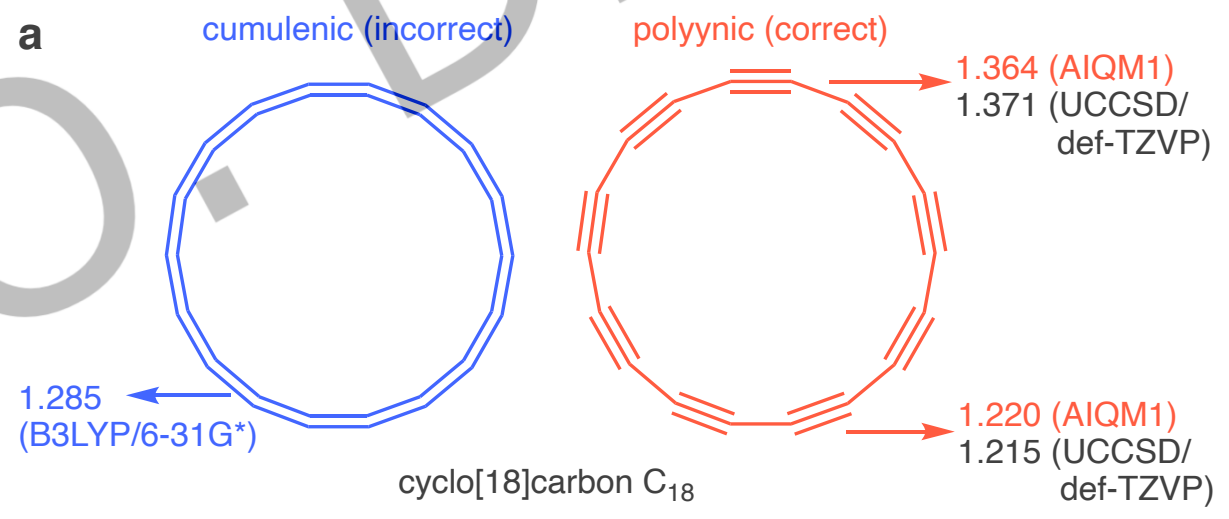
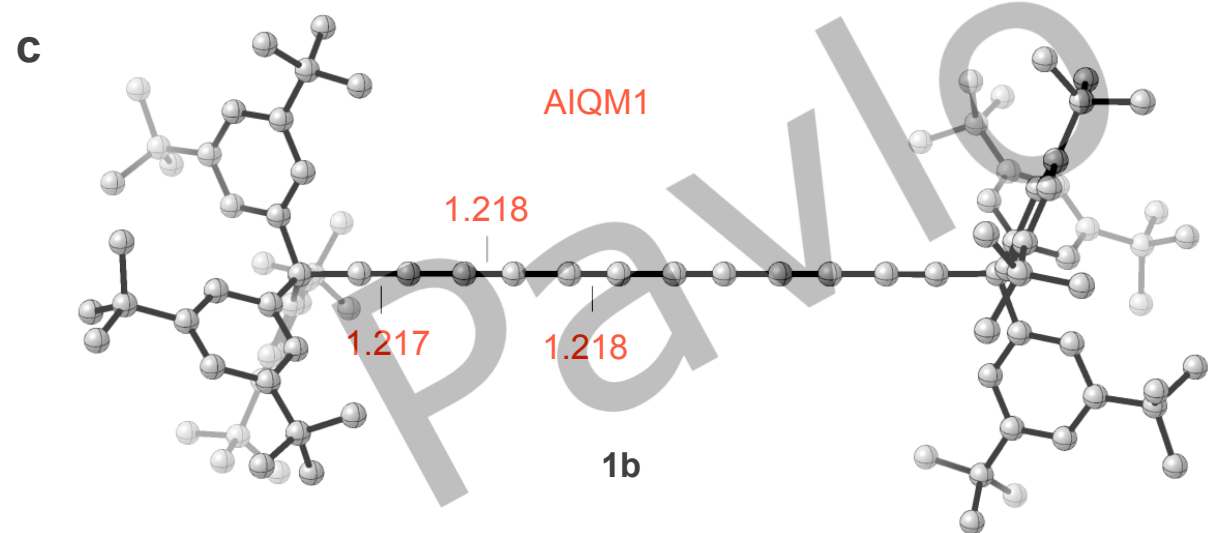
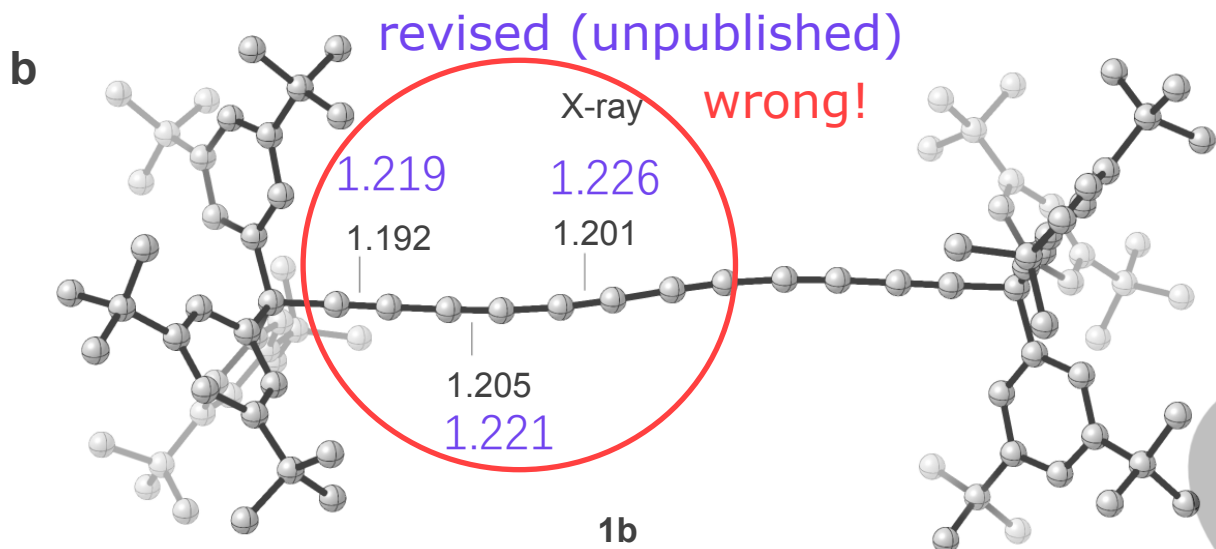
$\text{N}\equiv\text{N}$
1.098
1.097

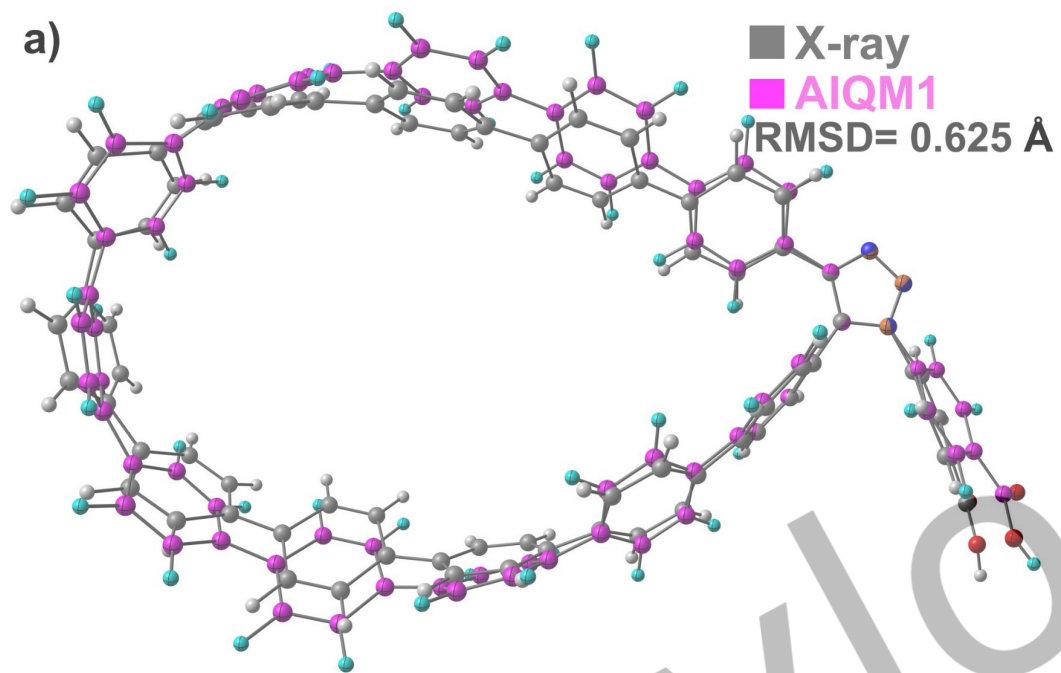
$^-\text{C}\equiv\text{O}^+$
1.128
1.125

b

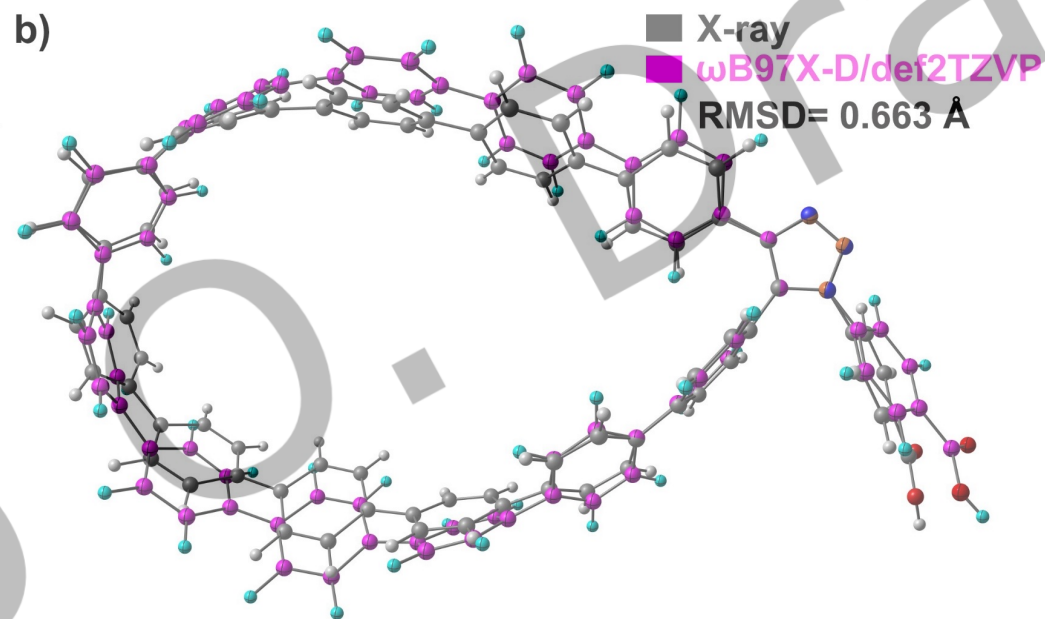
H_2O in CHNO
benchmark



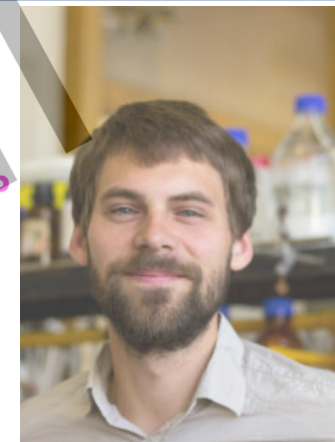




2 CPU-minutes



1200 CPU-minutes

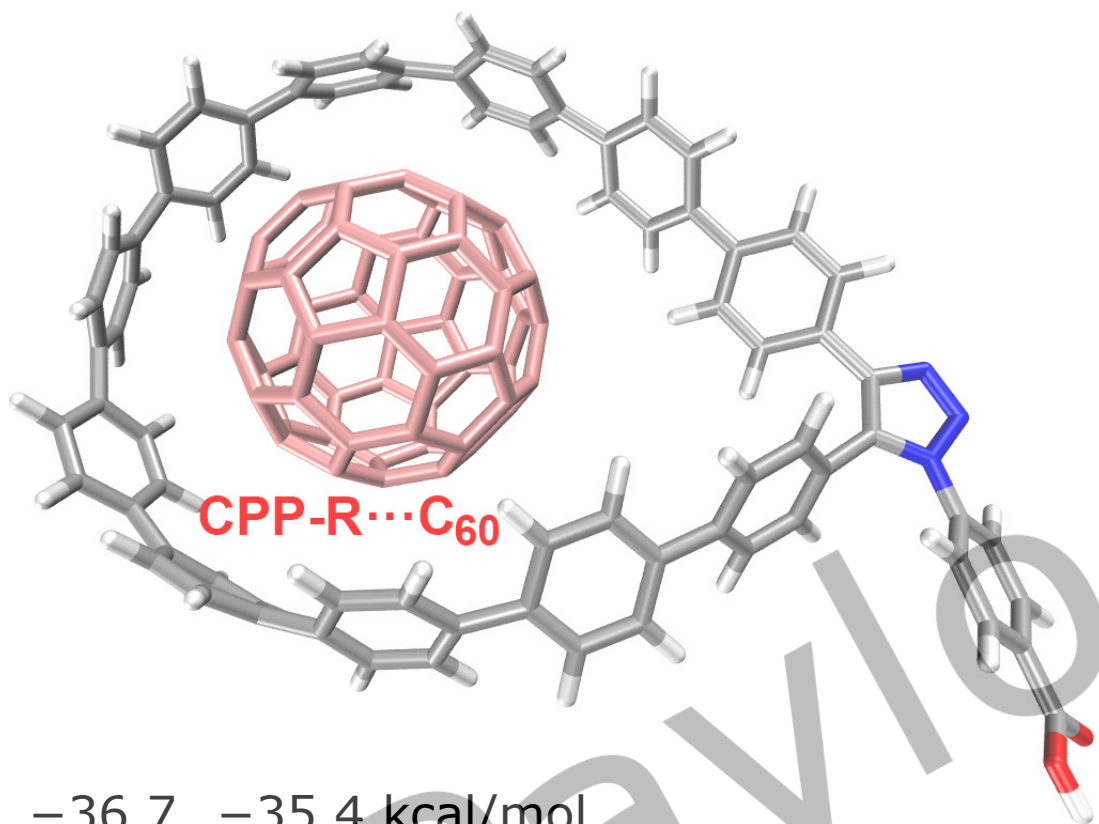


Tobias Schaub



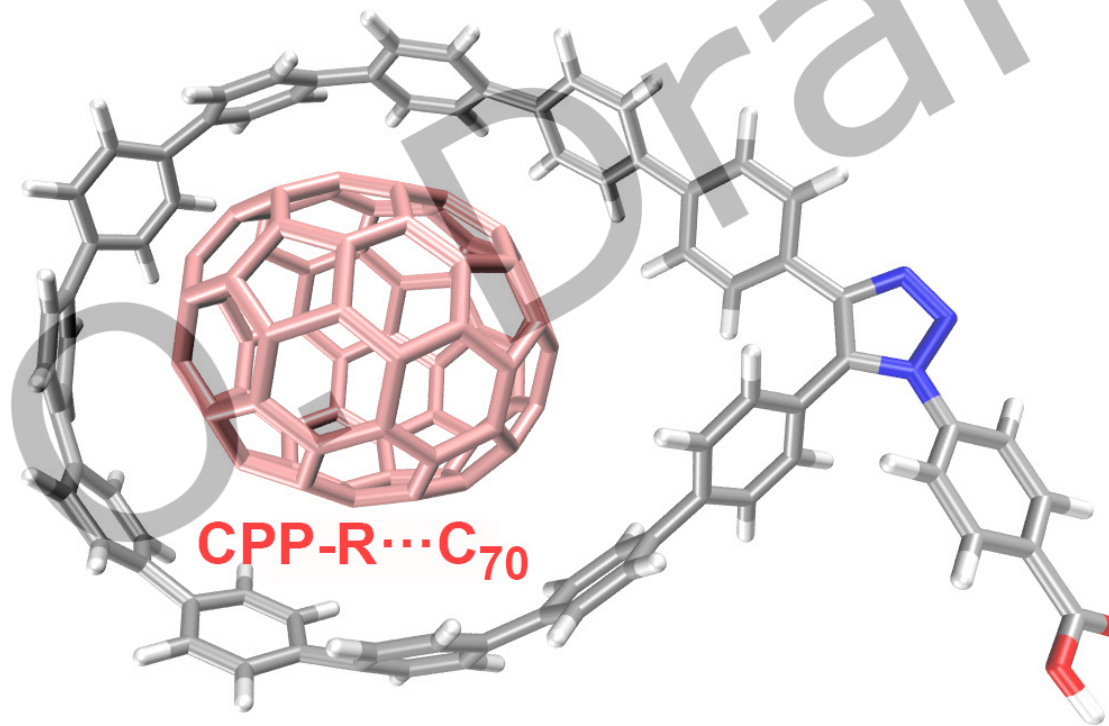
Yang Wudi

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 Macrocylic Polyparaphenylene Nanolassos via Copper-Free Click Chemistry. *Chem. Eur. J.* **2023**, 29, e202300668



–36.7...–35.4 kcal/mol

15 CPU-minutes



–41.9...–38.3 kcal/mol

30 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

Example ML-uni-1. Calculate the bond length in H₂ and H₂O molecules with ANI-1ccx and AIQM1 (you can try UAIQM if you want!).

Check:

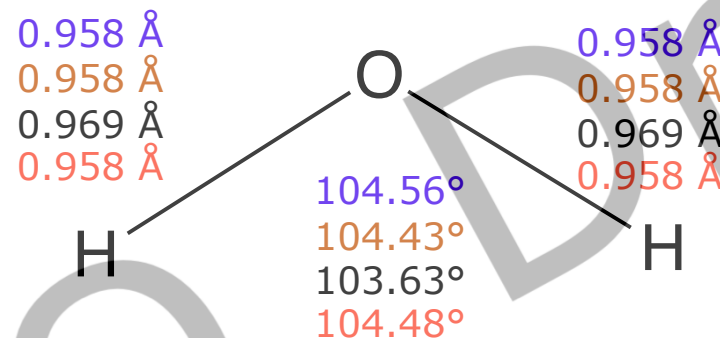
- method you used
- bond length (and angle for H₂O) you obtained
- how much time it took to complete the calculations

```
geomopt                # Request geometry optimization
ANI-1ccx
XYZfile='
2
H      0.0000000000000000      0.0000000000000000      0.0000000000000000
H      0.0000000000000000      0.0000000000000000      0.8000000000000000
'
optXYZ=h2_opt.xyz      # optimized geometry output
```


AIQM1 and ANI-1ccx are approaching CCSD(T)/CBS but AIQM1 \neq ANI-1ccx \neq CCSD(T)/CBS!

H₂ bond length:

- 0.4368 Å (ANI-1ccx)
- 0.726 Å (AIQM1)
- 0.7122 Å (HF/STO-3G)
- 0.7415 Å (KREG & FCI/aug-cc-pV6Z)
- 0.7414 Å (experiment)



ANI-1ccx

AIQM1

B3LYP/6-31G*

Experiment

A. R. Hoy and P. R. Bunker,

J. Mol. Spectrosc., **1979**, 74, 1-8

Any ML model might have limitations (like QM models too). Hence, always pay attention and use your expertise to check whether results are reasonable:

- other high-level QM calculations (can be unavailable or expensive)
- compare to experiment (maybe not reliable either!)
- check uncertainty (easiest and often works)

After geometry optimization, the next step is to calculate frequencies

Pavlo O. Dral

Toward Chemical Accuracy in Predicting Enthalpies of Formation with General-Purpose Data-Driven Methods

Peikun Zheng, Wudi Yang, Wei Wu, Olexandr Isayev,* and Pavlo O. Dral*

 Cite This: *J. Phys. Chem. Lett.* 2022, 13, 3479–3491

 Read Online

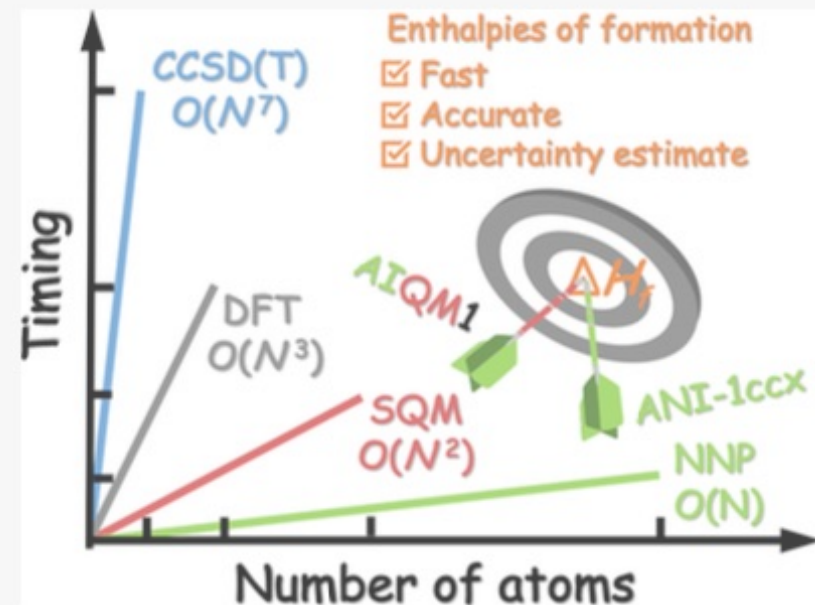
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 Article Recommendations

 Supporting Information

ABSTRACT: Enthalpies of formation and reaction are important thermodynamic properties that have a crucial impact on the outcome of chemical transformations. Here we implement the calculation of enthalpies of formation with a general-purpose ANI-1ccx neural network atomistic potential. We demonstrate on a wide range of benchmark sets that both ANI-1ccx and our other general-purpose data-driven method **AIQM1 approach the coveted chemical accuracy of 1 kcal/mol** with the speed of semiempirical quantum mechanical methods (AIQM1) or faster (ANI-1ccx). It is remarkably achieved without specifically training the machine learning parts of ANI-1ccx or AIQM1 on formation enthalpies. Importantly, we show that these data-driven methods provide statistical means for uncertainty quantification of their predictions, which we use to detect and eliminate outliers and revise reference experimental data. Uncertainty quantification may also help in the systematic improvement of such data-driven methods.



After geometry optimization, the next step is to calculate frequencies

Example ML-uni-2. Calculate frequencies in H₂, H₂O, and vinylacetylene molecules with ANI-1ccx.



vinylacetylene

Report:

- Are your optimized geometries true minima?
- What are the heats of formation?
- Is any of the calculations uncertain?

```
freq # Request frequency and thermochemistry calculations
ANI-1ccx
XYZfile=h2_opt.xyz # file with optimized geometry
```


Creation of the initial XYZ geometry of vinylacetylene takes time. We do provide you with the initial guess, but what is a faster way to get XYZ geometry for a new molecule?





what is xyz geometry of vinylacetylene?



I'm sorry, but the term "xyz geometry" is not specific enough for me to provide a precise answer. The "xyz" notation typically refers to the Cartesian coordinates of atoms in a molecule, specifying their positions in three-dimensional space. However, it doesn't specify the molecular geometry or bond angles.

Vinylacetylene is a compound with the chemical formula C_4H_4 . It consists of a vinyl group ($CH_2=CH-$), which is an alkene, attached to an acetylene group ($C\equiv CH$). The molecular geometry of vinylacetylene can be described based on the arrangement of its atoms.

In the vinyl group, the carbon atoms are sp^2 hybridized, forming a planar structure with bond angles of approximately 120 degrees. The acetylene group consists of two sp hybridized carbon atoms, which are linearly arranged with a bond angle of 180 degrees.

Overall, vinylacetylene has a linear molecular geometry due to the linear arrangement of the acetylene group. However, it's important to note that the actual molecular structure can be influenced by other factors such as steric effects or conjugation, which may slightly deviate from the idealized geometric description.



what are xyz coordinates of vinylacetylene molecule?



I apologize, but as an AI text-based model, I don't have access to real-time data or the ability to perform calculations. Therefore, I don't have the specific XYZ coordinates for the atoms in the vinylacetylene molecule.

To obtain the XYZ coordinates for vinylacetylene, you would typically need to use computational methods such as quantum chemical calculations or obtain experimental data from techniques like X-ray crystallography or spectroscopy.

If you have access to molecular modeling software or databases, you can input the chemical structure of vinylacetylene and generate the XYZ coordinates. Alternatively, you can consult research articles or databases that provide such information for vinylacetylene.

can you provide initial guess of internal coordinates of vinylacetylene?



Certainly! Here's an initial guess for the internal coordinates of vinylacetylene:

Assuming the vinylacetylene molecule is in a planar conformation, we can assign the following internal coordinates:

- Bond lengths:
 - C1=C2 (vinyl group): A typical value for a C=C double bond is around 1.34 Å.
 - C2-C3 (vinyl group): A typical value for a C-C single bond is around 1.54 Å.
 - C3-C4 (acetylene group): A typical value for a C-C triple bond is around 1.20 Å.
 - C4=H5 (acetylene group): A typical value for a C-H bond is around 1.09 Å.
- Bond angles:
 - C1=C2-C3 (vinyl group): Assuming a planar conformation, the bond angle can be approximately 120 degrees.
 - C2-C3-C4 (vinyl-acetylene connection): Assuming a planar conformation, the bond angle can be approximately 180 degrees.
 - C3-C4=H5 (acetylene group): Assuming a linear conformation, the bond angle can be approximately 180 degrees.
- Dihedral angle:
 - C1-C2-C3-C4: Assuming a planar conformation, the dihedral angle can be initially set at 0 degrees.

Please note that these are initial estimates and can vary based on the actual molecular structure, which would be best determined through accurate computational methods or experimental techniques.



Certainly! Here's an example of a Gaussian input file (Gaussian 09 format) that includes the initial guess of internal coordinates for vinylacetylene:

```

css
Copy code

%chk=vinylacetylene.chk
# opt freq b3lyp/6-31g(d) geom=connectivity

Title

O 1
C
C1      C2      C3      H4
C1      C2      C3      C4
H5      C4


C1      C2      1.34
C2      C3      1.54
C3      C4      1.20
C4      H5      1.09

C1=C2-C3      C2-C3-C4      C3-C4=H5
120           180           180

D 1 2 3 4
    
```

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In this input file:

 Regenerate response

Geometry for (1-Buten-3-yne) ¹A' C1

1910171554

InChI=1S/C4H4/c1-3-4-2/h1,4H,2H2 INChIKey=WFYPICNXBKQZGB-UHFFFA

CCSD(T)/6-31G*

Point group is C₁

Atom	Internal			Principal		
	x (Å)	y (Å)	z (Å)	a (Å)	b (Å)	c (Å)
C1	-0.6471	0.5025	0.0000	-0.6451	0.5050	0.0000
C2	0.7370	0.1141	-0.0000	0.7374	0.1113	-0.0000
C3	-1.6659	-0.3822	-0.0000	-1.6674	-0.3757	-0.0000
C4	1.9241	-0.1712	-0.0000	1.9234	-0.1786	-0.0000
H5	-0.8537	1.5746	0.0000	-0.8476	1.5779	0.0000
H6	-1.4909	-1.4569	-0.0000	-1.4965	-1.4511	-0.0000
H7	-2.7003	-0.0434	0.0001	-2.7005	-0.0330	0.0001
H8	2.9563	-0.4542	0.0003	2.9546	-0.4656	0.0003

tab delimited dump of previous table

Atom - Atom Distances (Å)

	C1	C2	C3	C4	H5	H6	H7	H8
C1		1.4375	1.3493	2.6579	1.0918	2.1334	2.1246	3.7282
C2	1.4375		2.4536	1.2209	2.1594	2.7261	3.4409	2.2910
C3	1.3493	2.4536		3.5962	2.1186	1.0889	1.0885	4.6228
C4	2.6579	1.2209	3.5962		3.2808	3.6490	4.6262	1.0703
H5	1.0918	2.1594	2.1186	3.2808		3.0977	2.4552	4.3165
H6	2.1334	2.7261	1.0889	3.6490	3.0977		1.8603	4.5589
H7	2.1246	3.4409	1.0885	4.6262	2.4552	1.8603		5.6716
H8	3.7282	2.2910	4.6228	1.0703	4.3165	4.5589	5.6716	

Maximum atom distance is 5.6716Å between atoms H7 and H8.

In some cases you can find the calculated geometries online

<https://cccbdb.nist.gov/exp2x.asp?casno=689974&charge=0>

Vibration analysis for molecule 1

Multiplicity: 1

This is a nonlinear molecule

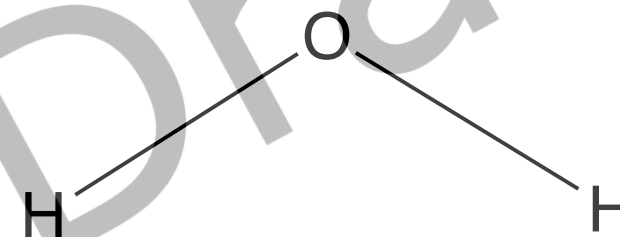
Mode	Frequencies (cm ⁻¹)	Reduced masses (AMU)	Force Constants (mDyne/A)
1	1654.6962	1.0829	1.7470
2	3850.4309	1.0449	9.1277
3	3931.4391	1.0817	9.8508

Thermochemistry for molecule 1

Standard deviation of NN contribution	:	0.00009088 Hartree	0.05703 kcal/mol
NN contribution	:	-0.00110508 Hartree	
Sum of atomic self energies	:	-63.04934947 Hartree	
ODM2* contribution	:	-13.33326549 Hartree	
D4 contribution	:	-0.00002289 Hartree	
Total energy	:	-76.38374293 Hartree	
ZPE-exclusive internal energy at 0 K:		-76.38374 Hartree	
Zero-point vibrational energy	:	0.02150 Hartree	
Internal energy at 0 K:		-76.36225 Hartree	
Enthalpy at 298 K:		-76.35847 Hartree	
Gibbs free energy at 298 K:		-76.37988 Hartree	
Atomization enthalpy at 0 K:		0.35062 Hartree	220.01876 kcal/mol
ZPE-exclusive atomization energy at 0 K:		0.37212 Hartree	233.50896 kcal/mol
Heat of formation at 298 K:		-0.09295 Hartree	-58.32770 kcal/mol

Wall-clock time: 4.54 s (0.08 min, 0.00 hours)

MLatom terminated on 25.04.2024 at 11:15:15



Gas-phase water!

Experiment^b: -57.8 kcal/mol

^b J.B.Pedley, R.D.Naylor, and S.P.Kirby, "Thermochemical Data of Organic Compounds", 2nd ed., Chapman and Hall, London, 1986.

Vibration analysis for molecule 1



Multiplicity: 1

This is a linear molecule

Mode	Frequencies (cm ⁻¹)	Reduced masses (AMU)	Force Constants (mDyne/A)
1	3500.7003	1.0078	7.2769

The program tells
you that H₂ is uncertain!
Treat with caution

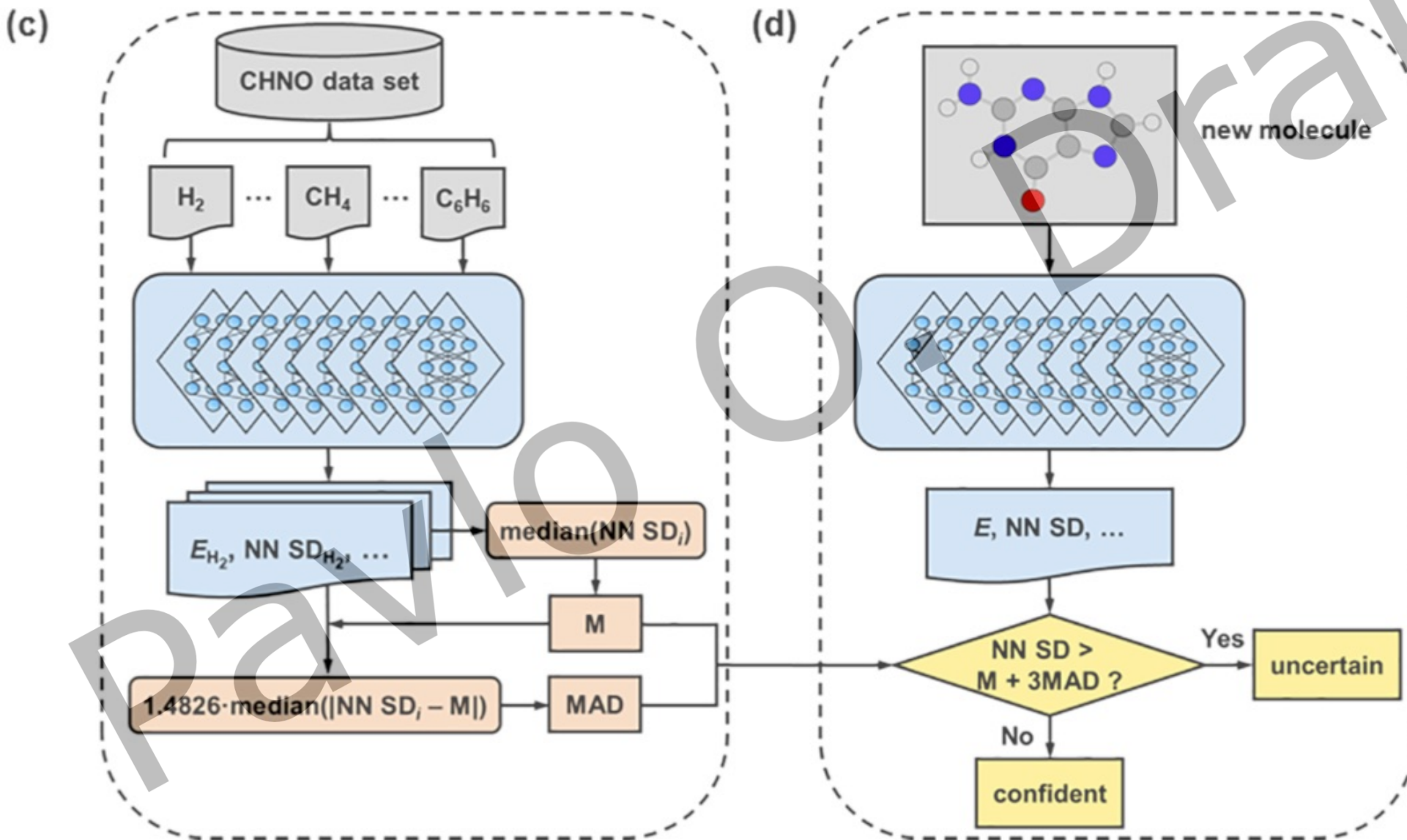
Thermochemistry for molecule 1

Standard deviation of NN contribution	:	0.00891919 Hartree	5.59688 kcal/mol
NN contribution	:	-0.00210675 Hartree	
Sum of atomic self energies	:	-0.08587317 Hartree	
ODM2* contribution	:	-1.09094346 Hartree	
D4 contribution	:	-0.00000889 Hartree	
Total energy	:	-1.17893227 Hartree	
ZPE-exclusive internal energy at 0 K:		-1.17893 Hartree	
Zero-point vibrational energy	:	0.00797 Hartree	
Internal energy at 0 K:		-1.17096 Hartree	
Enthalpy at 298 K:		-1.16765 Hartree	
Gibbs free energy at 298 K:		-1.18240 Hartree	

Uncertainty quantification of AIQM1 heats of formation:
P. Zheng, W. Yang, W. Wu, O. Isayev, P.O. Dral,
J. Phys. Chem. Lett. 2022, 13, 3479

Atomization enthalpy at 0 K:	0.16920 Hartree	106.17224 kcal/mol
ZPE-exclusive atomization energy at 0 K:	0.17717 Hartree	111.17663 kcal/mol
Heat of formation at 298 K:	-0.00455 Hartree	-2.85652 kcal/mol

* Warning * Heat of formation have high uncertainty!



H₂ bond length:

- 0.4368 Å (ANI-1ccx)
- 0.726 Å (AIQM1)
- 0.7122 Å (HF/STO-3G)
- 0.7415 Å (KREG & FCI/aug-cc-pV6Z)
- 0.7414 Å (experiment)

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Thermochemistry for molecule 1

Standard deviation of NN contribution	:	0.00008761 Hartree	0.05498 kcal/mol
NN contribution	:	0.00715111 Hartree	
Sum of atomic self energies	:	-133.90358074 Hartree	
ODM2* contribution	:	-20.63402319 Hartree	
D4 contribution	:	-0.00056531 Hartree	
Total energy	:	-154.53101813 Hartree	



vinylacetylene

ZPE-exclusive internal energy at 0 K:		-154.53102 Hartree	
Zero-point vibrational energy	:	0.06060 Hartree	
Internal energy at 0 K:		-154.47042 Hartree	
Enthalpy at 298 K:		-154.46492 Hartree	
Gibbs free energy at 298 K:		-154.49656 Hartree	

Experiment:
73 kcal/mol

Atomization enthalpy at 0 K:		1.29803 Hartree	814.52617 kcal/mol
ZPE-exclusive atomization energy at 0 K:		1.35863 Hartree	852.55199 kcal/mol
Heat of formation at 298 K:		0.11002 Hartree	69.04119 kcal/mol



vinylacetylene

original: 73

revised: 70.4

AIQM1: 69.1

G4: 69.1

Experiment: 73 kcal/mol

theory

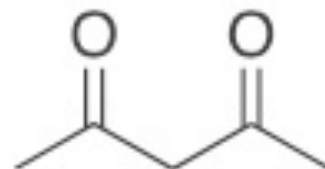
Heats of formation in kcal/mol

CHNO data set



vinylacetylene

original: 73
revised: 70.4
AIQM1: 69.1
G4: 69.1



acetylacetone

original: -91
revised: -89.9
AIQM1: -87.3
G4: -87.6



1,3-pyrimidine

exper.: 46.8
AIQM1: 44.5
G4: 44.3



acrolein

exper.: -18
AIQM1: -16.0
G4: -15.9

exp

theory

Heats of formation in kcal/mol

Example ML-uni-3.

Calculate heat of formation of H₂O with B3LYP/6-31G*.



vinylacetylene

Report:

- What is the heats of formation?
- Is this calculation uncertain?

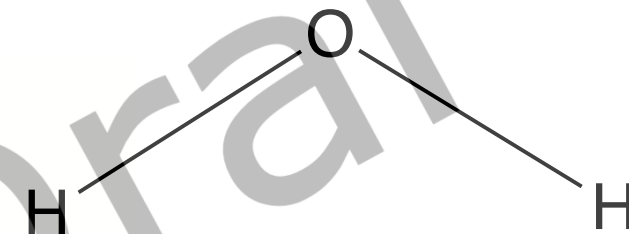
```
freq # Request frequency and thermochemistry calculations  
method=B3LYPG/6-31G* # Using PySCF instead of Gaussian  
qmprog=pyscf  
freqprog=pyscf  
XYZfile=h2_opt_B3LYP.xyz # file with optimized geometry
```

Vibration analysis for molecule 1

Multiplicity: 1

This is a nonlinear molecule

Mode	Frequencies (cm ⁻¹)	Reduced masses (AMU)	Force Constants (mDyne/A)
1	1705.0252	1.0829	1.8548
2	3765.4992	1.0453	8.7326
3	3888.7216	1.0813	9.6339



Gas-phase water!

Experiment: -57.8 kcal/mol

Thermochemistry for molecule 1

ZPE-exclusive internal energy at	0 K:	-76.40700 Hartree
Zero-point vibrational energy	:	0.02132 Hartree
Internal energy	at 0 K:	-76.38568 Hartree
Enthalpy	at 298 K:	-76.38190 Hartree
Gibbs free energy	at 298 K:	-76.40334 Hartree

No way to tell uncertainty!
Experiment can be also wrong as we saw!

Atomization enthalpy	at 0 K:	0.32573 Hartree	204.39938 kcal/mol
ZPE-exclusive atomization energy	at 0 K:	0.34705 Hartree	217.77910 kcal/mol
Heat of formation	at 298 K:	-0.06806 Hartree	-42.70844 kcal/mol

Heats of formation

	B3LYP/6-31G*	ωB97X/6-31G*	ωB97X-D/6-31G*	ωB97X-D4/def2-TZVPP	G4MP2	G4	AIQM1	AIQM1 (without outliers)	ANI-1ccx (without outliers)	ANI-1ccx	ANI-1ccx (without outliers)	
CHNO (ΔH_f)	2.63	6.72	4.09	3.83	3.20	2.74	0.90	0.75	0.84	0.60	1.76	0.92
BIGMOL20 (ΔH_f)	3.97	18.92	4.40	4.37	8.01	6.01	2.40	2.16	2.30	1.96	2.34	2.07
CONFORMERS30 (ΔH_f)	2.21	10.37	3.46	3.01	4.50	3.10	0.79	0.64	0.46	0.44	0.96	0.96
ISOMERS44 (ΔH_f)	1.16	8.08	3.57	3.53	4.52	3.78	0.44	0.37	0.42	0.42	1.34	0.59
ALKANES28 (ΔH_f)	1.15	11.17	7.07	6.26	5.12	3.06	0.59	0.53	0.97	0.24	2.67	0.65
G2 (ΔH_f)	2.59	4.99	4.31	4.07	2.60	2.39	0.60	0.52	0.97	0.44	2.62	0.62
G3 (ΔH_f)	2.90	8.66	3.48	3.26	4.28	3.30	0.74	0.68	0.73	0.68	1.08	0.97
HEDM-45 (ΔH_f)	5.55	9.06	4.33	3.90	3.46	3.48	1.20	2.27	3.80	0.96	2.87	1.25
PAH-103 (ΔH_f)	2.10	14.72	2.93	2.89	7.63	5.73	1.96	1.13	1.19	0.79	1.75	1.15
CHNO (ΔH_r)	1.92	1.75	1.41	1.39	1.32	1.29	0.94	1.02	1.06	0.22	2.63	0.68
CONFORMERS30 (ΔH_r)	1.36	1.19	1.09	1.09	1.29	1.28	1.28	1.27	1.35	1.20	1.37	1.37
ISOMERS44 (ΔH_r)	0.70	2.29	1.45	1.31	1.19	1.10	0.40	0.44	0.50	0.50	1.62	0.61
ALKANES28 (ΔH_r)	0.34	1.90	1.10	0.94	1.74	1.14	0.28	0.32	0.59	0.39	0.20	0.08
AF6 (ΔH_r)	1.32	3.07	0.55	1.68	1.28	0.73	1.02	1.05	0.45	—	3.67	—

'Outliers' – uncertain predictions

Mean absolute errors (MAEs) in kcal/mol of benchmarked methods for various data sets. MAEs of AIQM1 and ANI-1ccx

Example ML-uni-4.

Optimize and calculate frequencies of H_2 with ANI-1ccx but starting not from initial bond length of 0.7 Å as in the [previous task](#) but with 0.8 Å.

Questions:

1. Is the geometry you have obtained the same as in the previous task?
2. Is your optimized geometry true minimum?
3. What is its heats of formation?
4. Is this calculation certain?

