Aitomistic

NICOLAUS COPERNICUS UNIVERSITY IN TORUŃ

Towards Autonomous Computational Chemistry Research with AI and ML

Pavlo O. Dral

Xiamen University, China

Nicolaus Copernicus University in Toruń, Poland

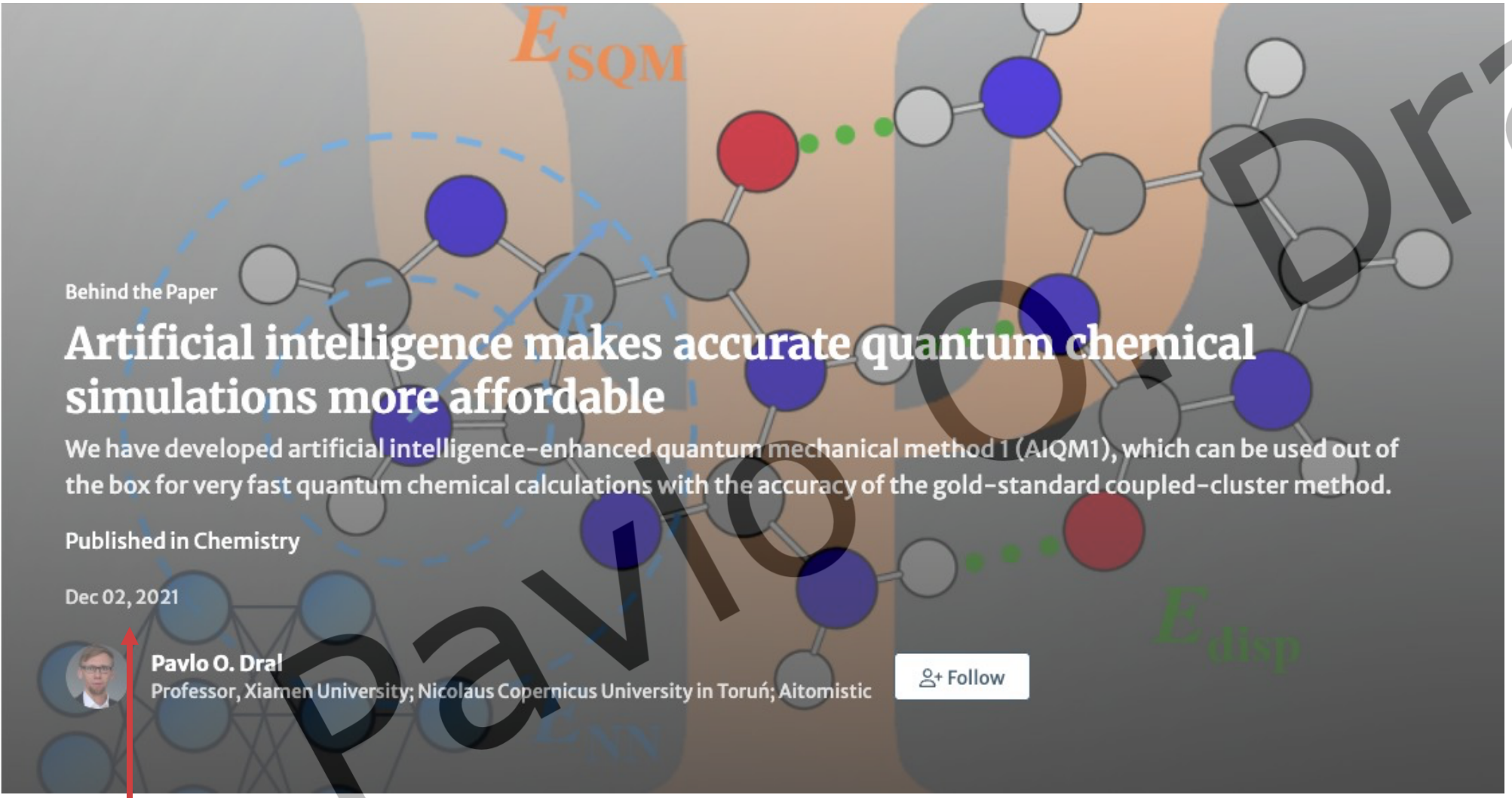
Aitomistic, Shenzhen, China

9 September 2026

Pavlo O. Dral

dr-dral.com

The Vision



ChatGPT:
Nov 30, 2022

https://communities.springernature.com/posts/artificial-intelligence-makes-accurate-quantum-chemical-simulations-more-affordable

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The Vision

learning (ML) – the very tool of AI we actually used in AIQM1), in school, I was fascinated by nature and was learning about it as much as I could. I quickly realized that it is impossible to learn everything I am interested in. The more I thought about it, the more obvious was to me that the human mind is just incapable of coping with all the information, which humanity generated, and this is likely to impose a natural barrier on how we can actually make a qualitative jump in our understanding of the world. Computers, in the long run, may overcome this barrier as they are not limited by biological constraints and can have access to all digitalized information. However, can computers by themselves make a qualitative jump in our understanding of nature? This is the first question.

Pavlo O. Dral

Dec 2, 2021

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Later, already in the university doing my master degree, I have had to run many quantum chemical (QC) simulations. It was exciting at first to witness how a computer can predict correctly, e.g., the geometry of a water molecule, but after I run many such simulations, I realized that many of them are quite repetitive and the second question is: can computers by themselves perform all these simulations, analyze results and write papers?

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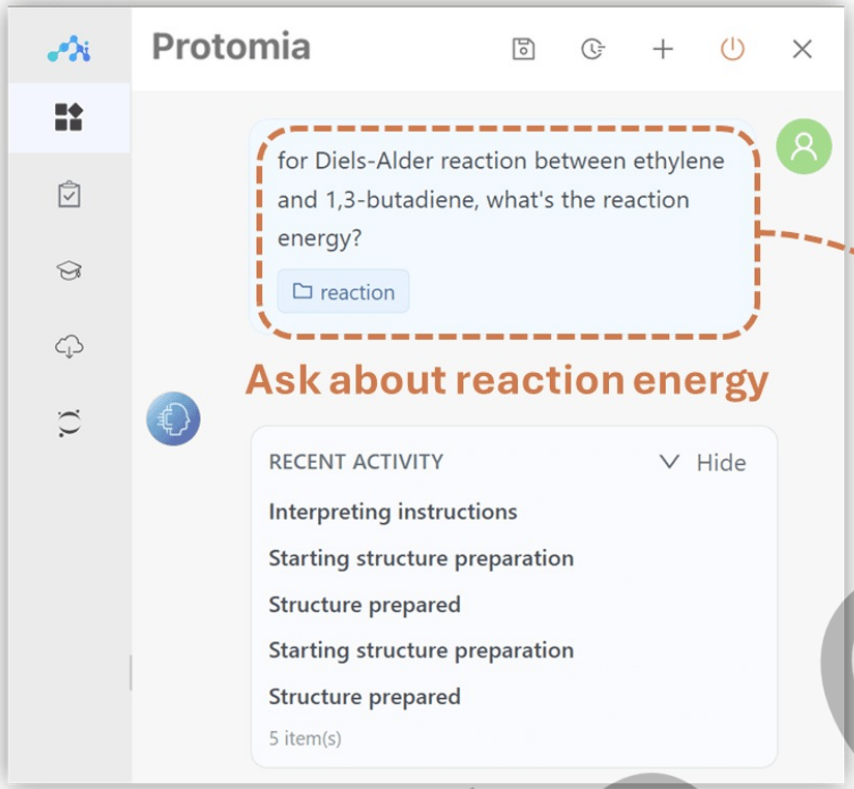

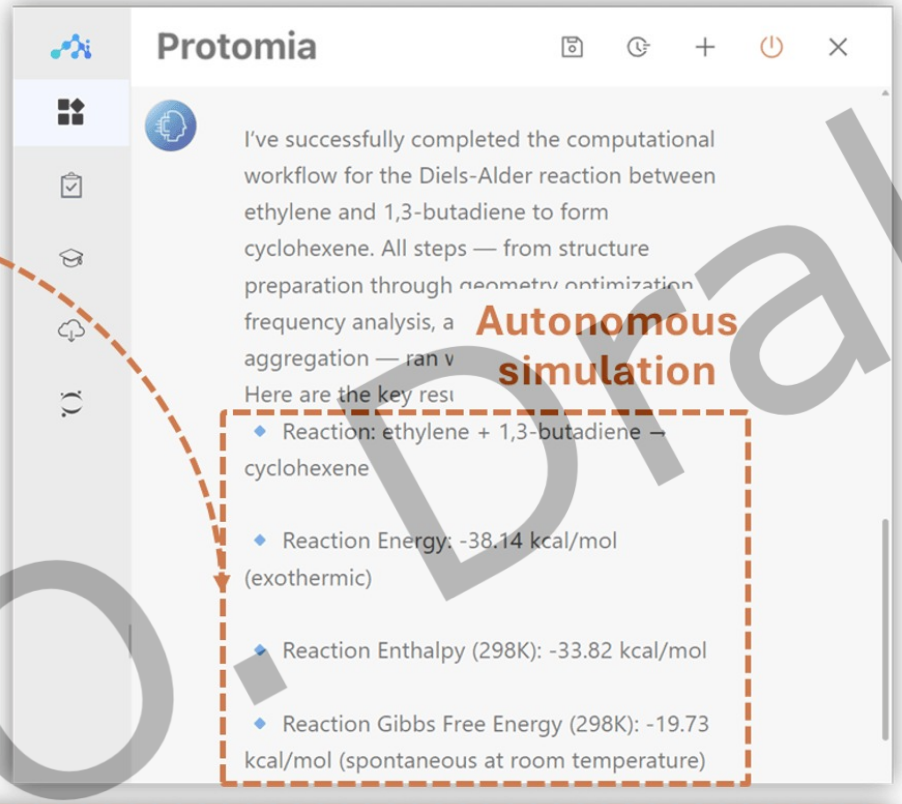

type	system/reaction	units	coefficient	E	H	G	method	output_molecule
System								
reactant	ethylene	hartree	1	-78.572	-78.5165	-78.542	B3LYP/6-31G	/aitomistic/hub/home/
reactant	1,3-butadiene	hartree	1	-155.96	-155.868	-155.9	B3LYP/6-31G	/aitomistic/hub/home/
product	cyclohexene	hartree	1	-234.592	-234.438	-234.473	B3LYP/6-31G	/aitomistic/hub/home/
Reactions/Relative energies								
reaction	ethylene + 1,3-butadiene -> cyclohexene	hartree		-0.06078	-0.05389	-0.03144		
reaction	ethylene + 1,3-butadiene -> cyclohexene	kcal/mol		-38.1393	-33.8159	-19.7303		
reaction	ethylene + 1,3-butadiene -> cyclohexene	kJ/mol		-159.575	-141.486	-82.5515		
constant	hartree_to_kcal_mol	kcal/mol		627.509				
constant	hartree_to_kj_mol	kJ/mol		2625.5				

Spreadsheet of reaction

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EXPLORER

- protomia_demo
  - DA_ethene_butadiene
    - 1-3-butadiene_opt_freq_AIQM2
    - cyclohexene_opt_freq_AIQM2
      - scr
      - README.md
      - cyclohexene_opt_freq_AIQM2.inp
      - cyclohexene_opt_freq_AIQM2.log
      - cyclohexene_opt_freq_AIQM2.xyz
      - slurm.sh
      - slurm_6655.err
      - slurm_6655.out
    - ethene_opt_freq_AIQM2
    - 1-3-butadiene_init.json
    - 1-3-butadiene_init.xyz
    - DA_ethene_butadiene.xlsx
    - README.md
    - cyclohexene_init.json
    - cyclohexene_init.xyz
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    - ethene_init.xyz
    - mini_paper.aux
    - mini_paper.log
    - mini_paper.out
    - mini_paper.pdf
    - mini_paper.tex
  - test

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Computational Chemistry Report — Generated by Protomia

May 27, 2026

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Despite its simplicity, this reaction is of fundamental interest for benchmarking computational methods, as it involves significant changes in bonding, conjugation, and strain upon cyclization.

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(exergonic) under standard conditions. The reaction is strongly enthalpically driven (ΔH = −40.31 kcal/mol), with the entropy penalty from combining two molecules into one partially offsetting the favorable enthalpy.

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now write a mini-paper in latex and make a pdf

I'll write a mini-paper in LaTeX about this Diels-Alder reaction and compile it to PDF. Let me first check the project directory for any existing files, then create the LaTeX document.

Ran 1 action

Starting step 1: listing the project directory contents to see existing results.

Ran 1 action

Updated while you were away

Step 1 done. Found the project directory with all species calculation folders and the summary spreadsheet. Now moving to step 2: writing the LaTeX mini-paper.

Ran 1 action

Step 2 done — the LaTeX mini-paper has been written. Now moving to step 3: compiling the LaTeX document to PDF using `pdflatex`.

Ran 3 actions

Step 3 done — the LaTeX compilation succeeded and the PDF is ready.

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- **Conclusions** and a short bibliography

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Pablo O. Drai

Pavlo O. Dral

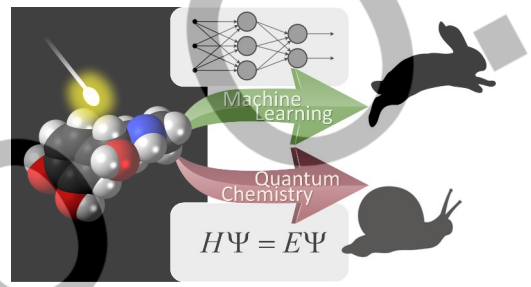
AI atomistic "Aitomistic" simulations

Professor

Email: dral@xmu.edu.cn

Research Areas: AI, AI agents, autonomous research, quantum chemistry, dynamics, excited states, reaction mechanisms, theoretical spectroscopy

MLatom.com



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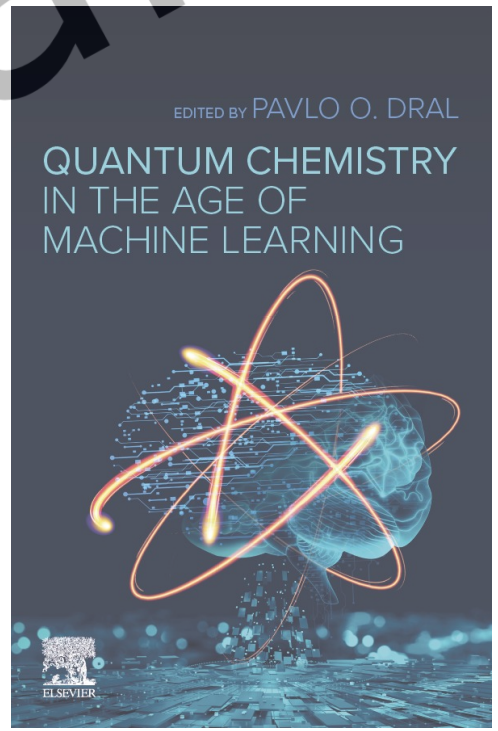


2025-Present : Aitomistic, co-founder

2024-Present : Nicolaus Copernicus University in Toruń, Professor

2021-Present : Xiamen University, Full Professor

2019-2021 : Xiamen University, Associate Professor

2013-2019 : Max-Planck-Institut für Kohlenforschung, Postdoc

2008-2013 : University of Erlangen-Nürnberg, M.Sc. & Ph.D.

2004-2010 : National Technical University of Ukraine "KPI", B.Sc. & M.Sc.

✓ **Selected papers:**

AI-DFT: ***Adv. Sci.*** *2024, 2408239*
AI platform: ***JCTC*** *2024, 20, 1193 | 2026, 22, 6557*
AI-quantum dynamics: ***Nat. Commun.*** *2022, 13, 1930*
AI-quantum mechanics: ***Nat. Commun.*** *2021, 12, 7022*
AI-excited states: ***Nat. Commun.*** *2026, 17, 4949*

Group website: dr-dral.com

Pavlo O. Dral

Aitomia Team: Academic Version

Pavlo O. Dral

Early implementations online since May 11, 2025

CHEMISTRY WORLD

NEWS

AI agents set to democratise computational chemistry

BY JULIA ROBINSON | 2 JANUARY 2026

While we'll have to wait to find that out, it's clear that significant change is already afoot. 'I'm pretty sure that in the future, people will wonder how people previously did quantum chemical simulations,' says Dral. 'Like we are now astonished at how people built the pyramids in Egypt.'

Aitomia

Status: Publicly available since 11 May 2025.

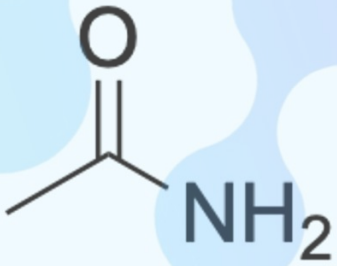
What it does: Aitomia assists researchers in all stages of their work, from setting up the calculations, providing possible options, automatically performing the simulations, and then helping to analyse the results in an understandable and reusable format. It supports a wide-array of AI-driven atomistic and quantum chemistry methods enabling essential computations such as energy calculations, geometry optimisations, molecular dynamics, thermochemistry, reaction and spectra simulations.

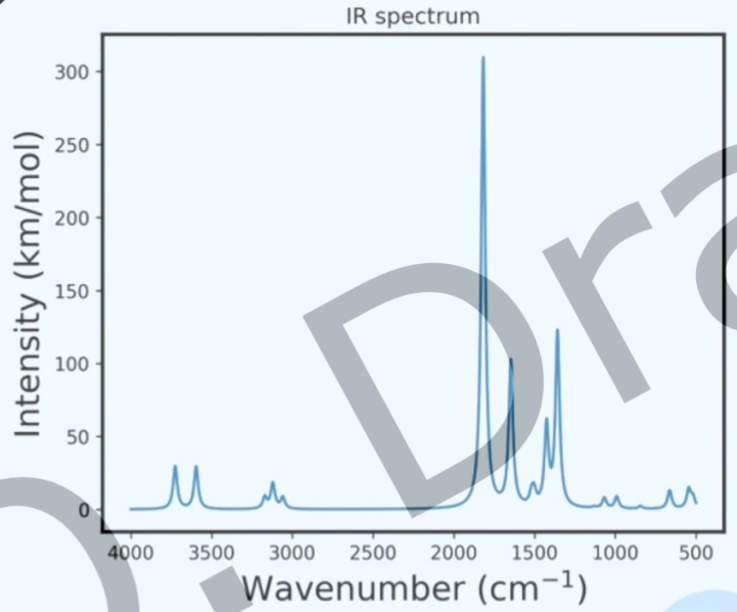
I used Aitomistic for teaching Applied Quantum Chemistry … It was amazing and students liked it so much.

By one of the independent professors

Pavlo O. Dral

Simulate IR spectrum for this molecule





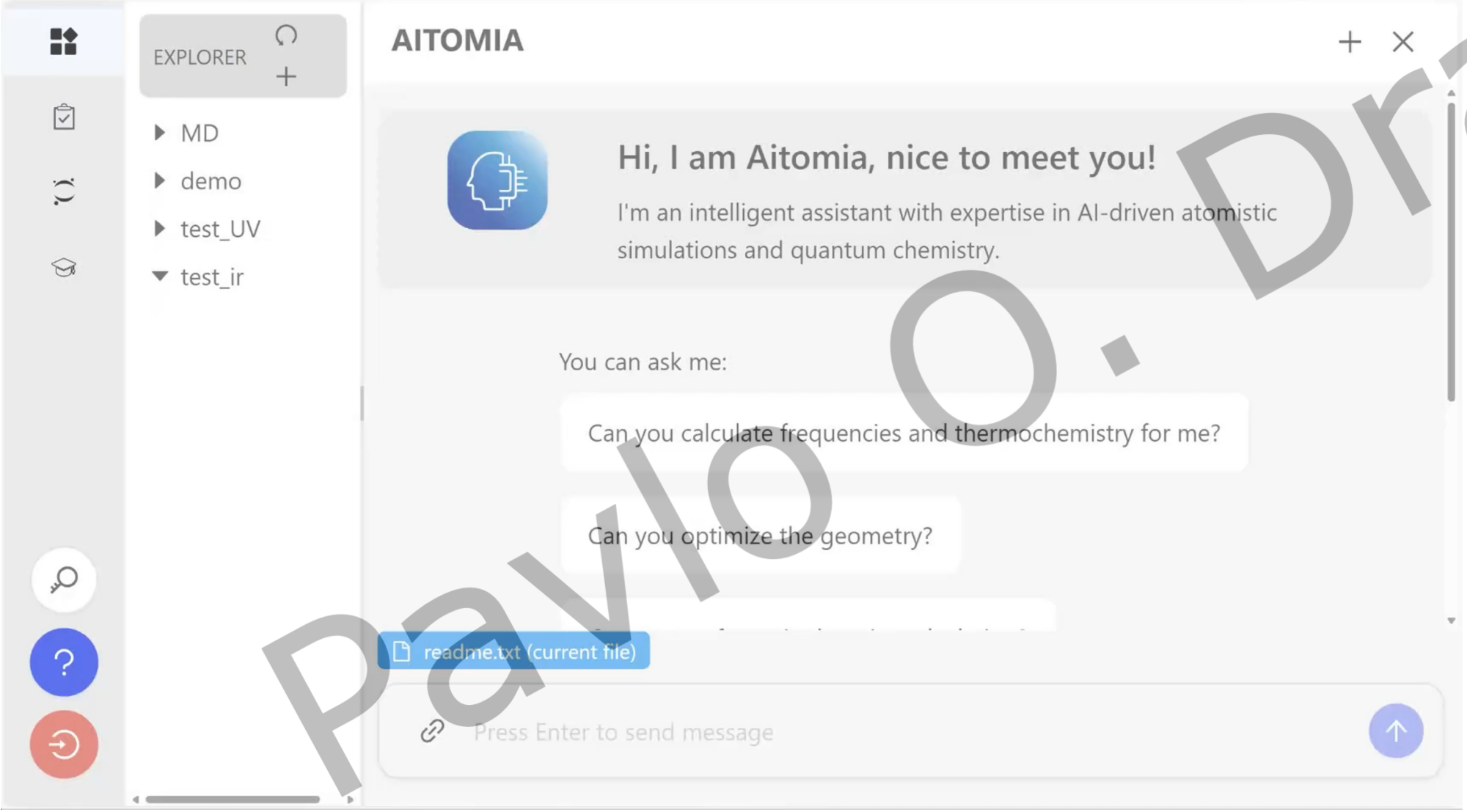
Sure!

Hello! I am *Aitomia*

Aitomistic

Pavlo O. Dral

Early implementations online since May 11, 2025



* Aitomia is the research framework introduced in 2025; **Protomia** is the modern architecture

https://atom.xmu.edu.cn (available for free when registered with an academic email)

https://aitomistic.xyz (registration and basic use free for everyone)

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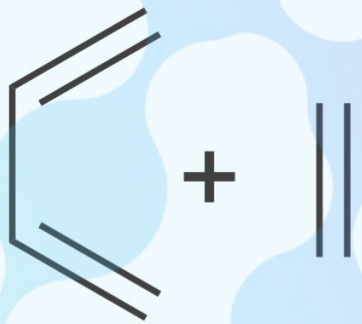
J. Hu, H. Nawaz, Y.-F. Hou, Y. Rui, L. Chi, Y. Chen*, A. Ullah*, P. O. Dral*. *JCTC* **2026**, *22*, 6557–6571

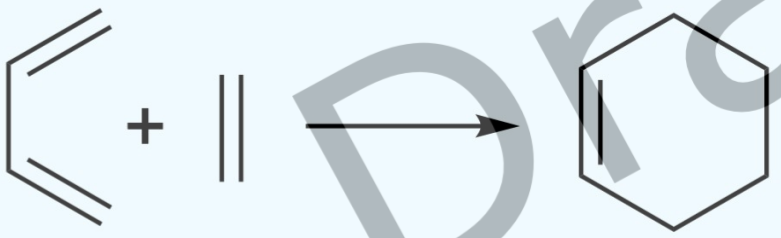
Aitomia: Intelligent Assistant for Aitomistic (AI+atomistic) and QM Simulations

Pavlo O. Dral

J. Hu, H. Nawaz, Y.-F. Hou, Y. Rui, L. Chi, Y. Chen*, A. Ullah*, P. O. Dral*. *JCTC* **2026**, *22*, 6557–6571

Simulate this reaction





ΔG=−25.7 kcal/mol

Sure!

Hello! I am *Aitomia*

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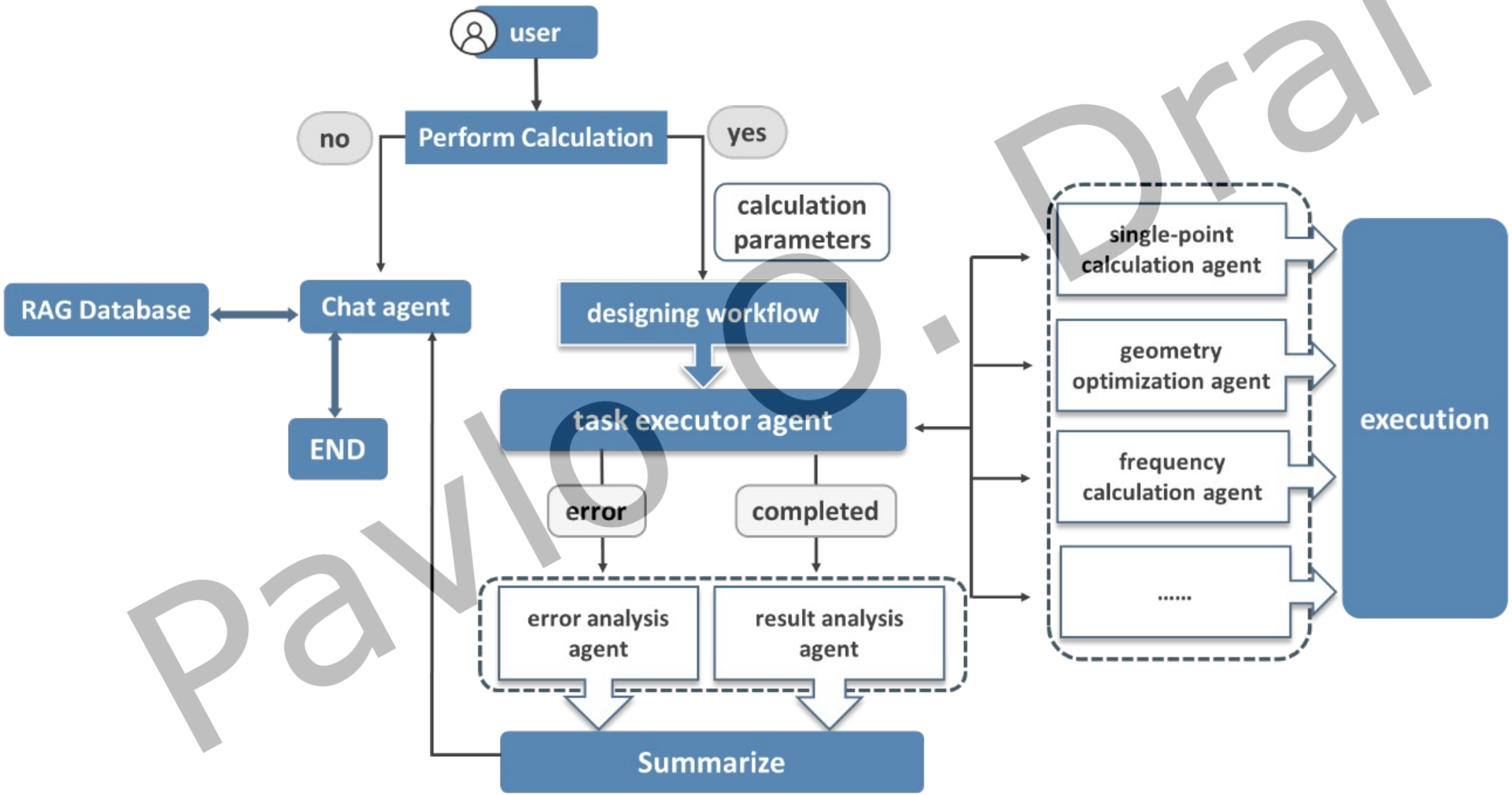
Autonomous simulations with AI agents



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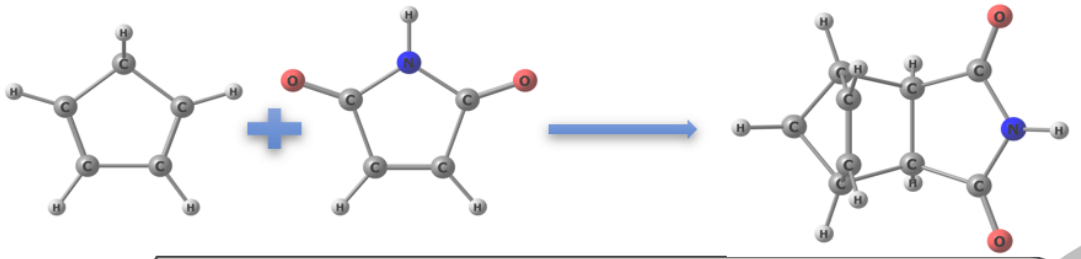

J. Hu, H. Nawaz, Y.-F. Hou, Y. Rui, L. Chi, Y. Chen*, A. Ullah*, P. O. Dral*. *JCTC* **2026**, *22*, 6557–6571

Calculate the reaction energy and thermodynamic properties for the Diels-Alder reaction between cyclopentadiene and maleimide using AIQM2. I will provide the adduct. Please generate the other required structures for me.

The user only provides the adduct structure. For this task, the structures of maleimide and cyclopentadiene are also required. I will call the initial structure generation agent to generate the missing structures needed to solve the user's problem.

For **adduct**, I will proceed with following calculations:
……
For **maleimide**, I'll follow this plan:
…..

We are calculating the reaction energy (ΔE), enthalpy change (ΔH), and Gibbs free energy change (ΔG) for Diels-Alder reaction.

cyclopentadiene +maleimide ⟶ adduct

1. Reaction energy (ΔE) = -33.73 kcal/mol
2. Enthalpy Change (ΔH) = -30.41 kcal/mol
3. Gibbs Free Energy Change (ΔG) = -15.

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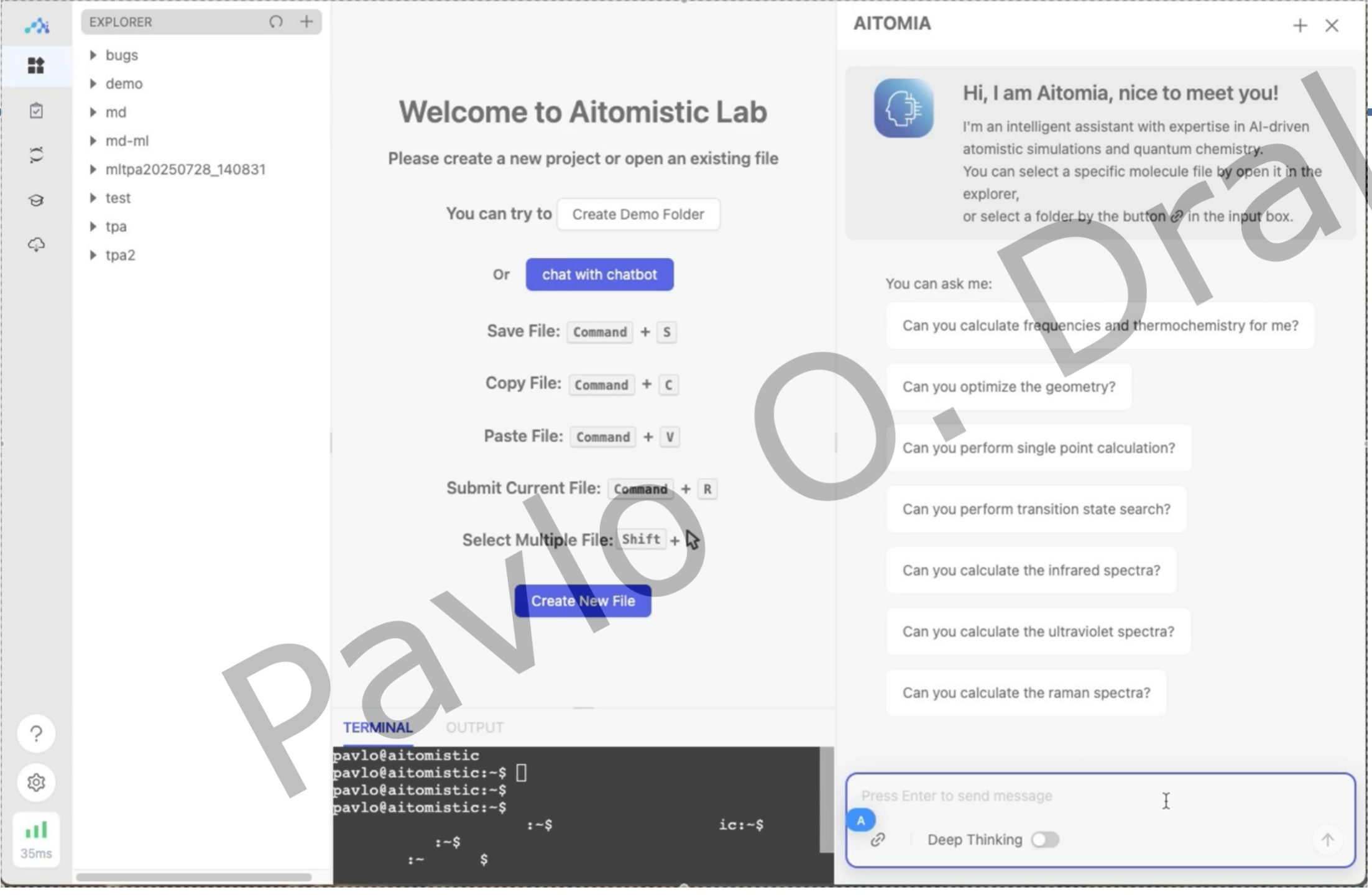

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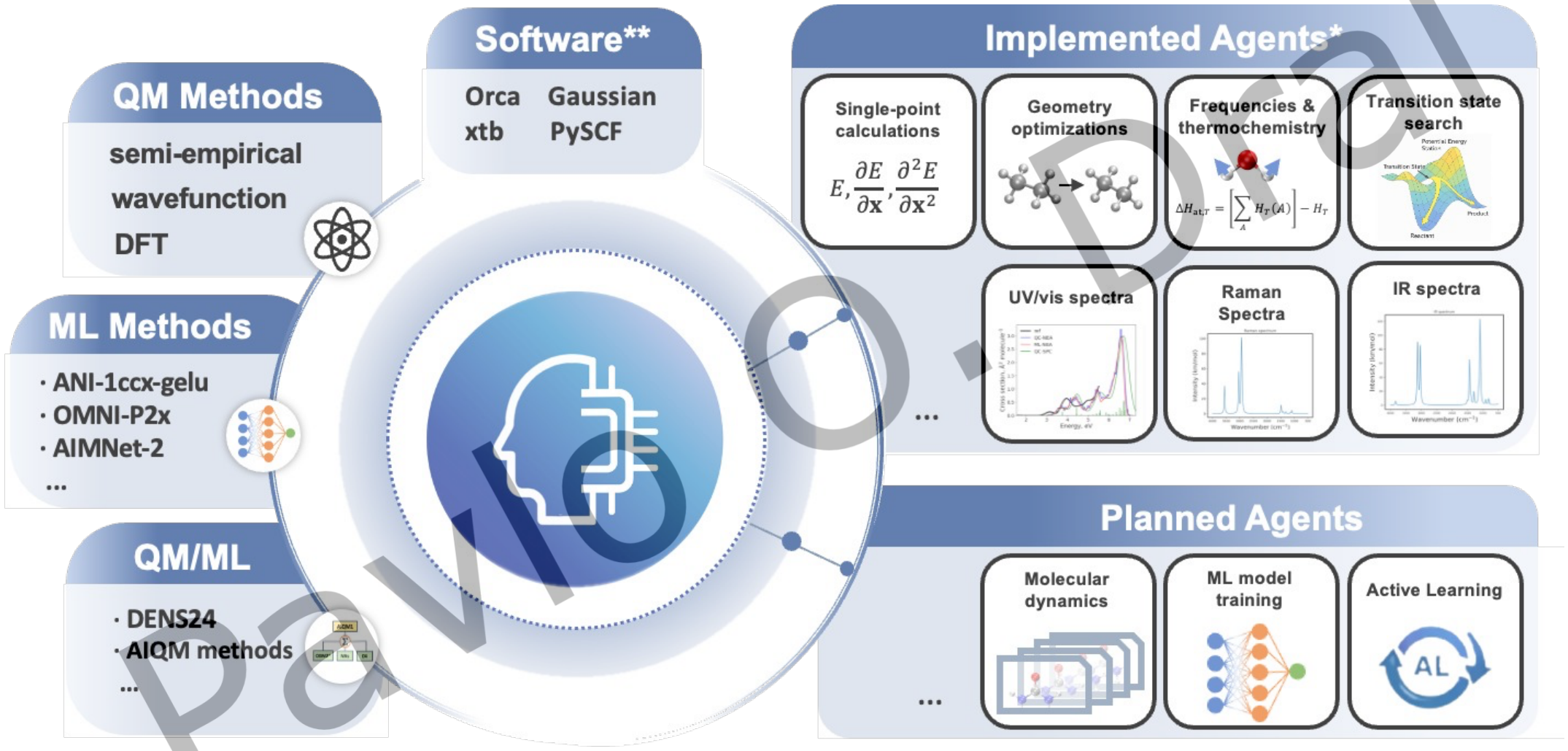
Pablo O. Drai

Assistant for aitomistic and QM simulations



*Implemented agents can be used in more complex workflows, such as reaction enthalpy calculations.
**Only software with permissive licenses is available online for registered users, while Aitomia supports more programs.

J. Hu, H. Nawaz, Y.-F. Hou, Y. Rui, L. Chi, Y. Chen*, A. Ullah*, P. O. Dral*. *JCTC* **2026**, *22*, 6557–6571

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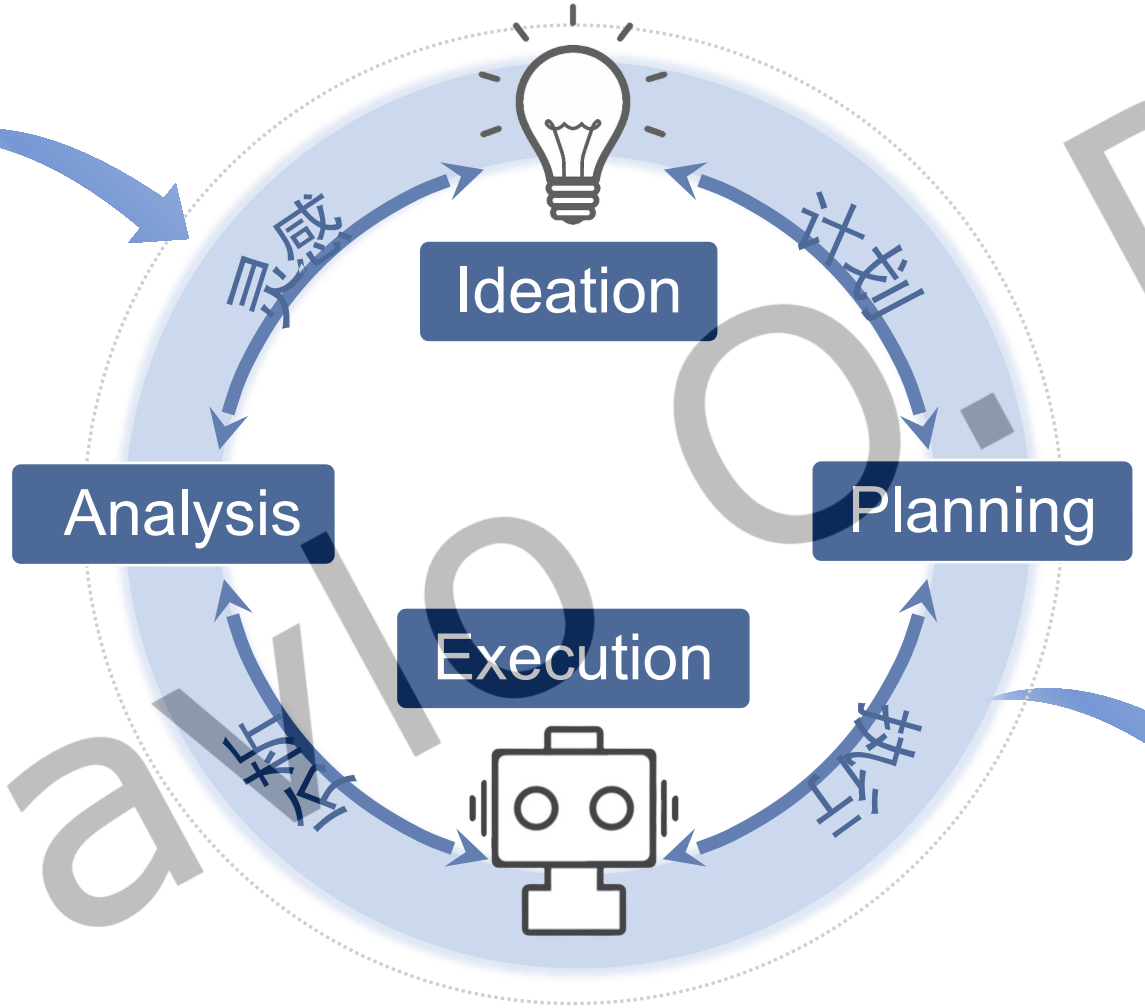
Track trends



- **Develop new methods**
- **Computational explorations**

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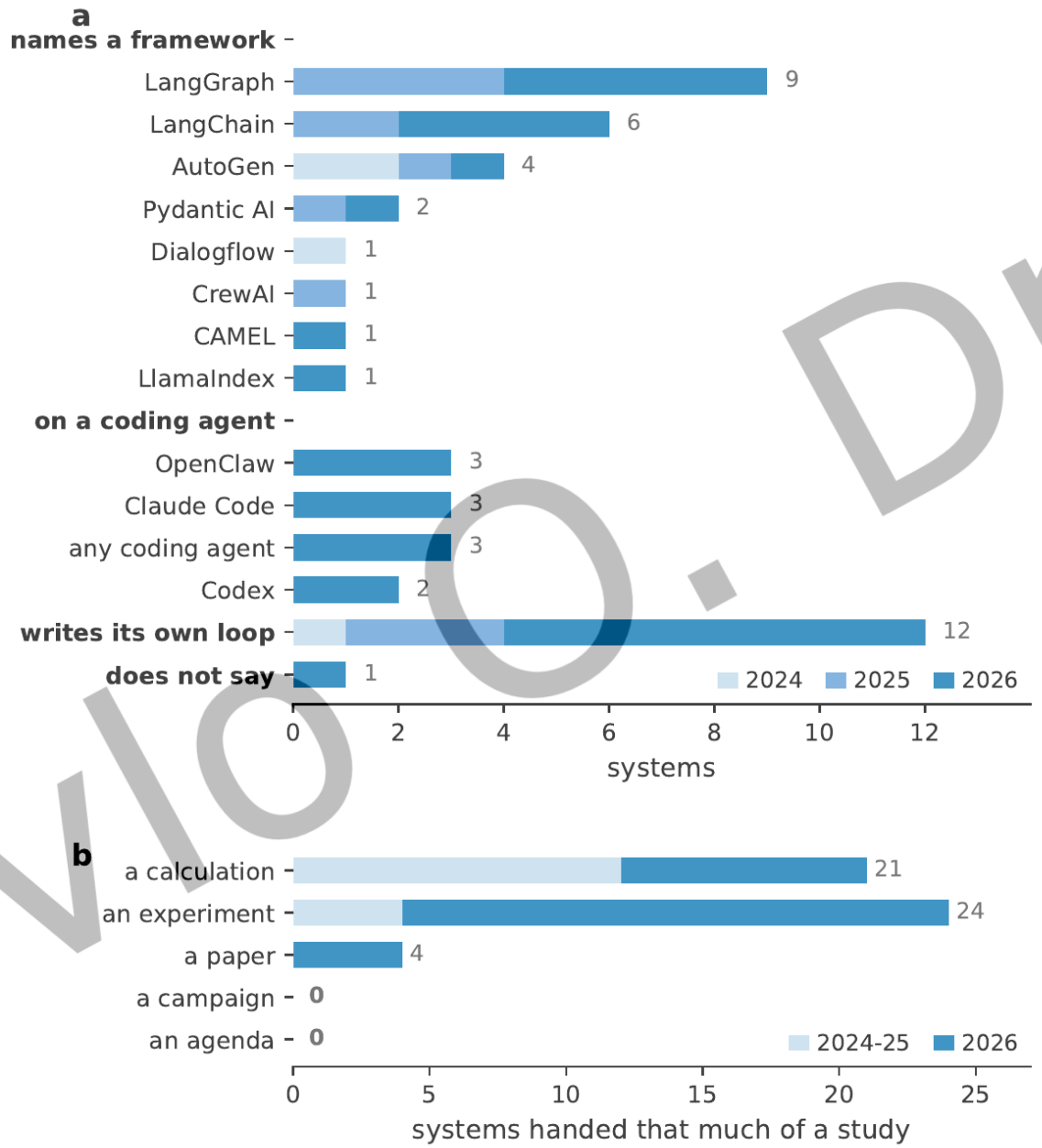

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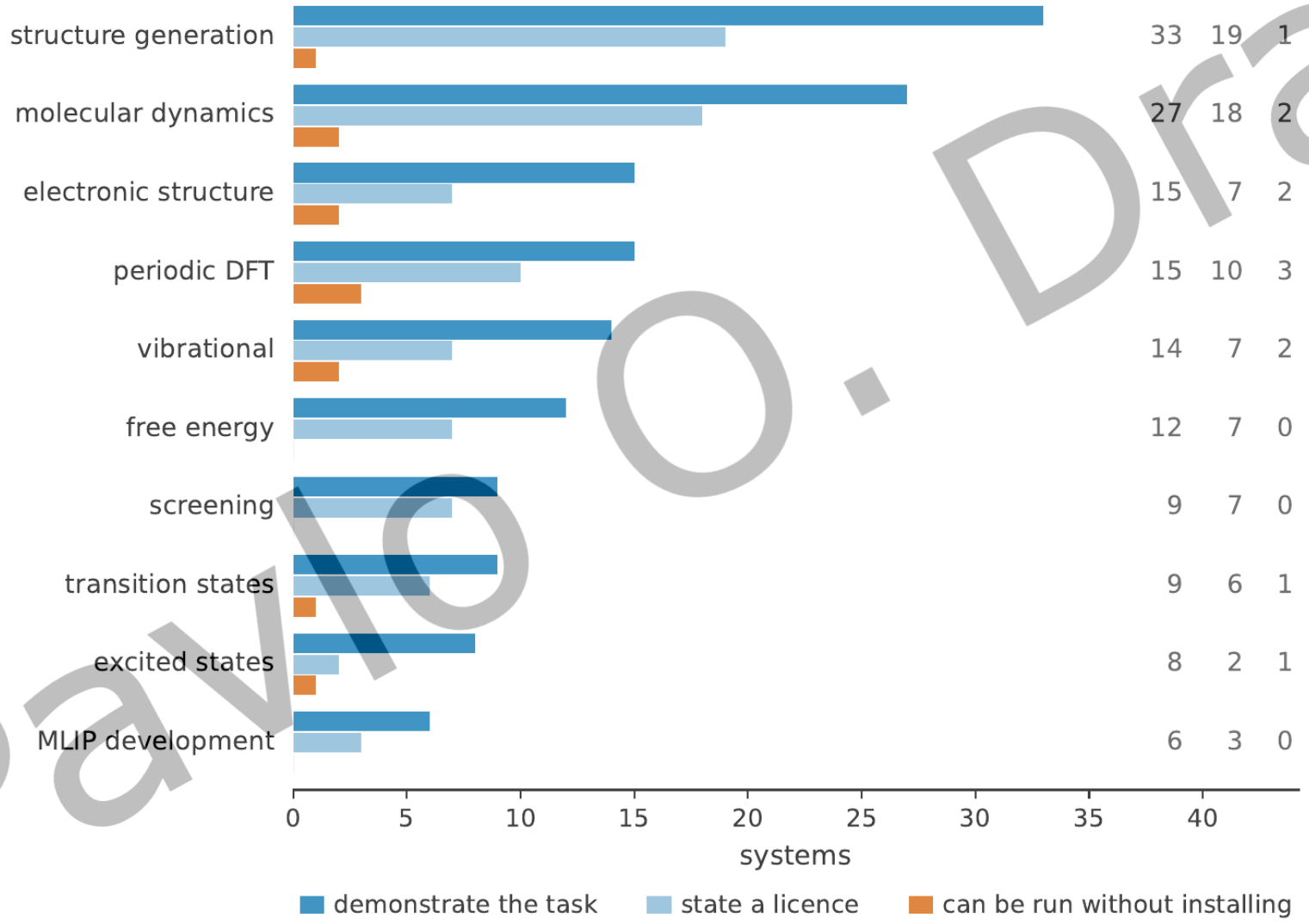
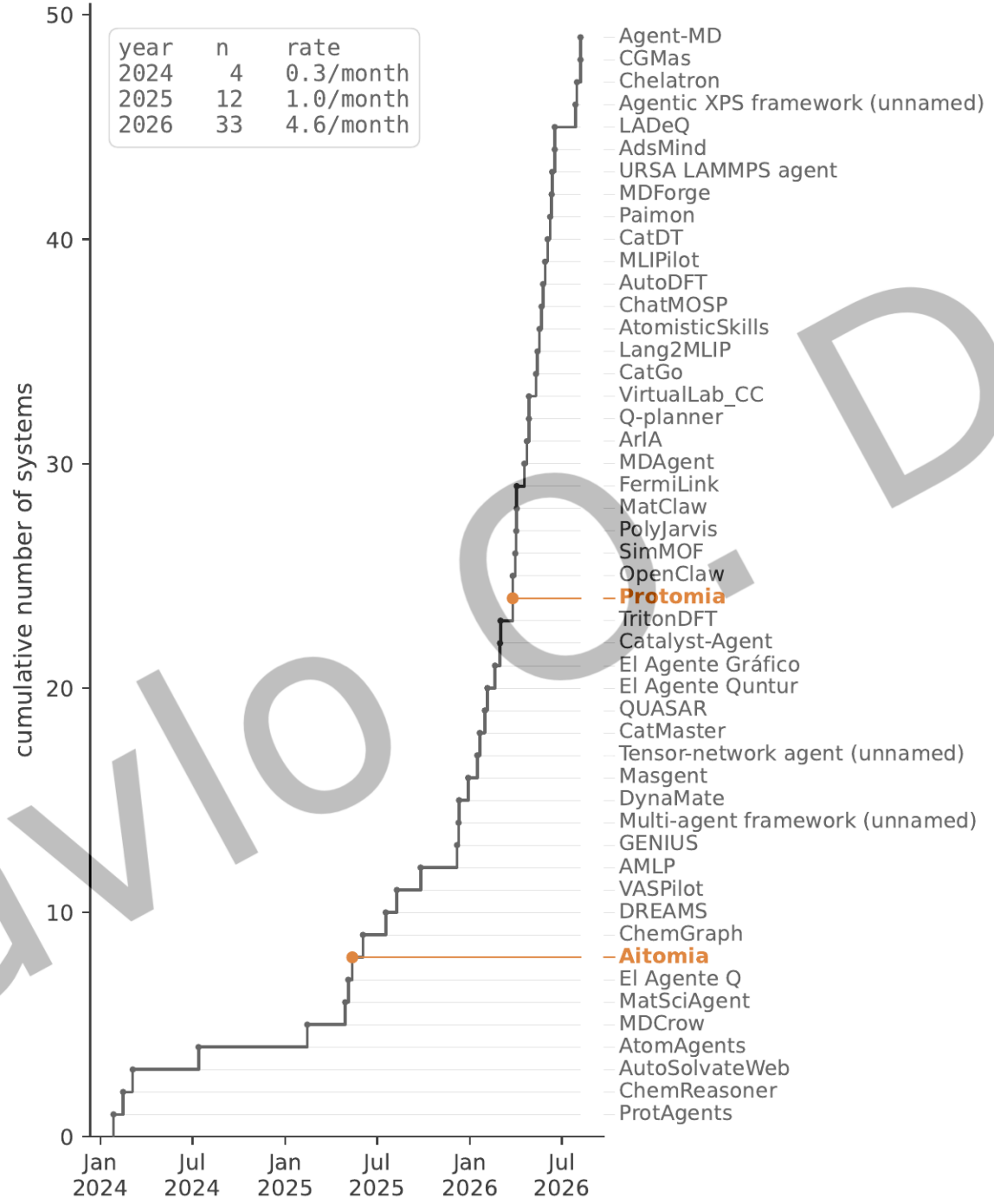
P. O. Dral, H. Nawaz, A. Ullah. Science Done on a Machine by a Machine: AI Agents in Computational Chemistry. **2026**. arXiv:2608.18508



Pavlo O. Dral

P. O. Dral, H. Nawaz, A. Ullah. Science Done on a Machine by a Machine: AI Agents in Computational Chemistry. **2026**. arXiv:2608.18508

P. O. Dral, H. Nawaz, A. Ullah. Science Done on a Machine by a Machine: AI Agents in Computational Chemistry. **2026**. arXiv:2608.18508



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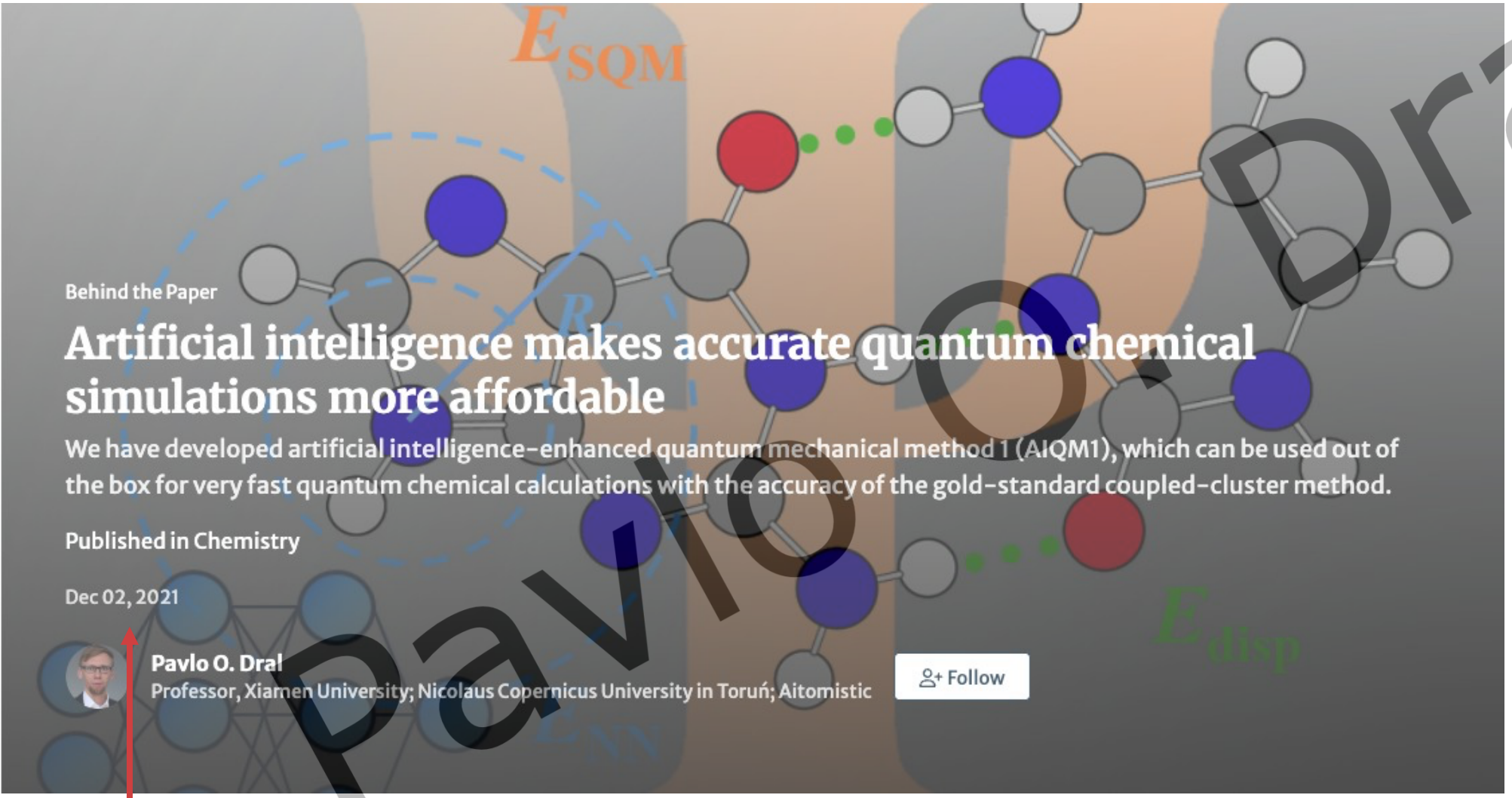
The Vision



ChatGPT:
Nov 30, 2022

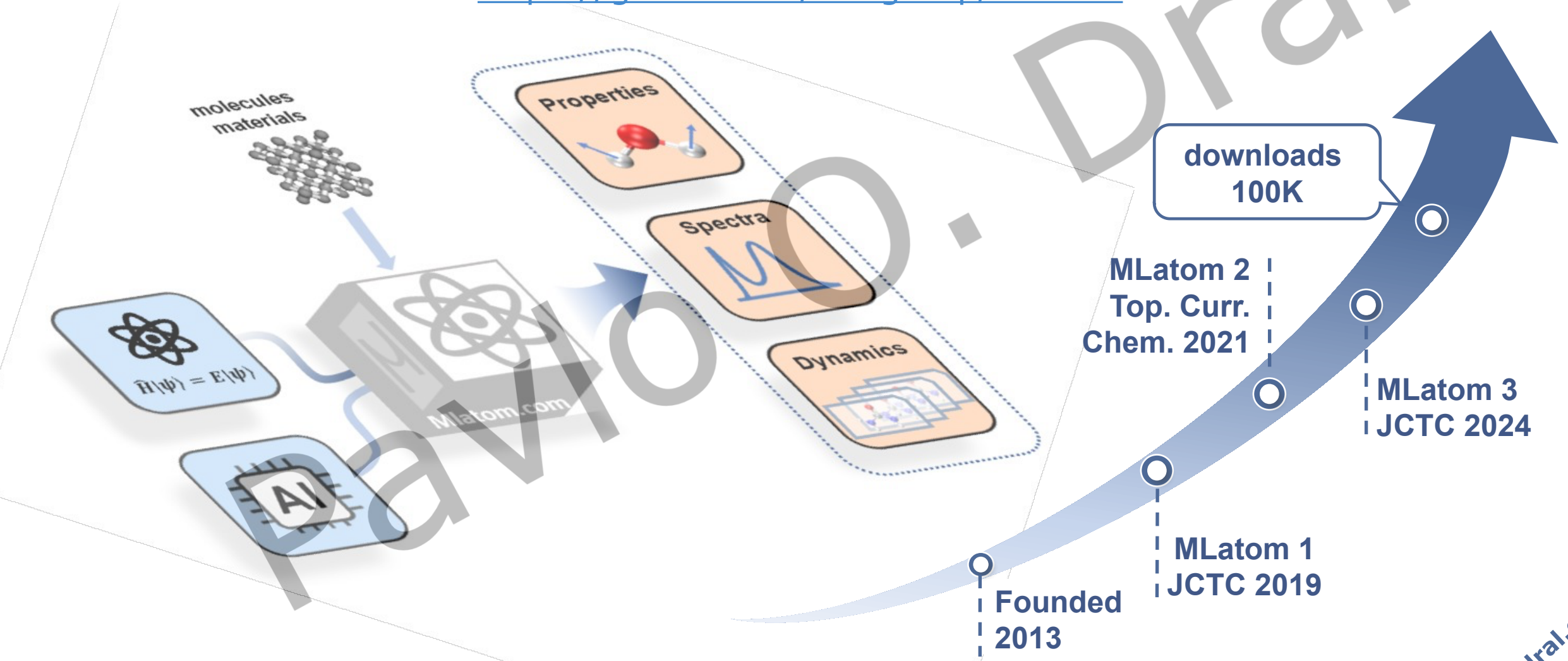
https://communities.springernature.com/posts/artificial-intelligence-makes-accurate-quantum-chemical-simulations-more-affordable

Pavlo O. Dral

Our AI ecosystem for computational chemistry

We develop MLatom – an open-source software ecosystem integrating AI and quantum chemistry

https://github.com/dralgroup/mlatom



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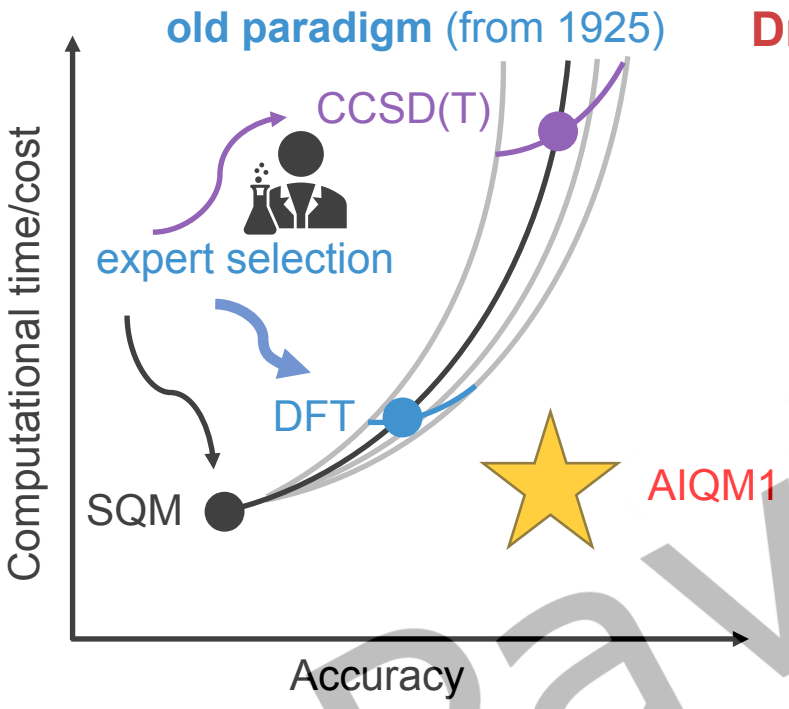
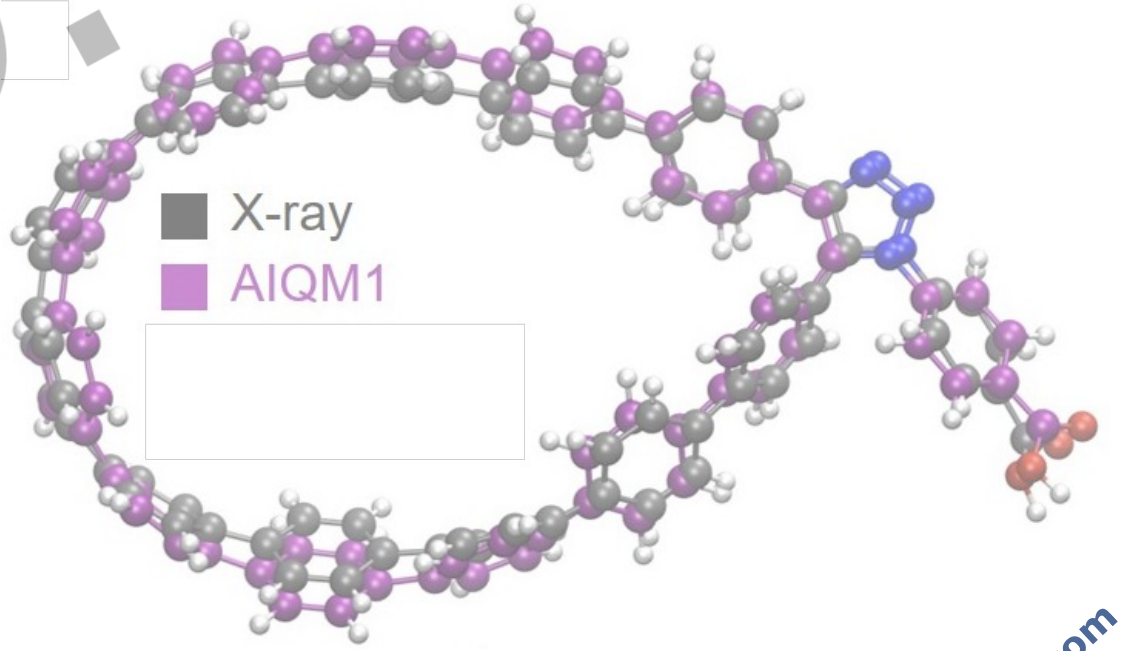
AIQM1

We developed AI models working out of the box, resolving their stability problem



Dral*, *et al. Nat. Commun.* 2021

AIQM1 vs DFT
2 vs 1200 CPU-min
0.625 vs 0.663 Å (RMSD)



AIQM1 vs typical DFT (B3LYP, PBE, ...)

- **Orders of magnitude faster**
- **Accuracy is usually higher**
  for closed-shell, neutral, CHNO molecules

Dral, *et al. J. Chem. Eur. J.* 2023, *29*, e202300668

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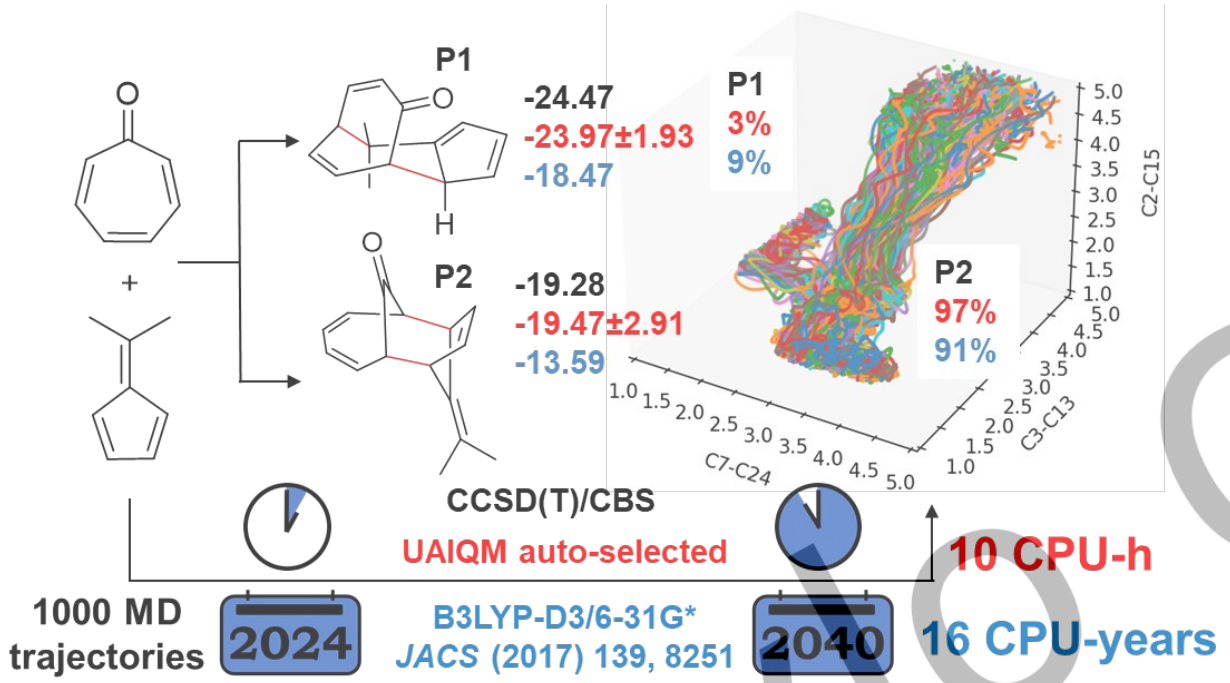
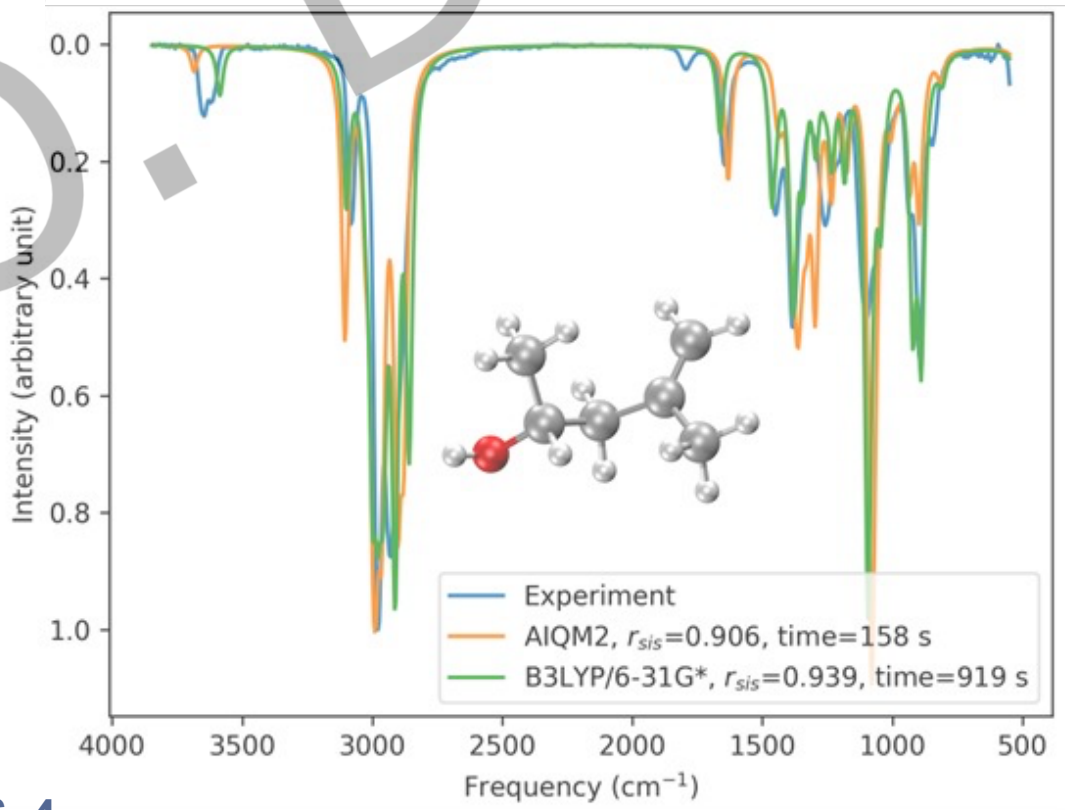
Foundational ML-based potentials



Fast, accurate, and trustworthy AI models for
快速、准确且可靠的人工智能模型用于

- reaction mechanisms, thermochemistry, IR and Raman spectra, MD, many chemical elements...



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

Selected publications on the models:

- Dral*, *et al. Nat. Commun.* 2021, *12*, 7022
- Dral*, *et al. J. Phys. Chem. Lett.* 2022, *13*, 3479; 2025, *16*, 4
- Dral*, *et al. Chem. Sci.* 2025, *16*, 15901

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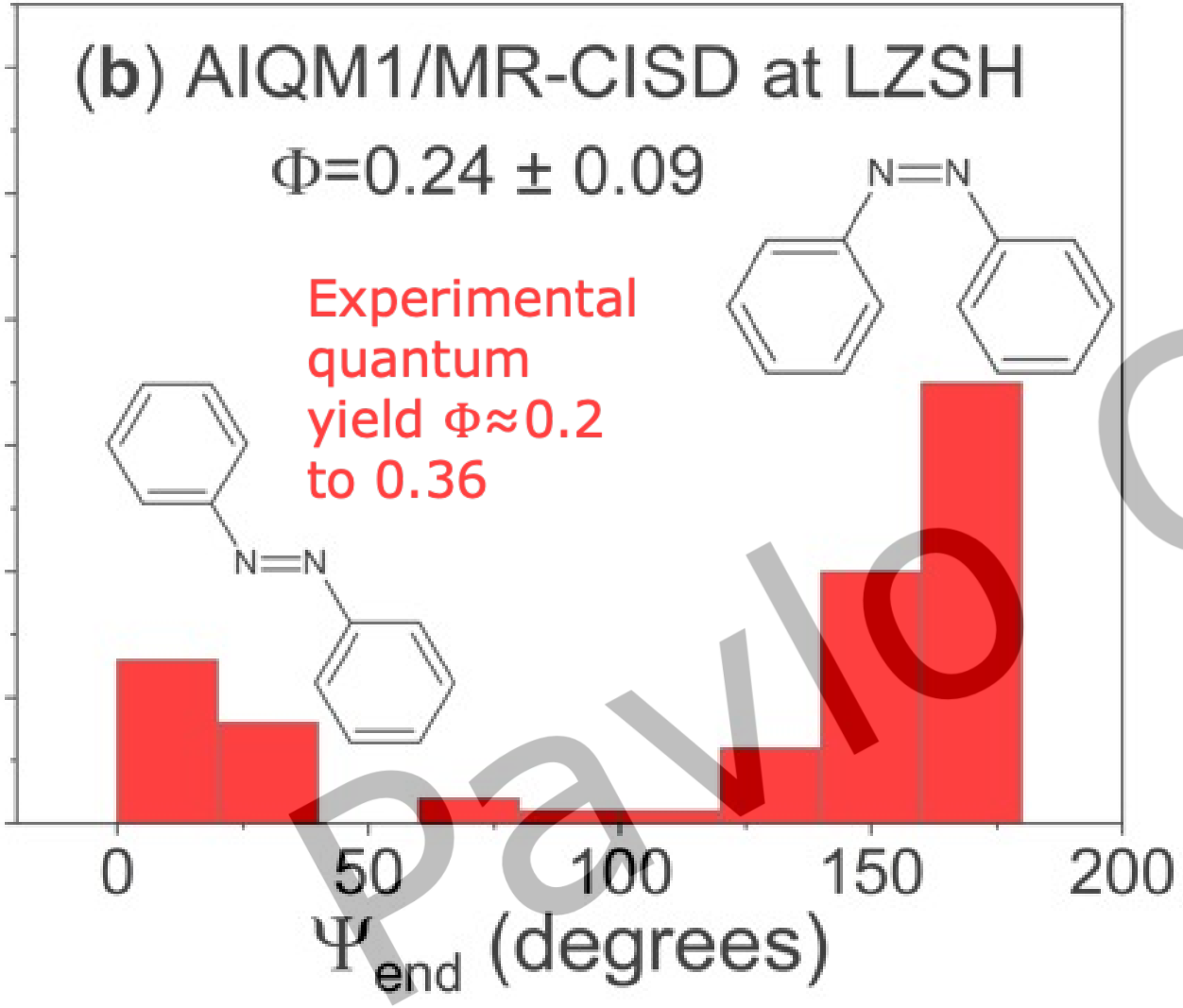
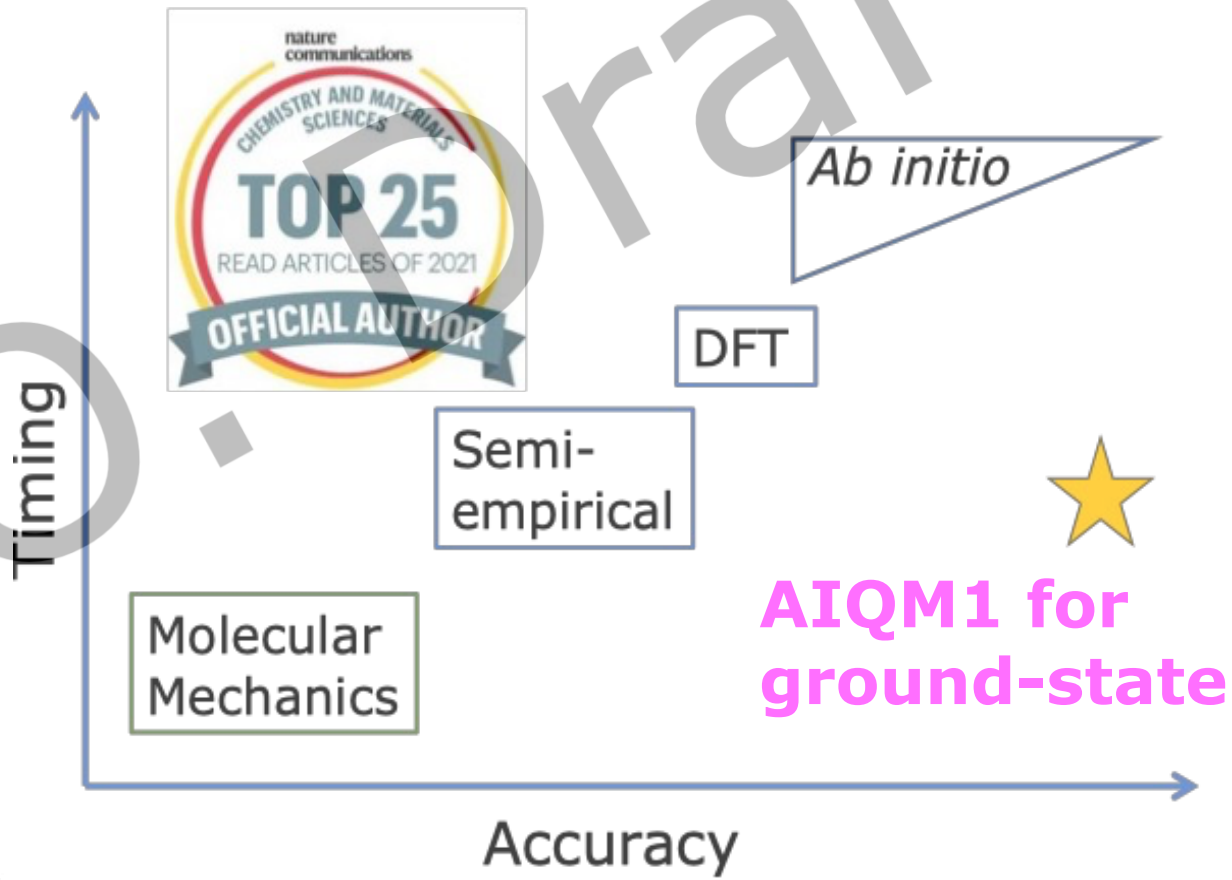
Δ-learning AIQM1 model for TSH





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

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

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Aitomistic

Handing off everything to Protomia

Protomia Solution 2.8.3

The molecule in your folder is **methane (CH_4)** (from `sp.xyz`), and I've submitted the AIQM2 orbital calculation to the cluster — it's running now (SLURM job 183853).

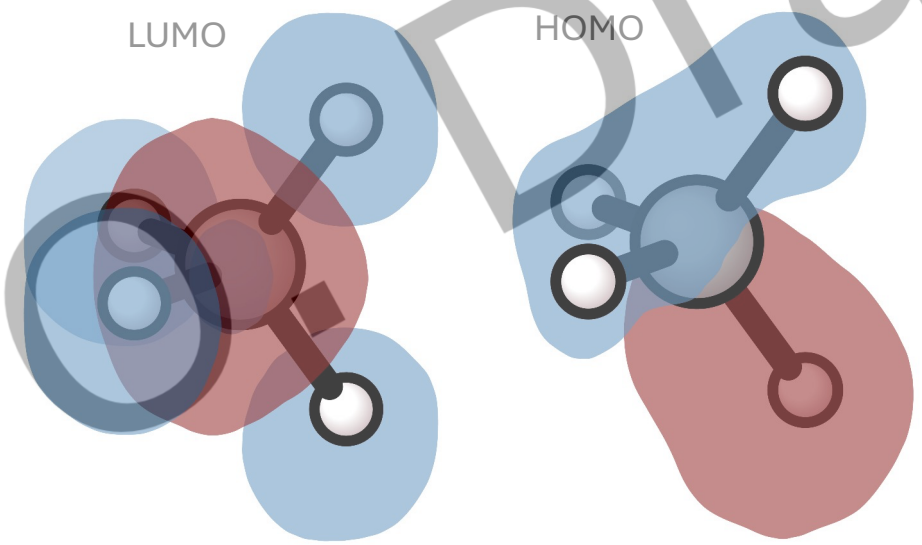
The job runs the single-point AIQM2 energy, then automatically renders the **HOMO** and **LUMO** molecular-orbital surface pictures, so you don't need to do anything else. It should finish quickly — I'll report the orbital energies (HOMO/LUMO in eV), the single-point energy, and the rendered orbital images to you as soon as it's done. Feel free to keep chatting in the meantime!

The methane (CH_4) AIQM2 orbital calculation has finished — here are the results:

Single-point energy (AIQM2): −40.464860 Hartree (dipole moment: 0.0 D, as expected for this T_{4s}-symmetric geometry)

Frontier molecular orbitals:

- **HOMO: −12.6931 eV**
- **LUMO: 4.4160 eV**
- **HOMO–LUMO gap: 17.1092 eV**



Visualization of HOMO and LUMO orbitals of methane calculated with AIQM2 by Protomia

Aitomistic Lab@XMU
atom.xmu.edu.cn

Docs of MLatom3
mlatom.com/docs

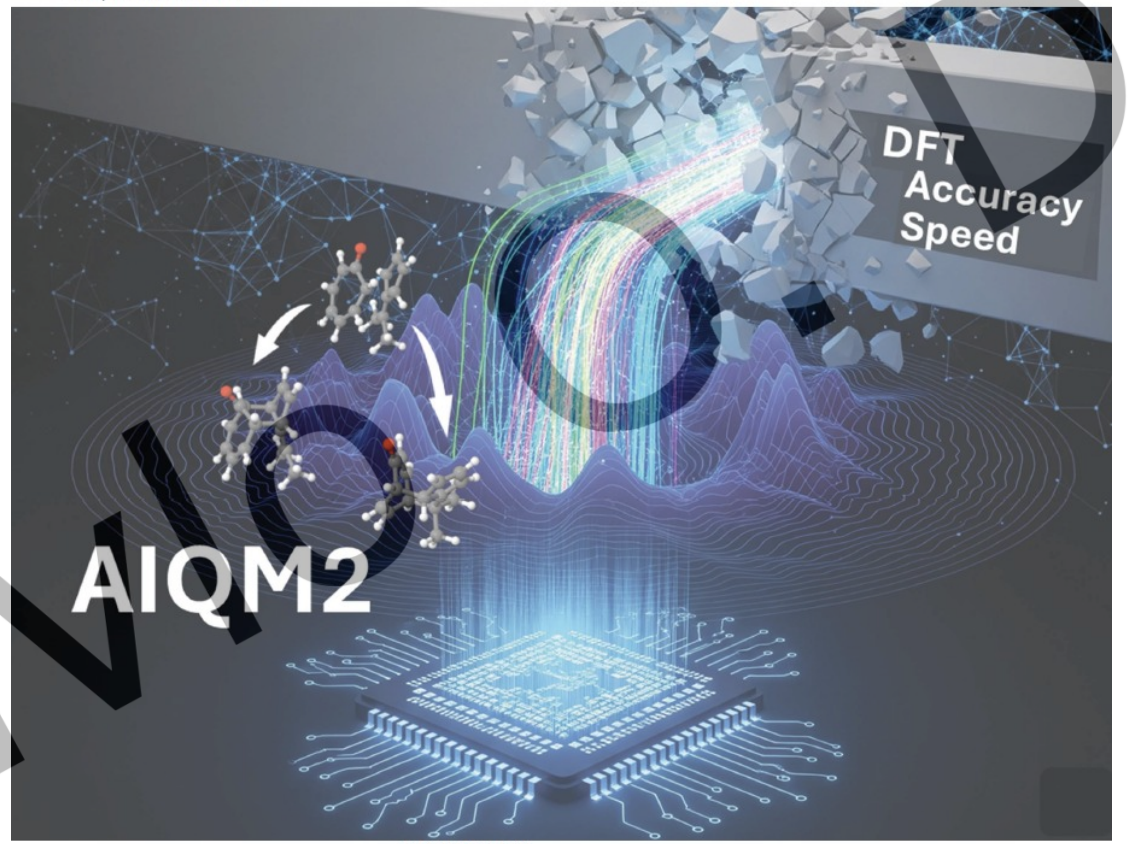
Pavlo Pral

Aitomistic

Volume 16
Number 35
21 September 2025
Pages 15745–16358

Chemical Science

rsc.li/chemical-science



ISSN 2041-6539

ROYAL SOCIETY OF CHEMISTRY

EDGE ARTICLE
Yuxinxin Chen and Pavlo O. Dral
AIQM2: organic reaction simulations beyond DFT

15 YEARS ANNIVERSARY

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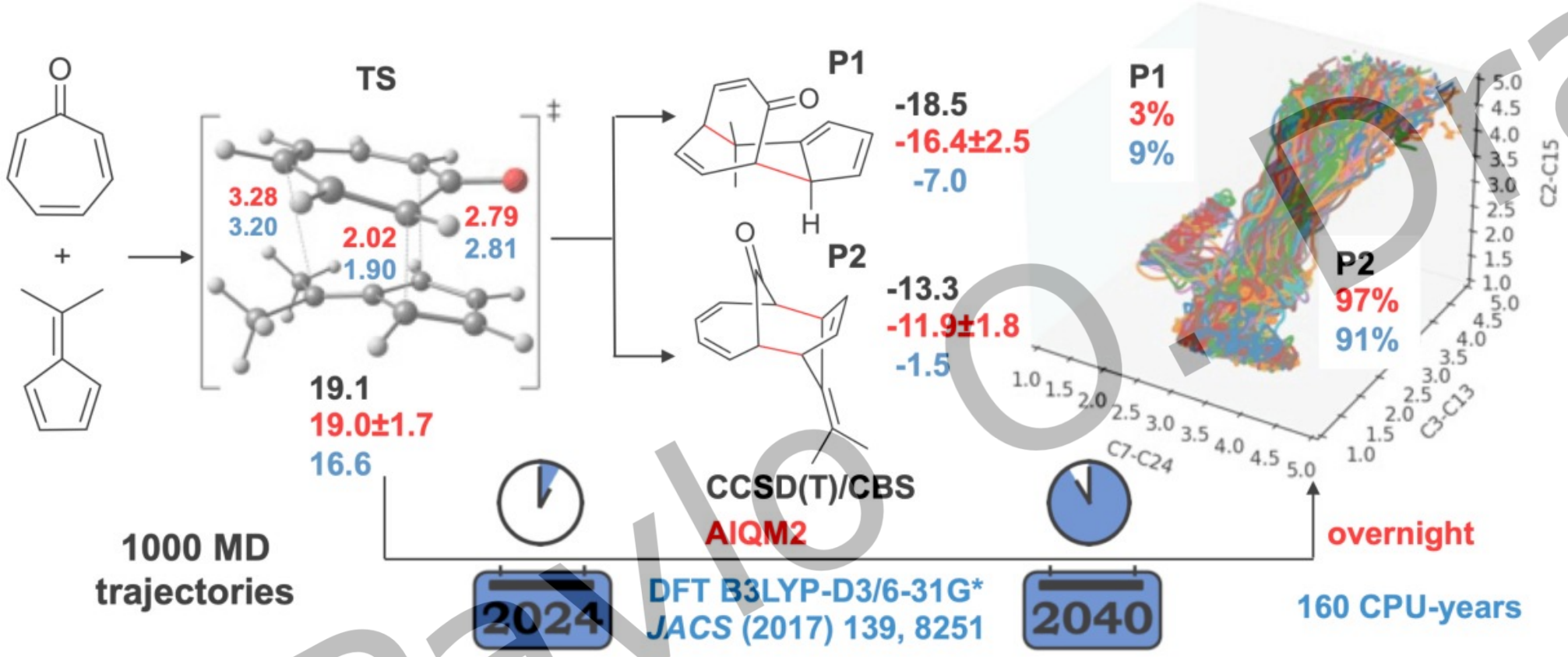
AIQM2



- Fast
- Accurate
- Trustworthy

Y. Chen, P. O. Dral. AIQM2: Organic Reaction Simulations Beyond DFT. *Chem. Sci.* **2025**, *16*, 15901

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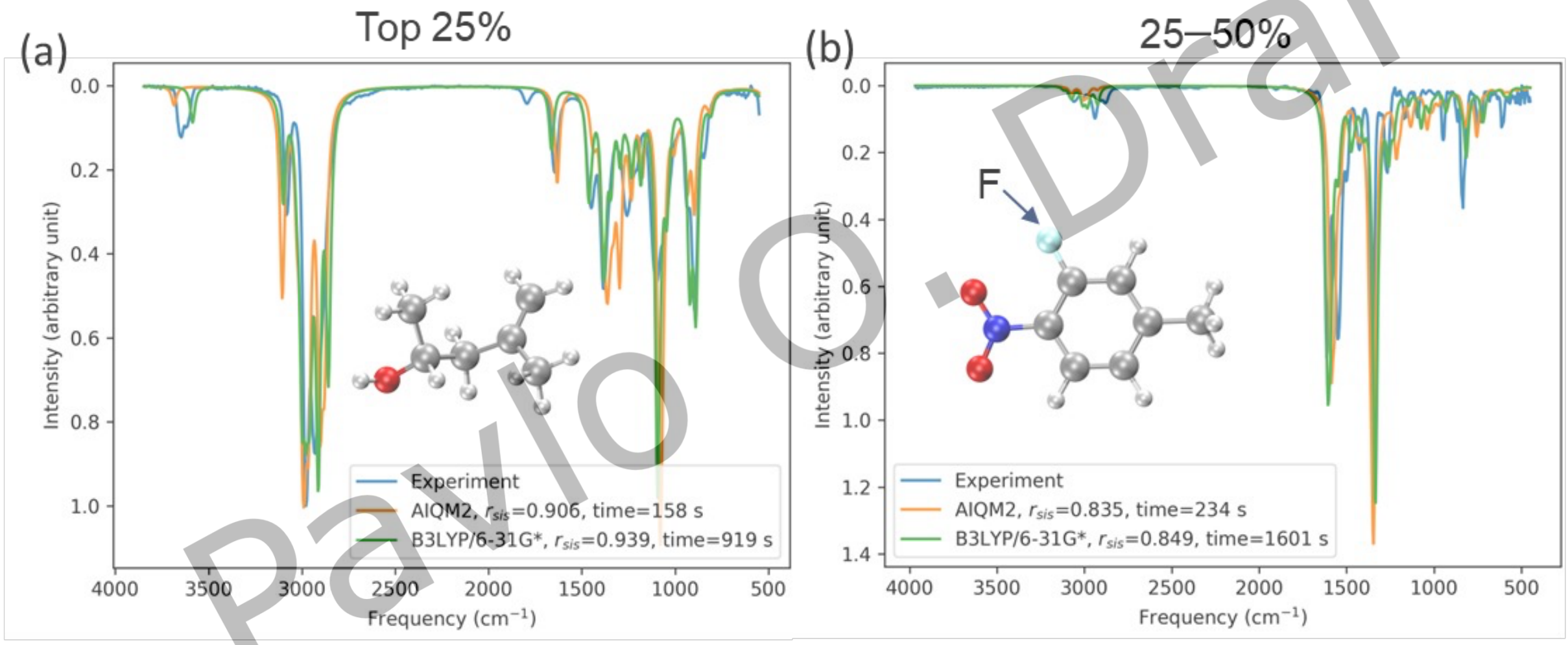
IR spectra with AIQM2



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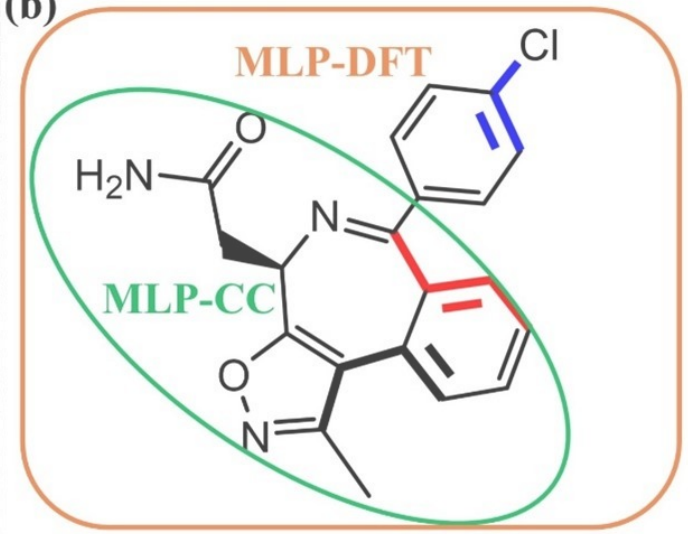
Y.-F. Hou, C. Wang, P. O. Dral. *J. Phys. Chem. A* **2025,** *129*, 3613.

(a)

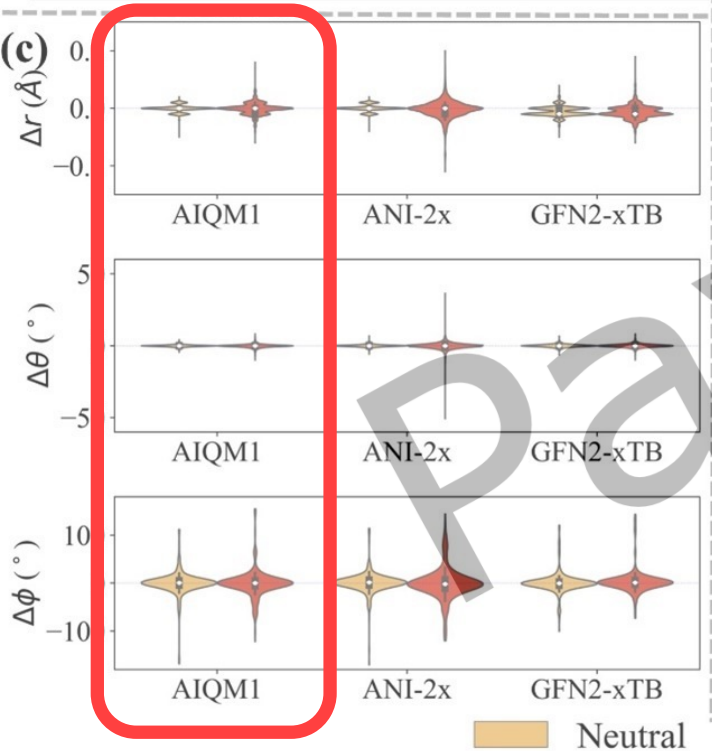
	Methods
M1	ONIOM2(DFT:MM)
M2	ONIOM2-EE(DFT:MM)
M3	ONIOM2(ANI-2x:MM)
M4	ONIOM2(ANI-1ccx:MM)
M4a	ONIOM3(ANI-1ccx:ANI-2x:MM)[b]
M5	ONIOM2(AIQM1:MM)[c]
M5a	ONIOM3(AIQM1:ANI-2x:MM)[b]
M6	ONIOM2(SE:MM)
M7	ONIOM3(DFT:SE:MM)
M8	ONIOM3(ANI-2x:SE:MM)
M9	ONIOM3(ANI-1ccx:SE:MM)
M9a	ONIOM4(ANI-1ccx:ANI-2x:SE:MM)[b]
M10	ONIOM3(AIQM1:SE:MM)[c]
M10a	ONIOM4(AIQM1:ANI-2x:SE:MM)[b]
M6R	ONIOM2(SE:MM)[d]

(b)

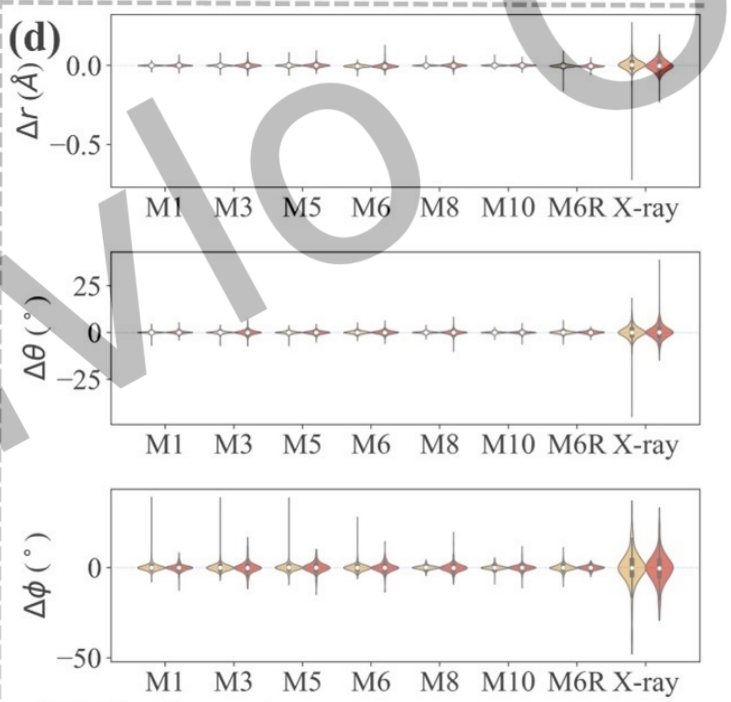


ONIOM2(MLP-CC:MLP-DFT)
ONIOM2(MLP:xTB)

(c)



(d)



Neutral Charged

Article | Open access | Published: 16 May 2024

Accelerating reliable multiscale quantum refinement of protein–drug systems enabled by machine learning

Zeyin Yan, Dacong Wei, Xin Li & Lung Wa Chung

Nature Communications **15**, Article number: 4181 (2024) | Cite this article

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Aitomistic

ACS Publications
Most Trusted. Most Cited. Most Read.

Search text, DOI, authors, etc.

Advanced Search

Integrating Machine Learning Interatomic Potentials with MMPBSA for Accurate Protein–Ligand Binding Free Energy Calculations

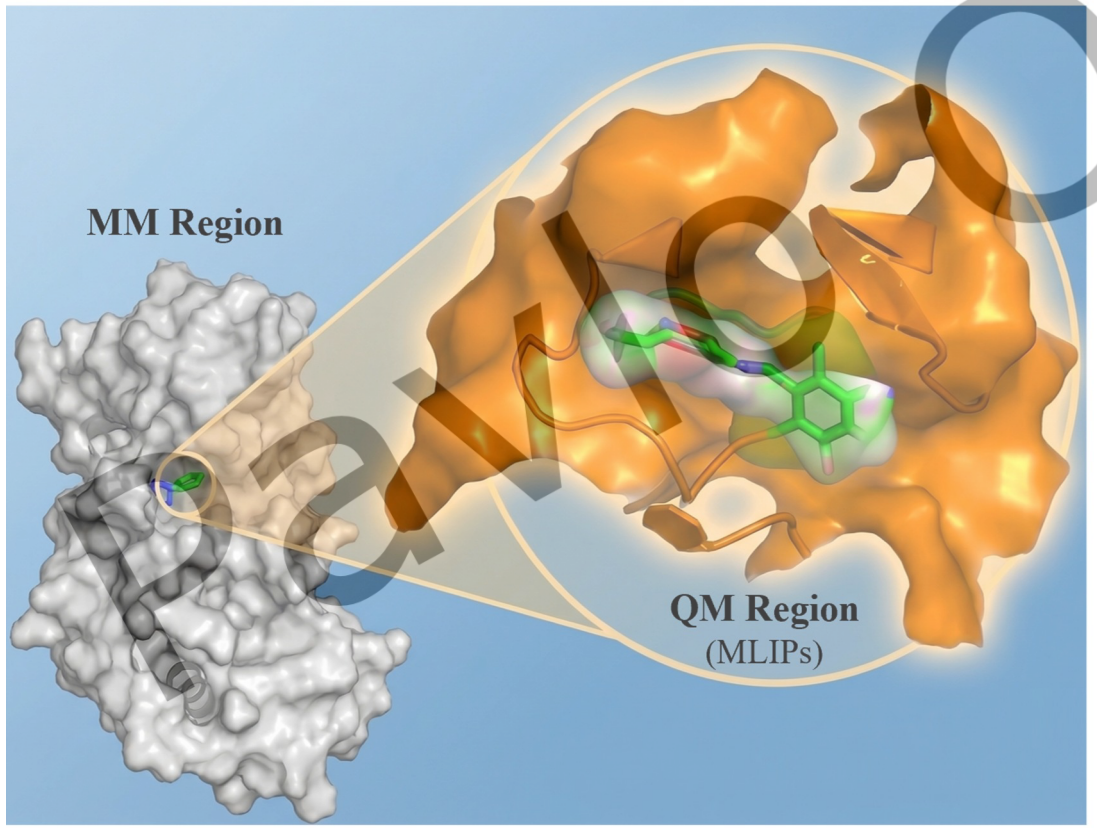
Xue-Xin Wei, Yuxinxin Chen, Yuedong Yang, Mingyuan Xu*, Pavlo O. Dral*, and Hongming Chen*

Open PDF

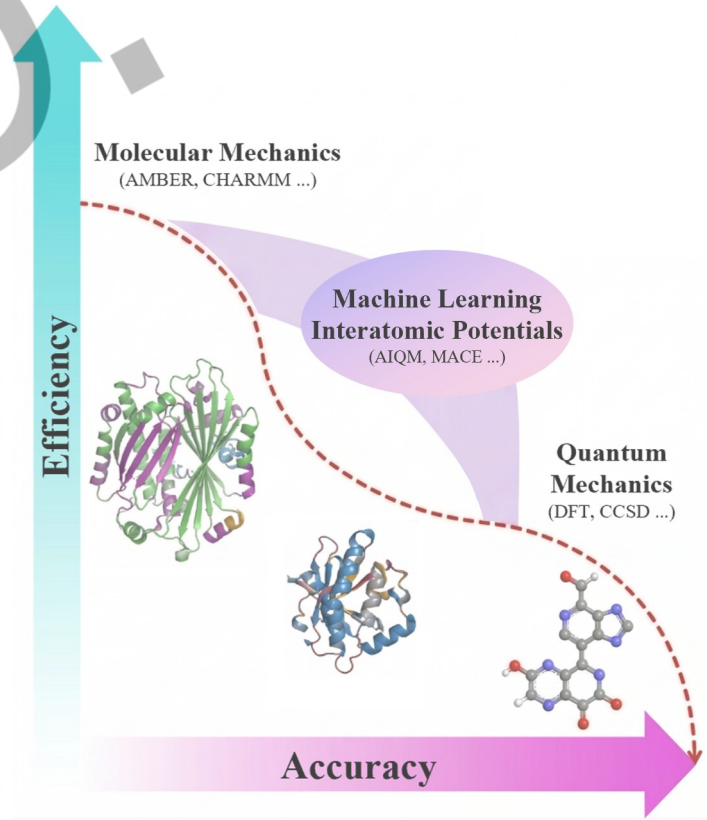
Supporting Information (1)

XMU

ONIOM(MLIP:MM)



Accuracy Meets Efficiency



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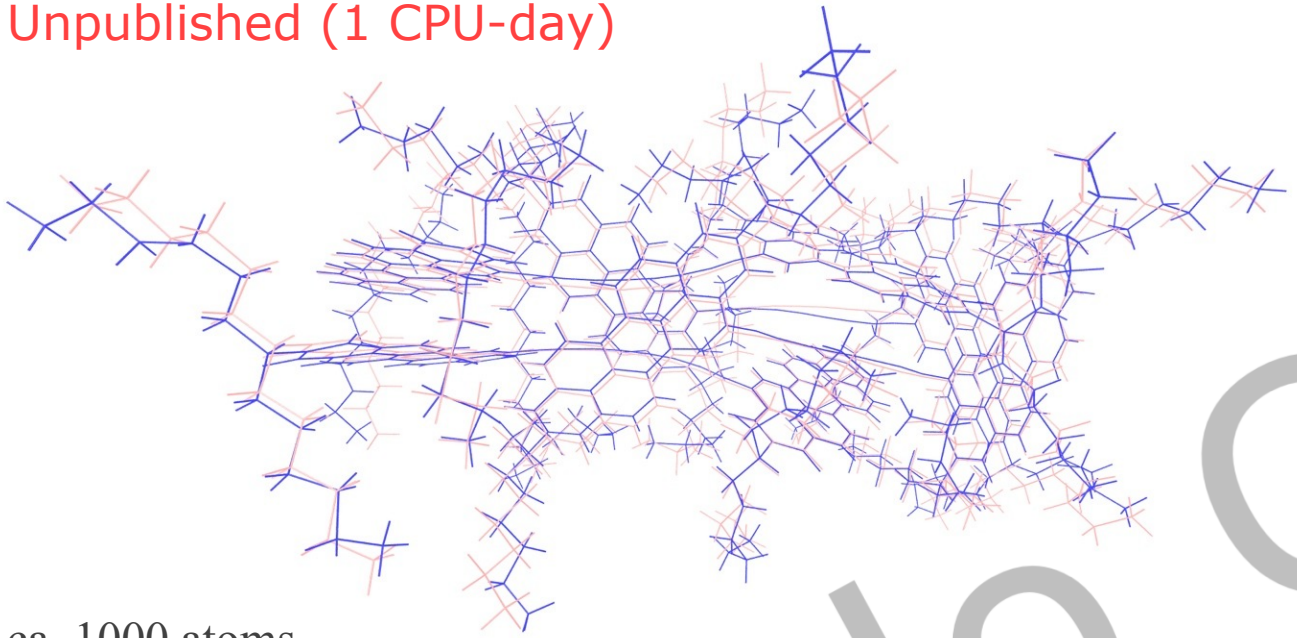
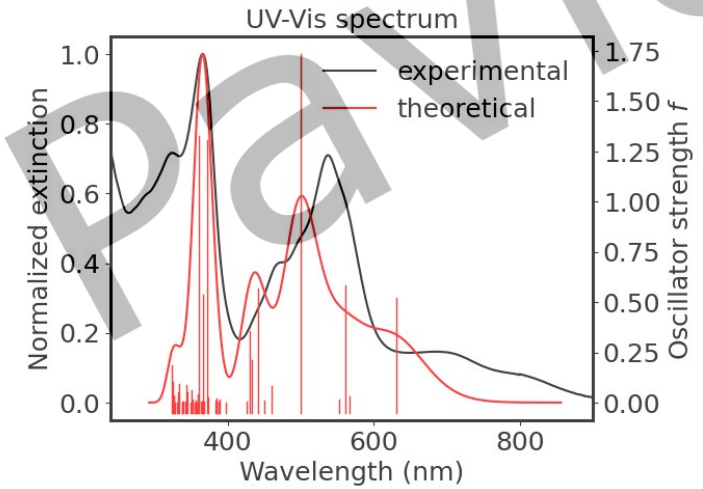
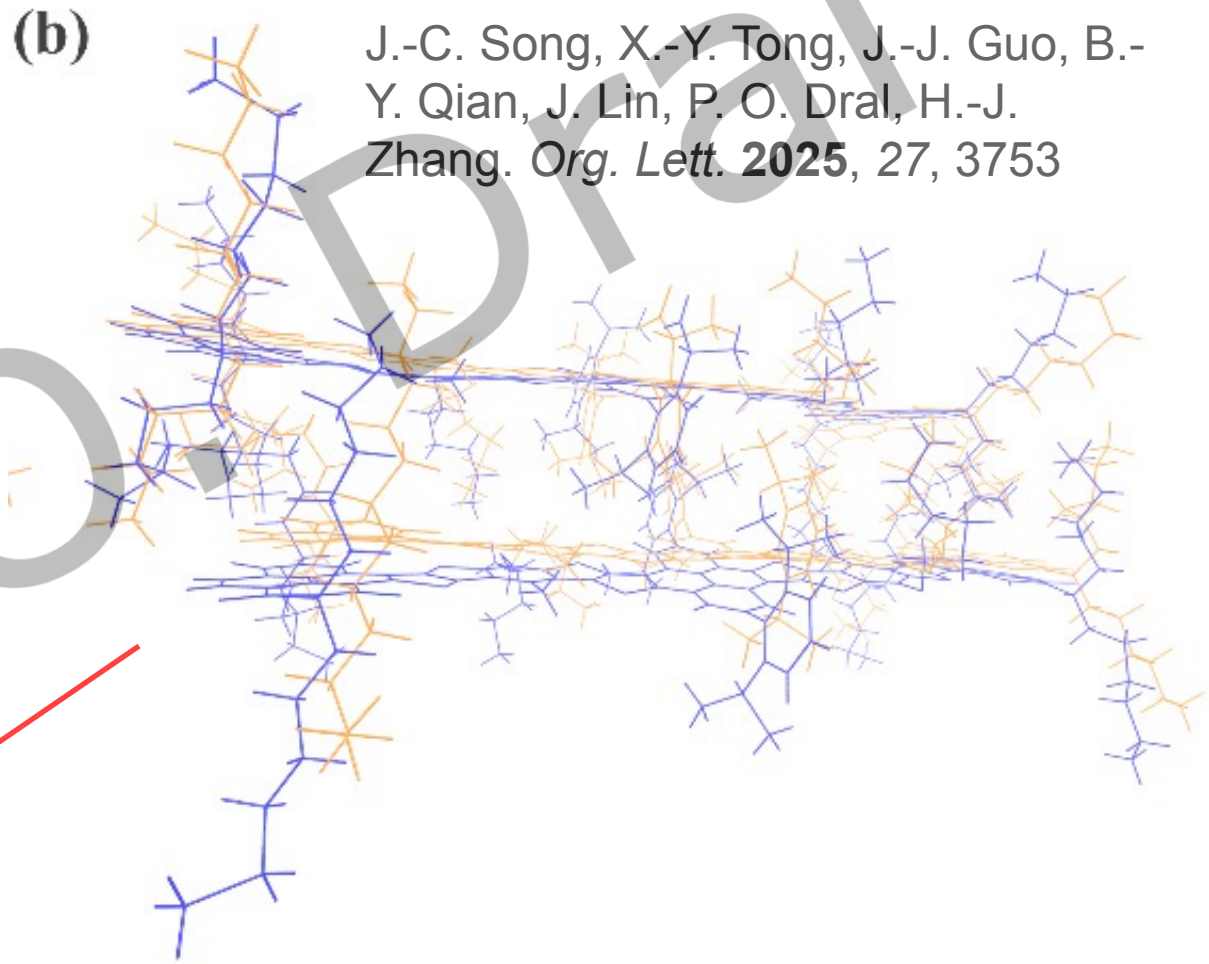
Unpublished (1 CPU-day)



ca. 1000 atoms,
agreement with crystallographic structure: 0.63 Å





J.-C. Song, X.-Y. Tong, J.-J. Guo, B.-Y. Qian, J. Lin, P. O. Dral, H.-J. Zhang. *Org. Lett.* **2025**, *27*, 3753

714 atoms,
agreement with crystallographic structure: 2.948 Å

Pavlo O. Dral

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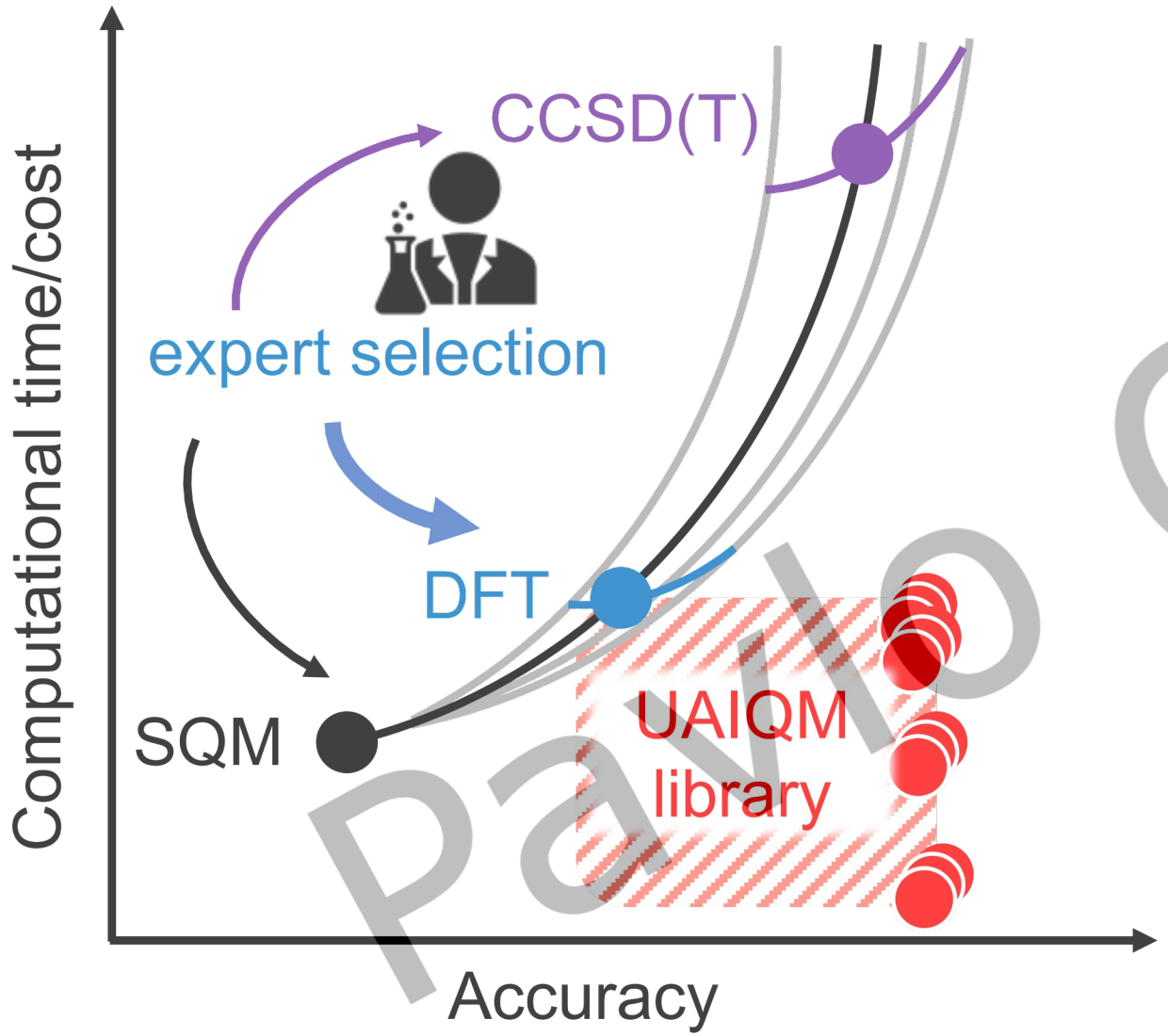
UAIQM: Universal and Updatable AI-QM models



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

name	keywords in MLatom	version	target level	baseline	dispersion	recommended elements
-	uaiqm_nobaseline@dft	20240606	DFT	-	D4 (ωB97X)	H C N O
ANI-1ccx	uaiqm_nobaseline@cc	20190701	CC	-	-	H C N O
-	uaiqm_nobaseline@cc	20240606	CC	-	D4 (ωB97X)	H C N O
AIQM1@DFT	uaiqm_odm2star@dft	20211202	DFT	ODM2*	D4 (ωB97X)	H C N O
AIQM1	uaiqm_odm2star@cc	20211202	CC	ODM2*	D4 (ωB97X)	H C N O
-	uaiqm_odm2star@cc	20240308	CC	ODM2*	D4 (ωB97X)	H C N O
AIQM2@DFT	uaiqm_gfn2xtbstar@dft	20240106	DFT	GFN2-xTB*	D4 (ωB97X)	H C N O
AIQM3@DFT	uaiqm_gfn2xtbstar@dft	20240619	DFT	GFN2-xTB*	D3bj (b97-3c)	H C N O F S Cl
AIQM4@DFT (?)	uaiqm_gfn2xtbstar@dft	20240730	DFT	GFN2-xTB*	D3bj (b97-3c)	H B C N O F Si P S Cl As Se Br I
AIQM2	uaiqm_gfn2xtbstar@cc	20240106	CC	GFN2-xTB*	D4 (ωB97X)	H C N O
AIQM3	uaiqm_gfn2xtbstar@cc	20250115	CC	GFN2-xTB*	D3bj (b97-3c)	H C N O F S Cl
-	uaiqm_wb97x631gp@cc	20230924	CC	ωB97X/6-31G*	D4 (ωB97X)	H C N O
-	uaiqm_wb97xdef2tzvpp@cc	20230923	CC	ωB97X/def2-TZVPP	D4 (ωB97X)	H C N O
-	uaiqm_wb97xdef2tzvpp@cc	20240227	CC	ωB97X/def2-TZVPP	D4 (ωB97X)	H C N O
-	uaiqm_wb97xdef2tzvpp@cc	20240228	CC	ωB97X/def2-TZVPP	D4 (ωB97X)	H C N O

Pavlo O. Dral

Aitomistic

More accurate description of more elements...

Excellent ~CCSD(T) level

Supported max. DFT level

Unsupported

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIIIB	VIIIB	VIIIB	IB	IIB	IIIA	IVA	VA	VIA	VIIA	VIIIA
1 H Hydrogen 1.01																	2 He Helium 4.00
3 Li Lithium 6.94	4 Be Beryllium 9.01											5 B Boron 10.81	6 C Carbon 12.01	7 N Nitrogen 14.01	8 O Oxygen 16.00	9 F Fluorine 19.00	10 Ne Neon 20.18
11 Na Sodium 22.99	12 Mg Magnesium 24.31											13 Al Aluminum 26.98	14 Si Silicon 28.09	15 P Phosphorus 30.97	16 S Sulfur 32.06	17 Cl Chlorine 35.45	18 Ar Argon 39.95
19 K Potassium 39.10	20 Ca Calcium 40.08	21 Sc Scandium 44.96	22 Ti Titanium 47.87	23 V Vanadium 50.94	24 Cr Chromium 52.00	25 Mn Manganese 54.94	26 Fe Iron 55.85	27 Co Cobalt 58.93	28 Ni Nickel 58.69	29 Cu Copper 63.55	30 Zn Zinc 65.38	31 Ga Gallium 69.72	32 Ge Germanium 72.63	33 As Arsenic 74.92	34 Se Selenium 78.97	35 Br Bromine 79.90	36 Kr Krypton 83.80
37 Rb Rubidium 85.47	38 Sr Strontium 87.62	39 Y Yttrium 88.91	40 Zr Zirconium 91.22	41 Nb Niobium 92.91	42 Mo Molybdenum 95.95	43 Tc Technetium (98)	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.91	46 Pd Paladium 106.42	47 Ag Silver 107.87	48 Cd Cadmium 112.41	49 In Indium 114.82	50 Sn Tin 118.71	51 Sb Antimony 121.76	52 Te Tellurium 127.60	53 I Iodine 126.90	54 Xe Xenon 131.29
55 Cs Cesium 132.91	56 Ba Barium 137.33	57 - 71 Lanthanides	72 Hf Hafnium 178.49	73 Ta Tantalum 180.95	74 W Tungsten 183.84	75 Re Rhenium 186.21	76 Os Osmium 190.23	77 Ir Iridium 192.22	78 Pt Platinum 195.08	79 Au Gold 196.97	80 Hg Mercury 200.59	81 Tl Thallium 204.38	82 Pb Lead 207.20	83 Bi Bismuth 208.98	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222)
87 Fr Francium (223)	88 Ra Radium (226)	89 - 103 Actinides	104 Rf Rutherfordium (265)	105 Db Dubnium (268)	106 Sg Seaborgium (271)	107 Bh Bohrium (270)	108 Hs Hassium (277)	109 Mt Meitnerium (276)	110 Ds Darmstadtium (281)	111 Rg Roentgenium (280)	112 Cn Copernicium (285)	113 Nh Nihonium (284)	114 Fl Flerovium 289	115 Mc Moscovium (288)	116 Lv Livermorium (293)	117 Ts Tennessine (294)	118 Og Oganesson (294)

Charged species, radicals, dissociations, multi-reference cases, bigger systems...

57 La Lanthanum 138.91	58 Ce Cerium 140.12	59 Pr Praseodymium 140.91	60 Nd Neodymium 144.24	61 Pm Promethium (145)	62 Sm Samarium 150.36	63 Eu Europium 151.96	64 Gd Gadolium 157.25	65 Tb Terbium 158.93	66 Dy Dysprosium 162.50	67 Ho Holmium 164.93	68 Er Erbium 167.26	69 Tm Thulium 168.93	70 Yb Ytterbium 173.05	71 Lu Lutetium 174.97
89 Ac Actinium (227)	90 Th Thorium 232.04	91 Pa Protactinium 231.04	92 U Uranium 238.03	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (259)	103 Lr Lawrencium (262)

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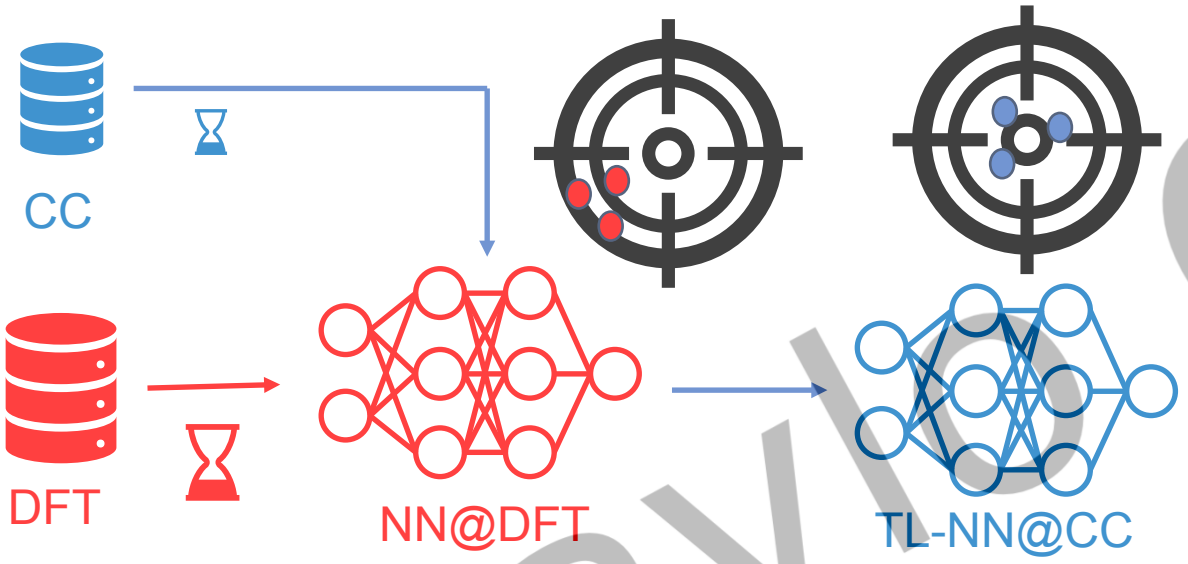
Transfer learning/Fine-tuning



- × two-step training
- × separate models
- × cannot be trained on combined databases

Fine-tuning of AIQM, ANI, OMNI-P models: https://aitomistic.com/mlatom/tutorial_finetuning.html

Seyedeh Fatemeh Alavi, Yuxinxin Chen, Yi-Fan Hou, Fuchun Ge, Peikun Zheng, Pavlo O. Dral. ANI-1ccx-gelu Universal Interatomic Potential and Its Fine-Tuning: Toward Accurate and Efficient Anharmonic Vibrational Frequencies. *J. Phys. Chem. Lett.* **2025**, *16*, 483

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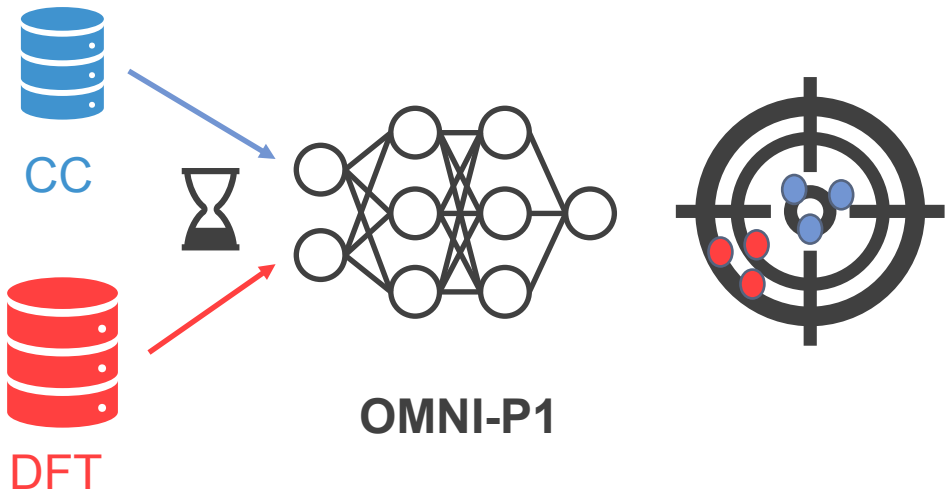
All-in-one AI model



- ✓ easy to train and predict
- ✓ single model
- ✓ can be trained on combined databases

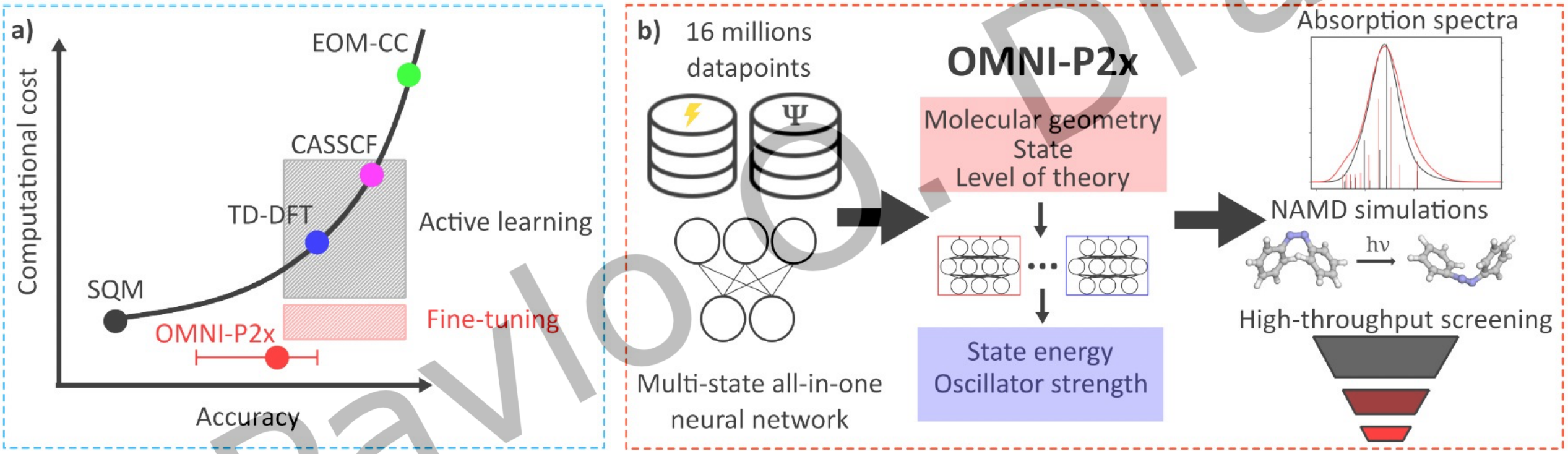
Pavlo O. Dral

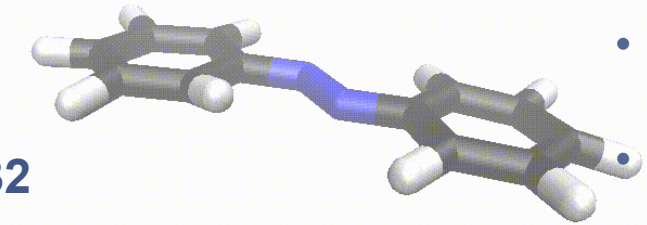
Y. Chen, P. O. Dral. All-in-one foundational models learning across quantum chemical levels. **2024**. *Preprint on ChemRxiv*: https://doi.org/10.26434/chemrxiv-2024-ng3ws

AI models for excited states

First-ever excited-state NNP

- **Much more difficult than ground state**





- **photodynamics**
- **photoreaction quantum yields**
- **...**

Selected publications:

OMNI-P2x: Dral. Nat. Commun., 2026, *17*, 4949.

Novel architecture: Dral*, *et al. npj Comput. Mater.* 2025, *11*, 132

Dral*, Barbatti*. *Nat. Rev. Chem.* 2021, *5*, 388

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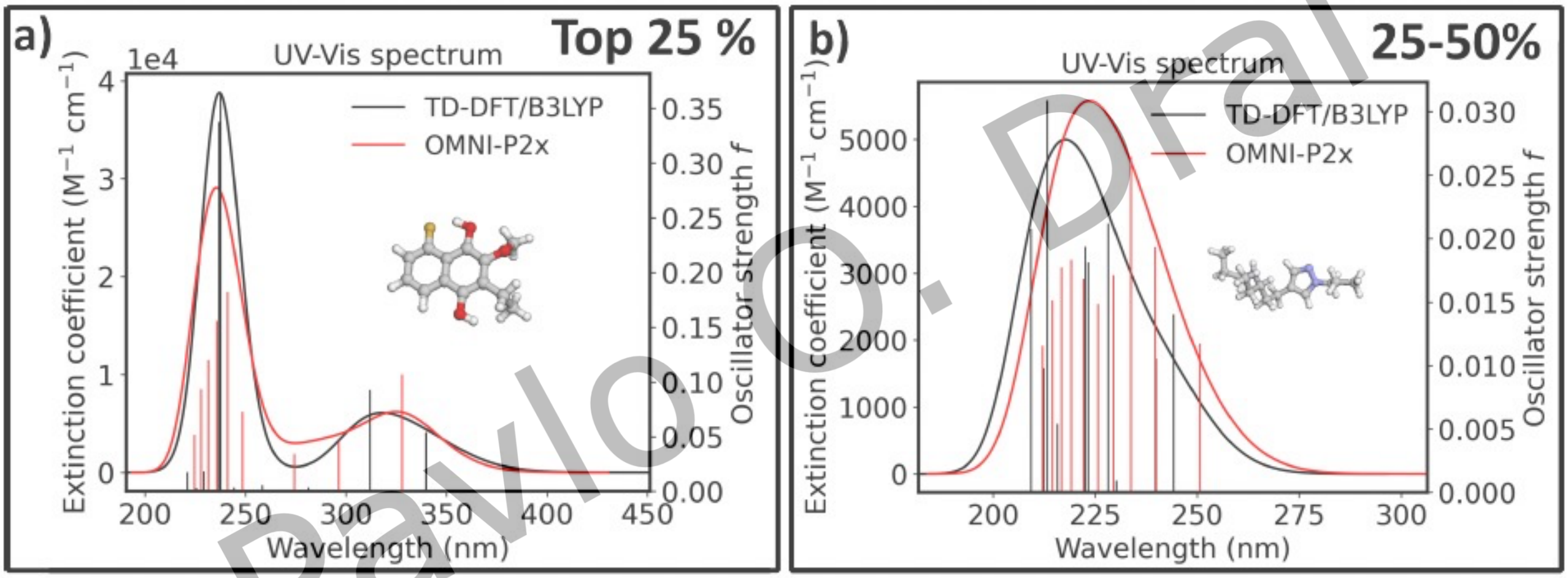
dr-dral.com

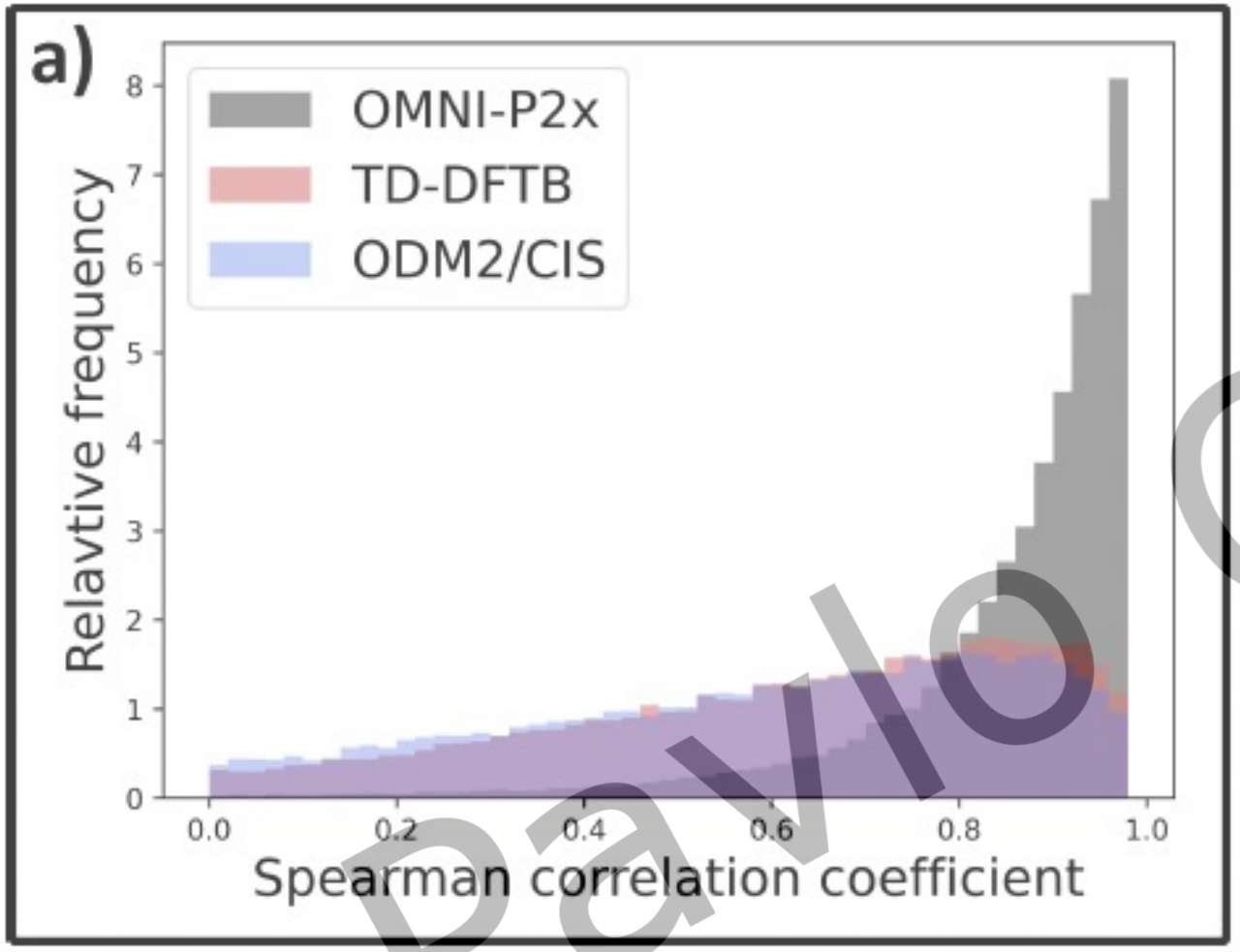
OMNI-P2x – the first universal excited-state potential

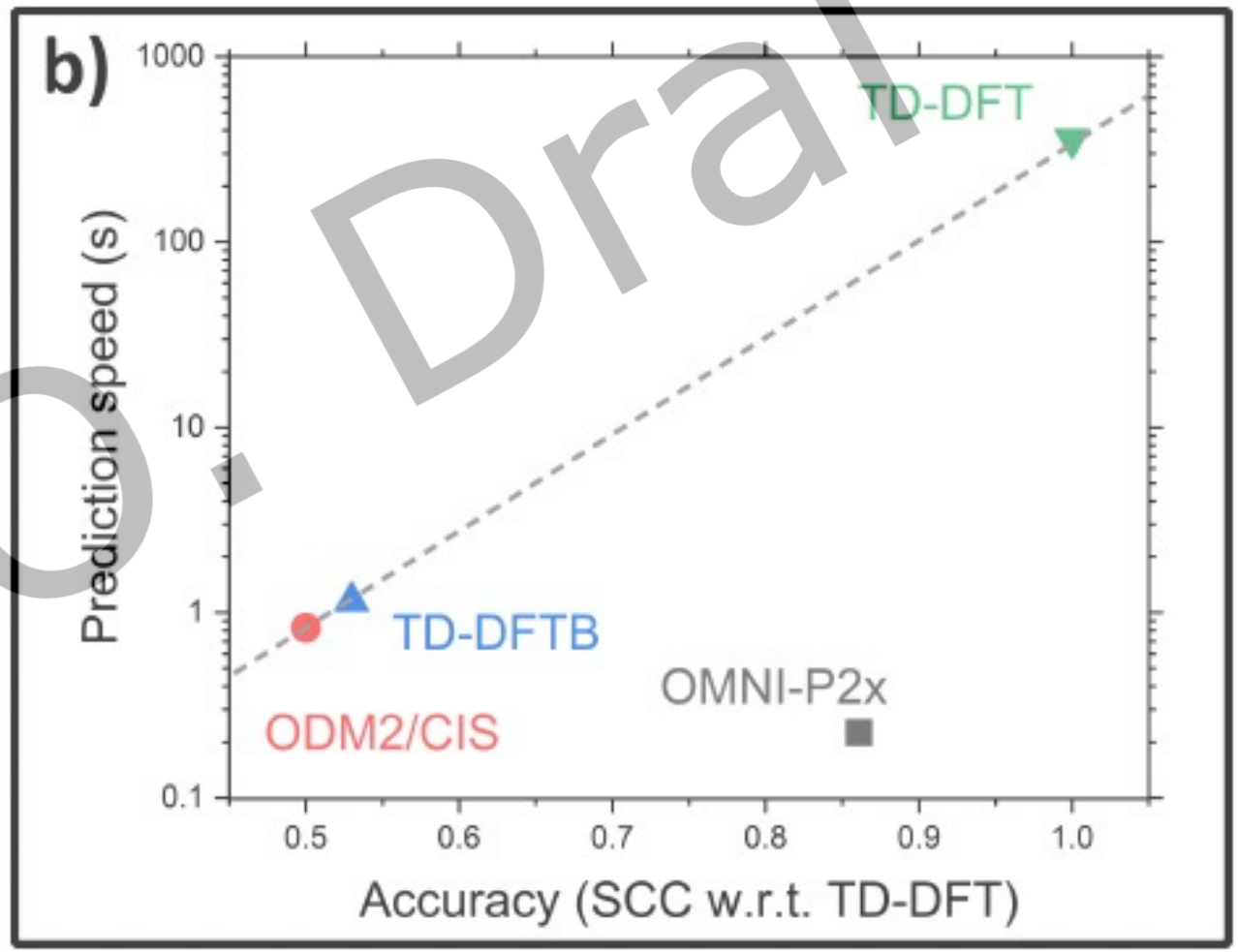


Pavlo O. Dral

M. Martyka, X.-Y. Tong, J. Jankowska, P. O. Dral. *Nat. Commun.* **2026**, *17*, 4949

OMNI-P2x – the first universal excited-state potential





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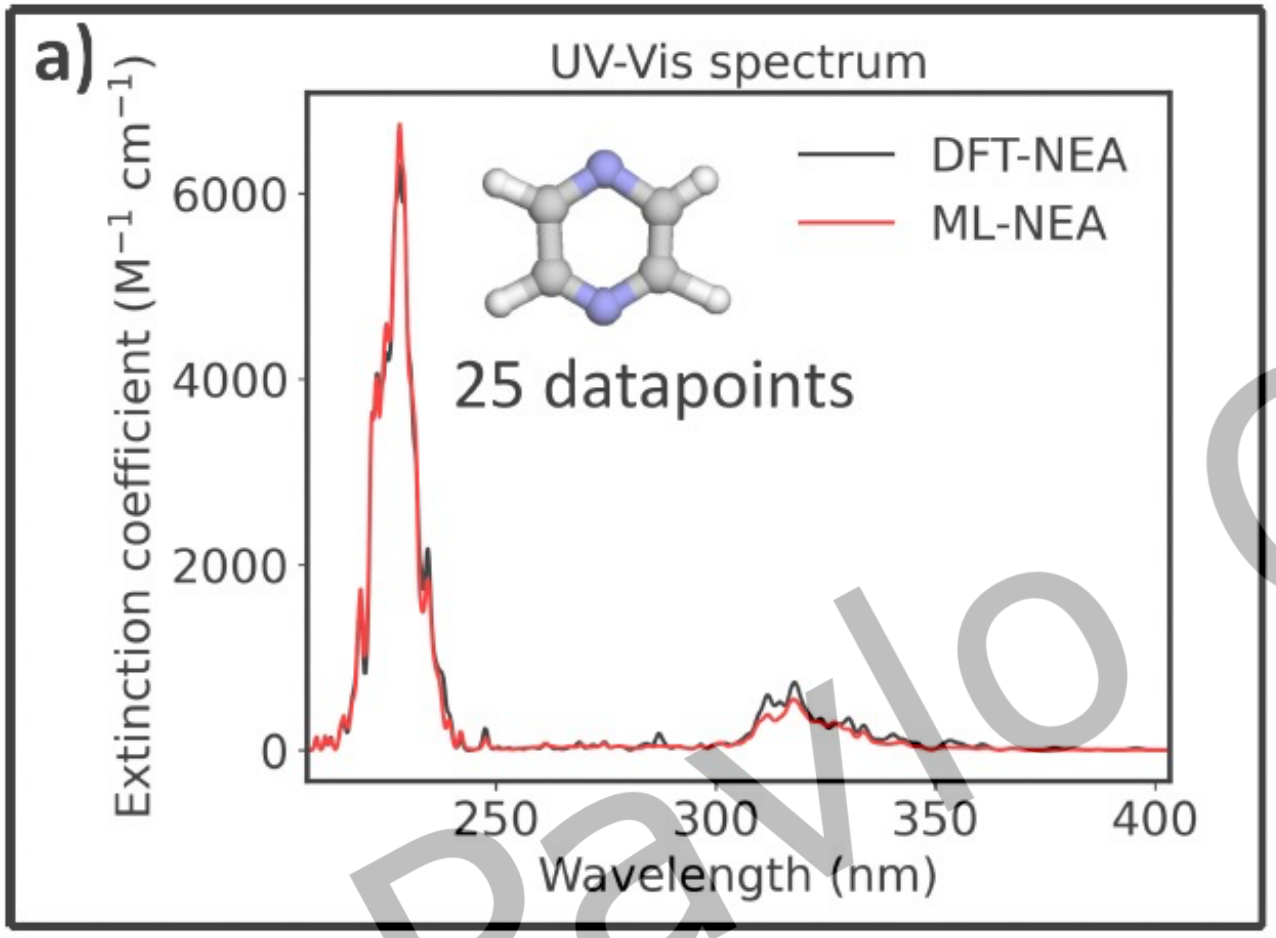
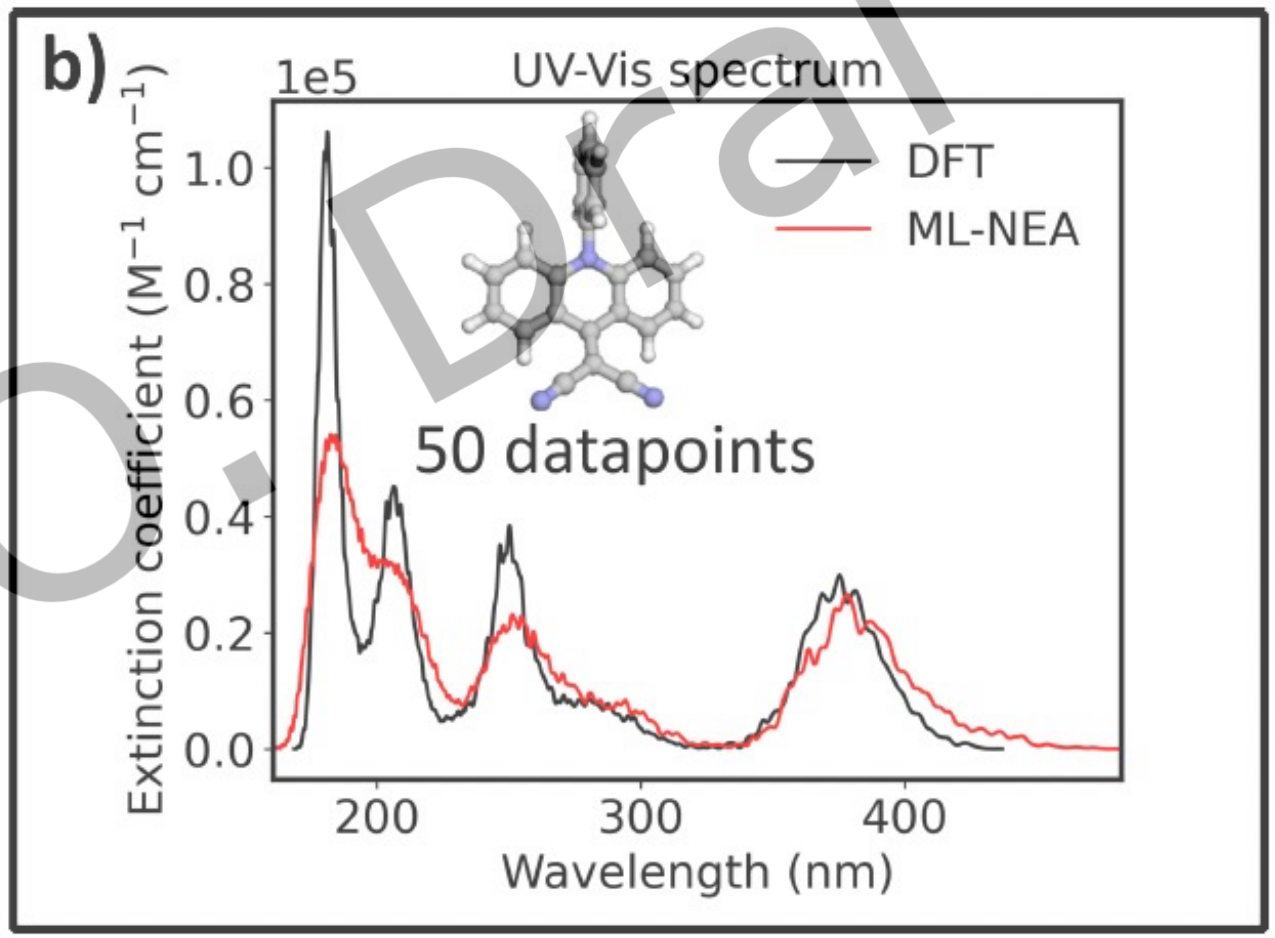
M. Martyka, X.-Y. Tong, J. Jankowska, P. O. Dral. *Nat. Commun.* **2026**, *17*, 4949

ML-NEA via fine-tuning OMNI-P2x





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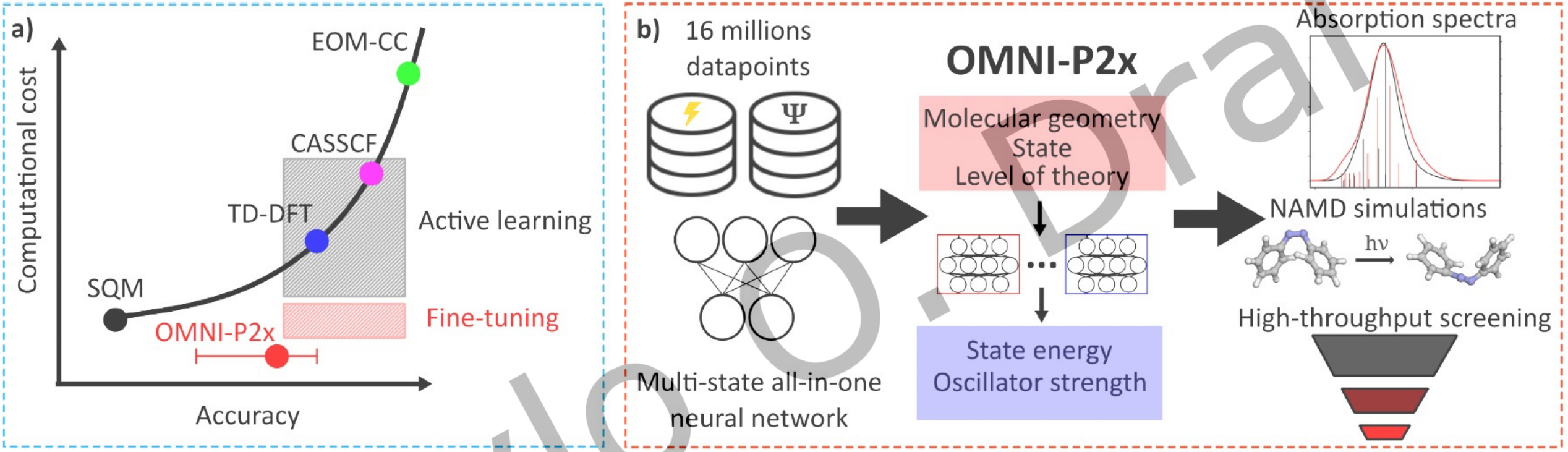
M. Martyka, X.-Y. Tong, J. Jankowska, P. O. Dral. *Nat. Commun.* **2026**, https://doi.org/10.1038/s41467-026-71380-5.

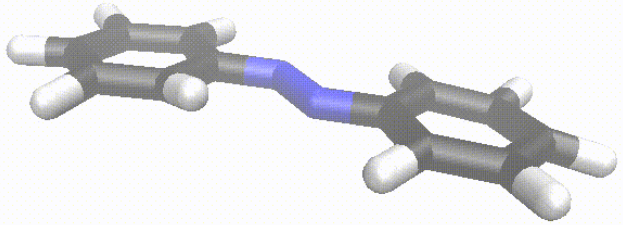
NONADIABATIC DYNAMICS

Pavlo O. Dral

OMNI-P2x: The first-ever universal potential for excited states



Active transfer learning (ATL) → robust nonadiabatic dynamics:



M. Martyka, X.-Y. Tong, J. Jankowska, P. O. Dral. *Nat. Commun.* **2026**, https://doi.org/10.1038/s41467-026-71380-5.

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Active learning

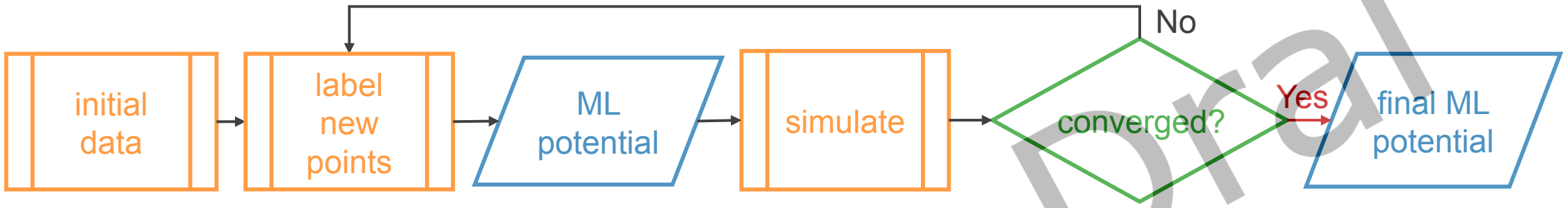

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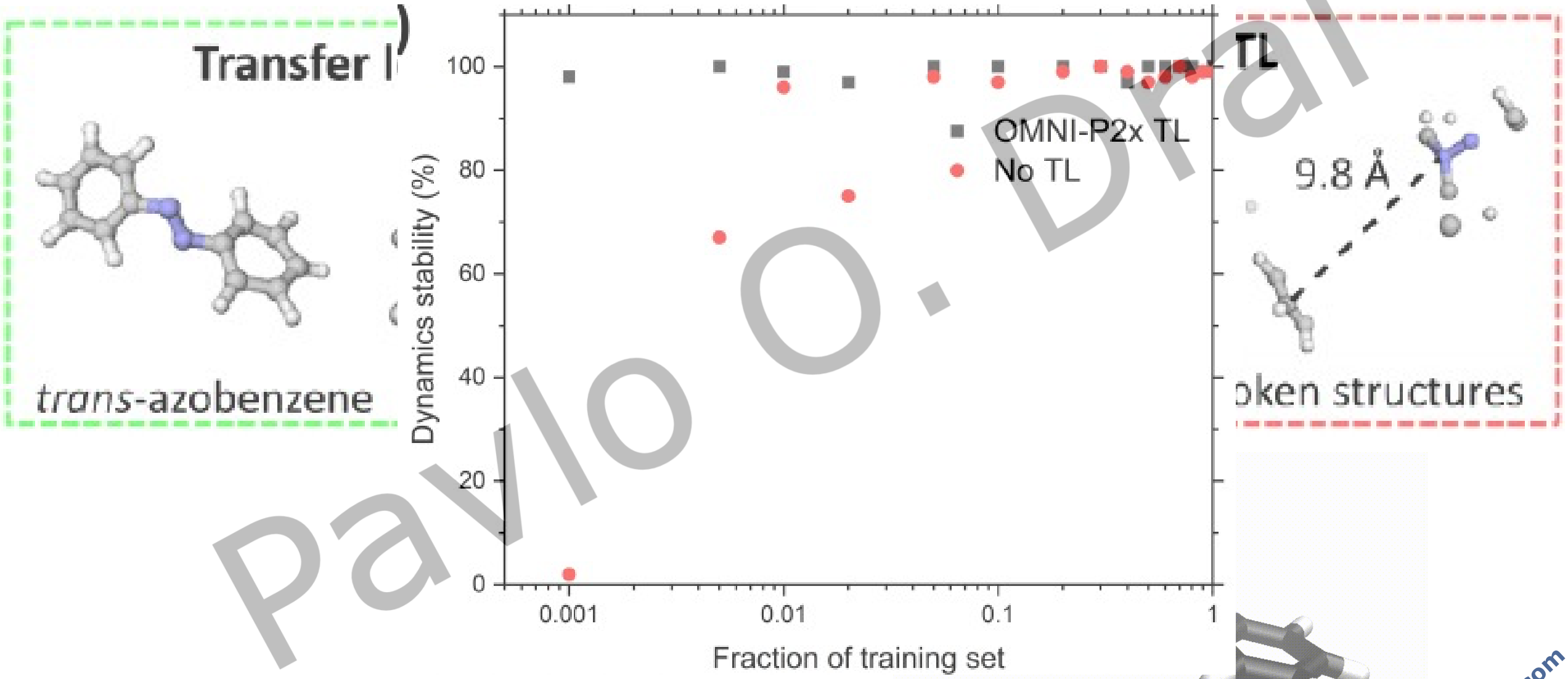
Figure from: Y.-F. Hou, L. Zhang, Q. Zhang, F. Ge, P. O. Dral, J. Chem. Theory Comput. 2024, 20, 7744

Fine-tuned OMNI-P2x can yield more stable NAMD



M. Martyka, X.-Y. Tong, J. Jankowska, P. O. Dral. *Nat. Commun.* **2026**, https://doi.org/10.1038/s41467-026-71380-5.

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Aitomistic

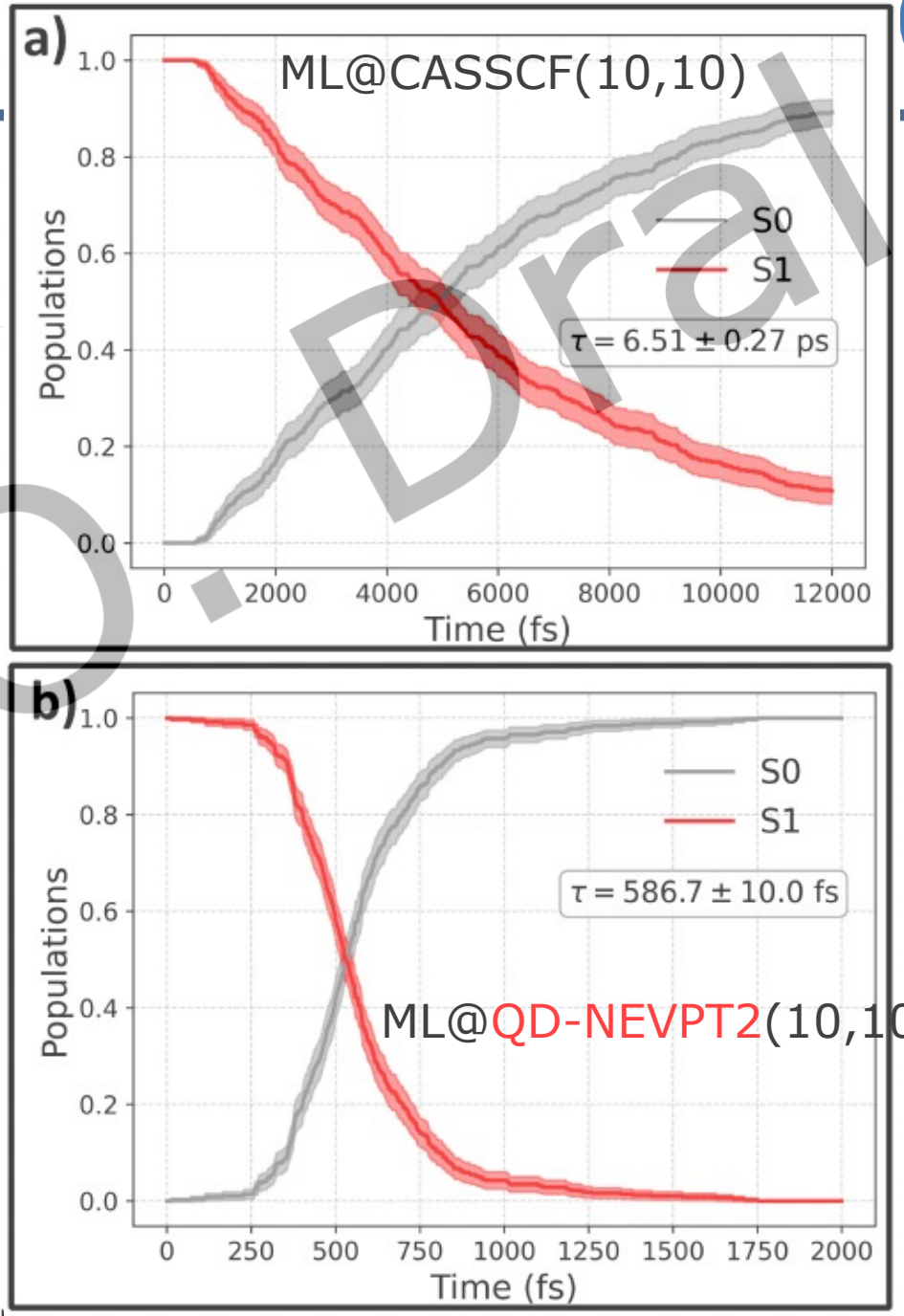
From the journal:
Chemical Science

Gradients not needed: ML-driven propagation of nonadiabatic molecular dynamics without reference gradients

Mikołaj Martyka, Joanna Jankowska, Hans Lischka and Pavlo O. Dral

Abstract

The recent development of machine learning (ML) methods for quantum chemistry has tremendously boosted the efficiency of molecular calculations. In this work, we use ML to enable nonadiabatic molecular dynamics (NAMD) simulations without access to the analytical energy gradients from the underlying electronic structure method. By fine-tuning our foundational model for excited-states, OMNI-P2x, on energies alone, and leveraging automatic differentiability to obtain forces, we eliminate the gradient computation bottleneck that restricts calculations, such as NAMD, to methods with available analytical derivatives. Firstly, we validate the method on the benchmark system, fulvene, demonstrating that gradient-free ML potentials accurately reproduce NAMD populations and dynamics across multiple levels of theory: AIQM1/MRCI, CASSCF, and MRSF-TDDFT. This enables, for the first time, performing dynamicsat the QD-NEVPT2 level, where analytical gradients remain unavailable. We further benchmark the protocol on cyclohexadiene photoinduced ring-opening, where gradient-free training on XMS-CASPT2 energies reproduces reference dynamics with high accuracy, and compare them to QD-NEVPT2 results. Finally, we apply the approach to trans-azobenzene, a prototypical molecular photoswitch, by performing fully dimensional simulations of its photoisomerization dynamics at the CASSCF and QD-NEVPT2 levels, establishing the highest-level excited-state simulations of this photoreaction to date.



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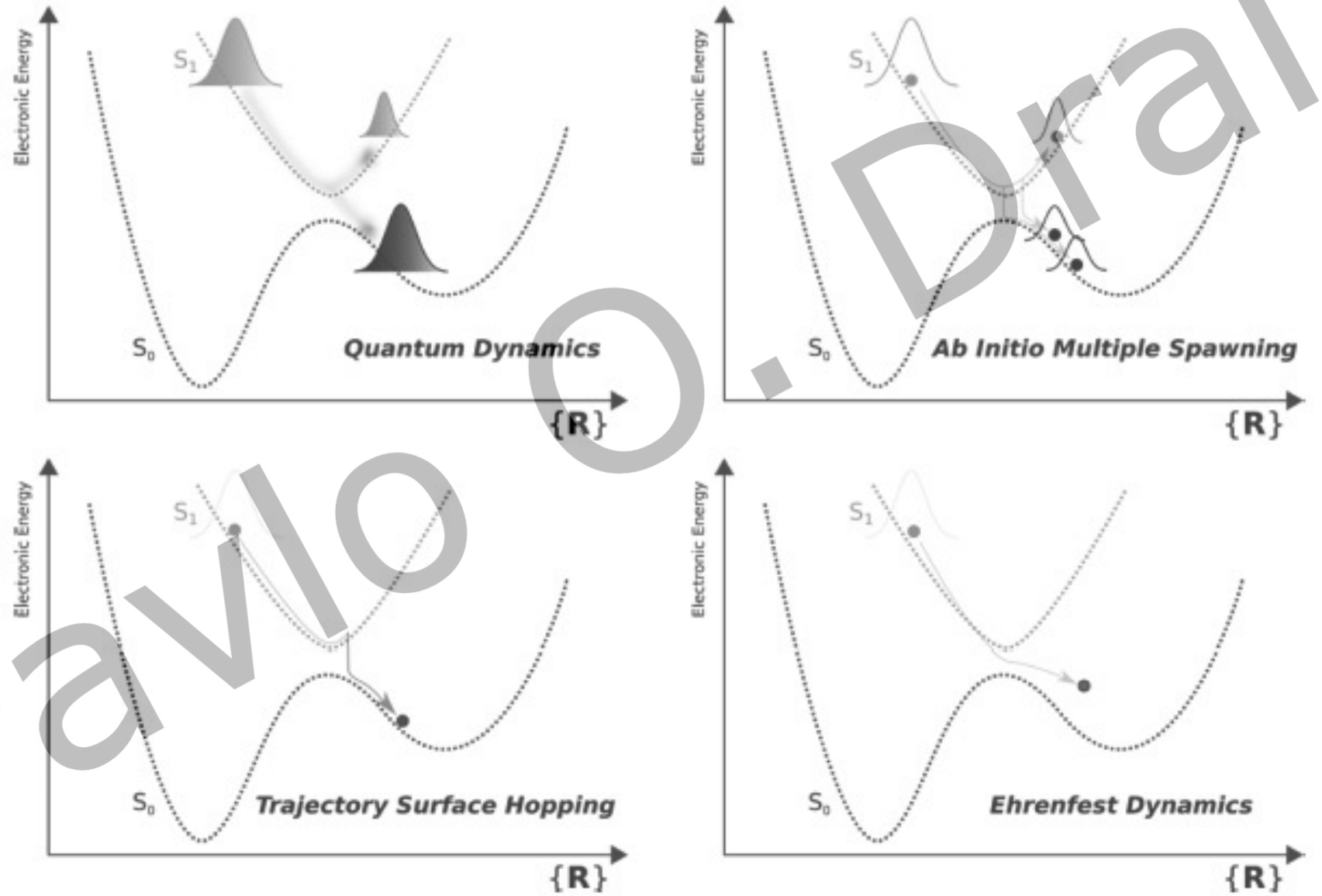
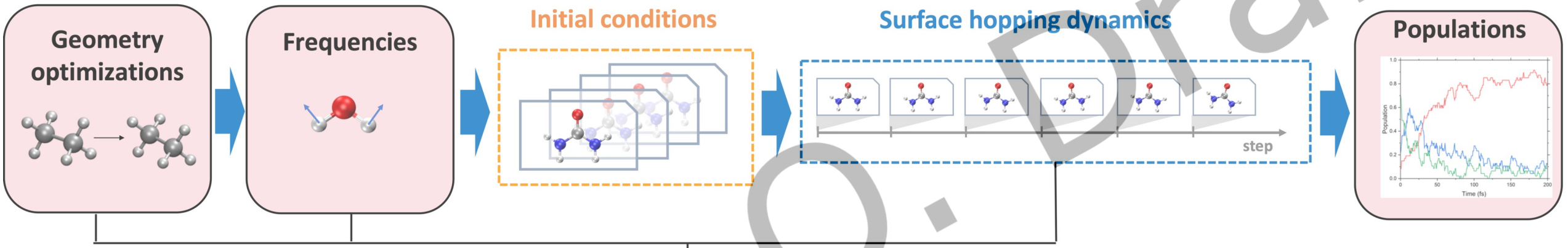


Pavlo O. Dral

B. F. E. Curchod, T. J. Martínez, *Chem. Rev.* **2018,** *118*, 3305

Surface-hopping dynamics in MLatom



Single point calculations

$$E, \frac{\partial E}{\partial \mathbf{x}}, \frac{\partial^2 E}{\partial \mathbf{x}^2}$$

```
aiqm1=mlatom.models.methods(method='AIQM1')
geomopt=mlatom.optimize_geometry(model=aiqm1, ...)
...
mlatom.namd.surface_hopping_md(model=model, ...)
```

Models

- HF, MP2, CC; ADC(2), CASSCF; ...
- B3LYP; ωB97x; ...
- PM6, GFN2-xTB; AM1, PM3, OMx; ...
- AIQM1; AIQM1@DFT; AIQM1@DFT*
- ANI-1x, ANI-2x; ANI-1ccx; ...
- ANI, PhysNet, DPMD; DeepPot-SE, MACE; ...
- KREG, sGDML; KRR-CM, GAP-SOAP; ...

L. Zhang, S. Pios, M. Martyka, F. Ge, Y. F. Hou, Y. Chen, L. Chen, J. Jankowska, M. Barbatti, P. O. Dral. *JCTC*, **2024**, *20*, 5043–5057

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Surface-hopping dynamics in MLatom

MLatom Interfaces

MLatom.com

Quantum Chemistry

COLUMBUS:	CASSCF/MRCI
MNDO:	AM1/PM3/OMx/ODMx ...
AIQM1:	MNDO + TorchANI
Molcas:	CASSCF/CASPT2
BAGEL:	CASSCF/CASPT2

Turbomole PySCF Gaussian ORCA

Machine Learning

DPMD DeepPotSE GAP - SOAP
(p)KREG ANI/MS-ANI MACE
sGDML PhysNet
KRR

Based on the available properties (energies, gradients and NACs), the surface hopping scheme is chosen.

Interface with:
BDF, OpenQP

Surface Hopping Schemes

Current Stage

Fully Automated Workflow

Custom Models

Different quantum chemical methods or machine learning models can be combined.

Flexible Analysis Tools

The surface hopping trajectories can be analyzed using easy-to-use built-in functions.

Integration of AI agents

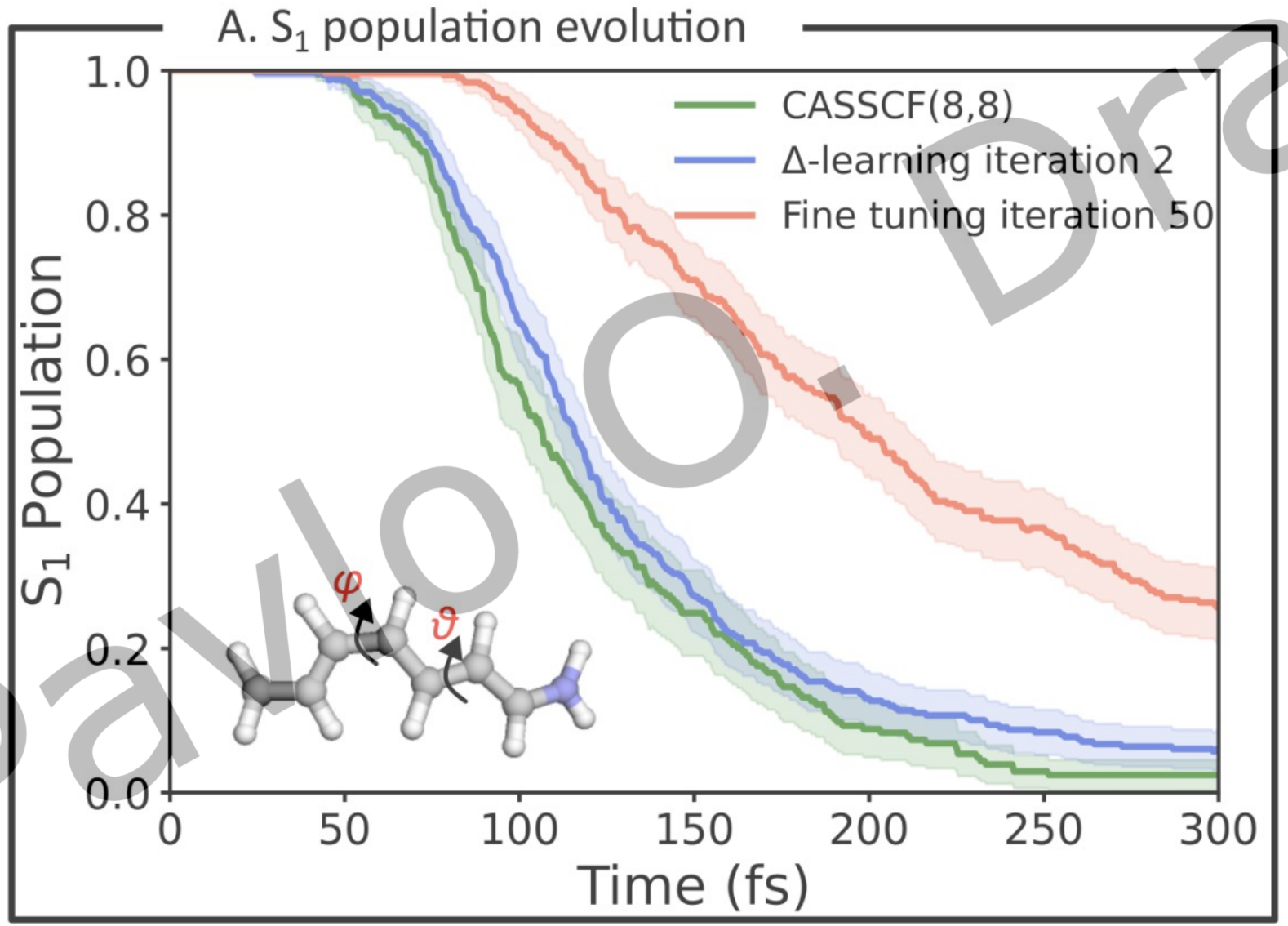
The current implementation will be integrated with AI agents using the Aitomia platform.

Pavlo O. Dral

J. Martinka, M. Martyka, B. Medhi, J. Pittner, P. O. Dral, *J. Chem. Theory Comput.* **2026**, *22*, 2467

Active Delta Learning for NAMD

Solution for molecules with many conformers



M. Martyka, M. Barbatti, J. Jankowska, P. O. Dral. *Faraday Discuss.* **2026** *accepted.*

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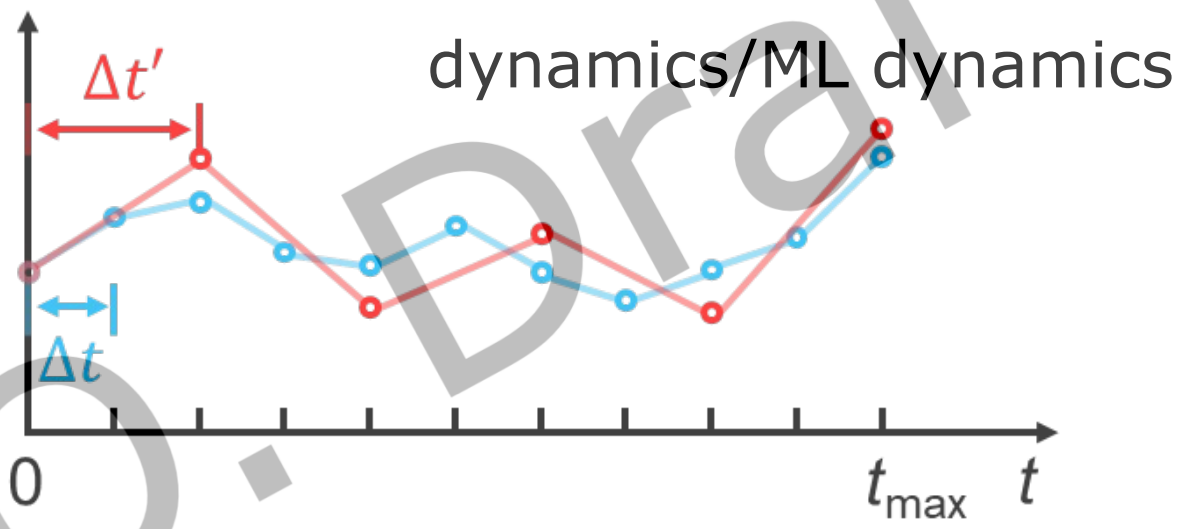
Can we do better?



dynamics propagation is

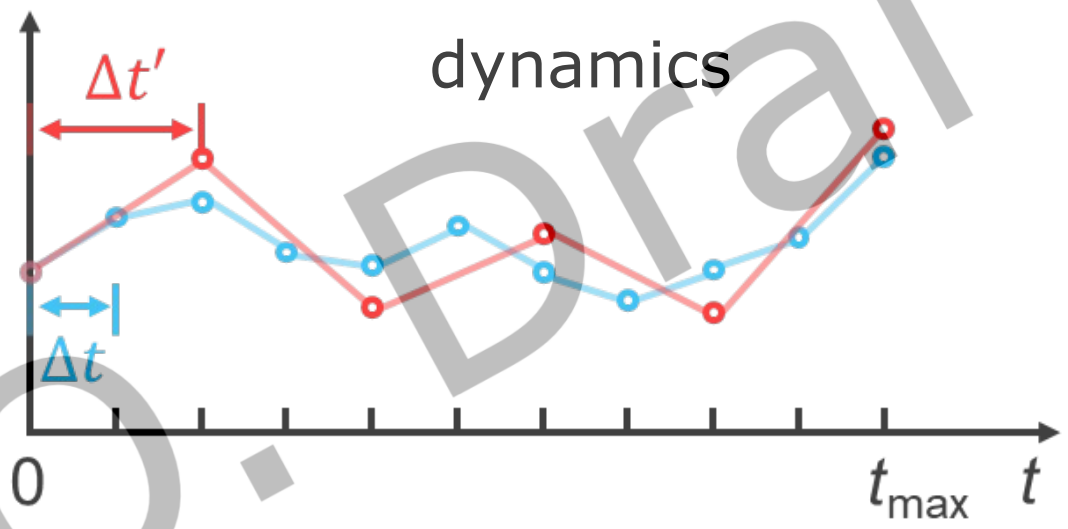
- ~~computationally expensive~~
- recursive (iterative)

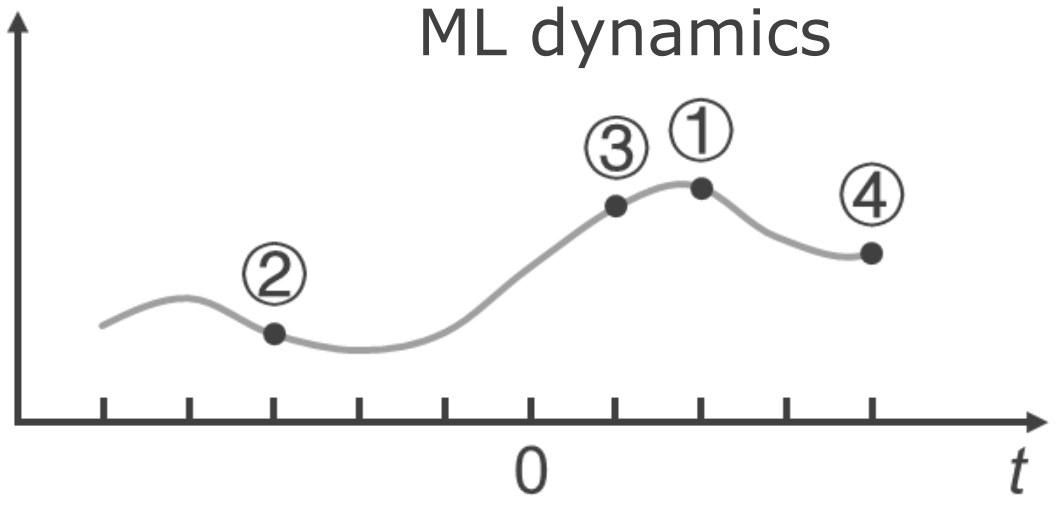
Pavlo O. Dral

Can we do better?

dynamics propagation is

- ~~computationally expensive~~
- ~~recursive (iterative)~~





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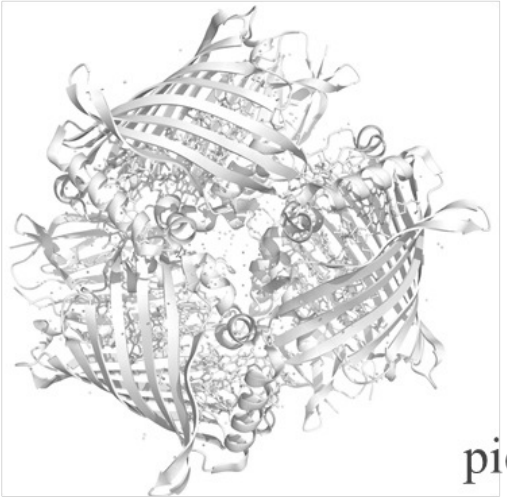
AI-QD (artificial intelligence-based quantum dynamics)

γ = characteristic frequency
λ = reorganization energy
T = temperature

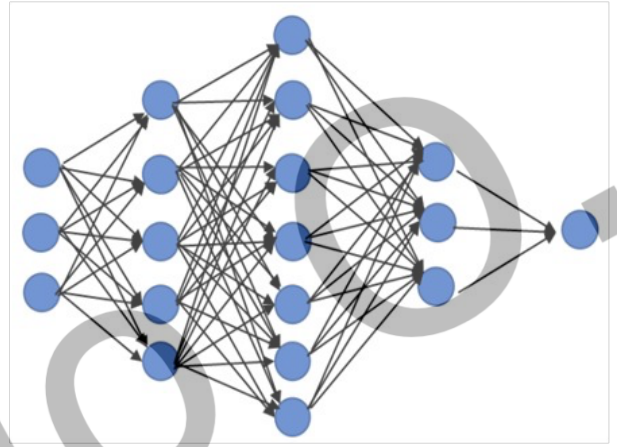
PDB code: 3ENI

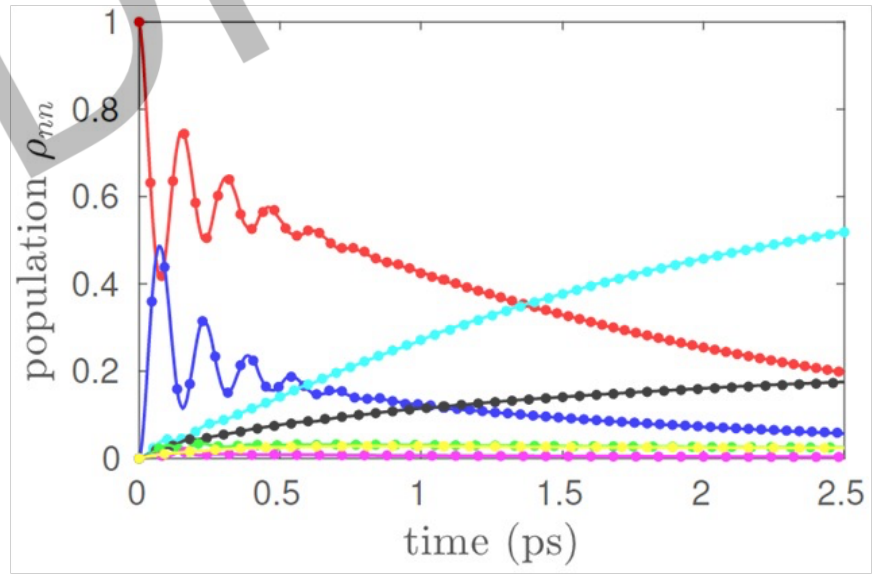


γ, λ, T

pico-second watch

2.5ps





Dots: Reference
Line: AI-QD

7-sites Fenna–Matthews–Olson (FMO) complex

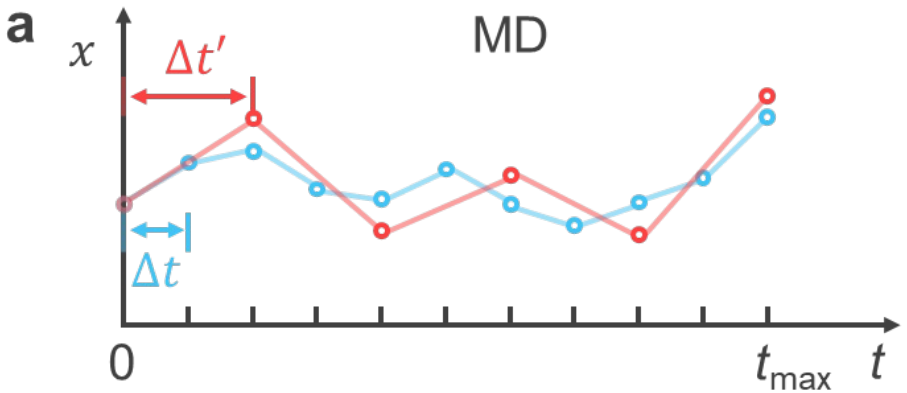
A. Ullah, P. O. Dral. Predicting the future of excitation energy transfer in light-harvesting complex with artificial intelligence-based quantum dynamics. *Nat. Commun.* **2022**, *13*, 1930

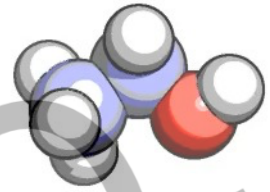
Pavlo O. Dral

AI for Direct Prediction of Dynamics 分子动力学直接预测的 AI 方法

We introduced a radically different way to do MD, 100x faster than with ML potentials

我们提出了一种全然不同的分子动力学方法，其速度比机器学习势快 100 倍。

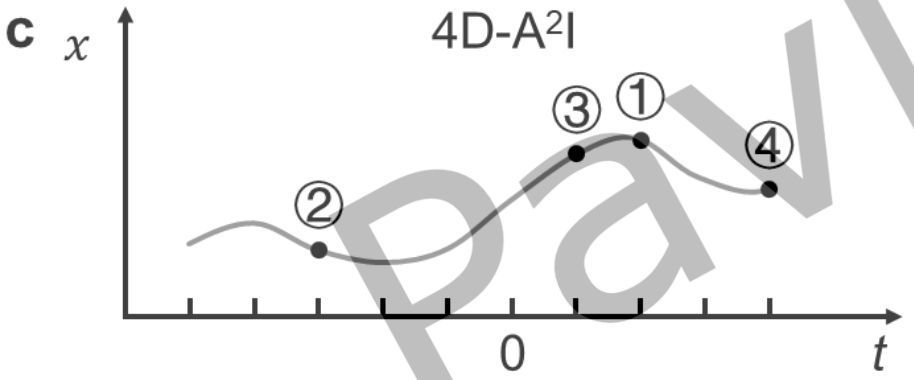


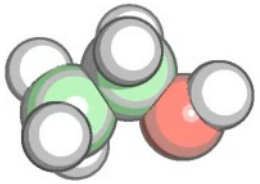


Reference MD

Almost everyone thought it was impossible due to the vast phase space of multi-atomic systems

几乎所有人都认为这是不可能的，因为多原子体系具有巨大的相空间





Directly AI-generated MD

0.0 fs

Dral*, *et al.* in *Nat. Commun.* 2022, *13*, 1930; *JPCL* 2023, *14*, 7732; *JCTC* 2026, *22*, 1549

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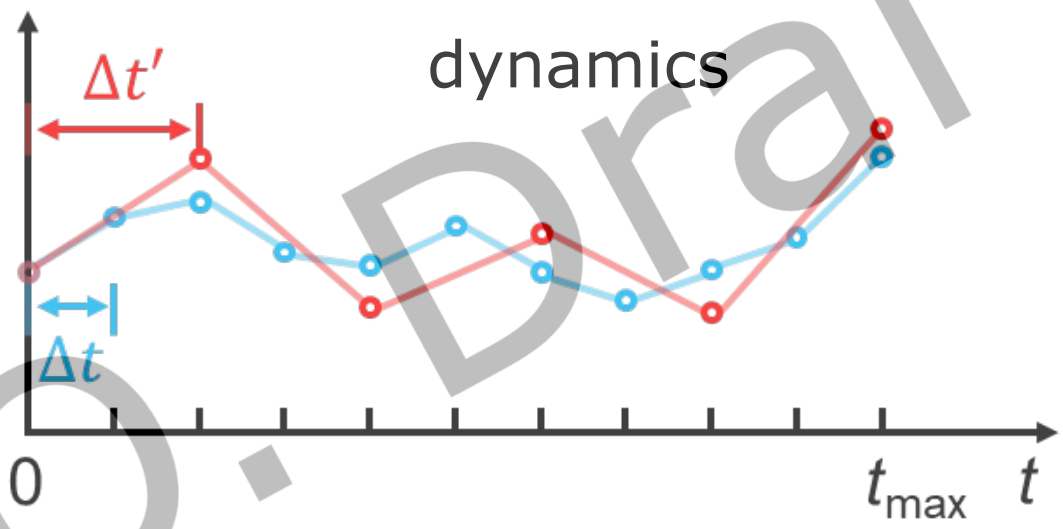
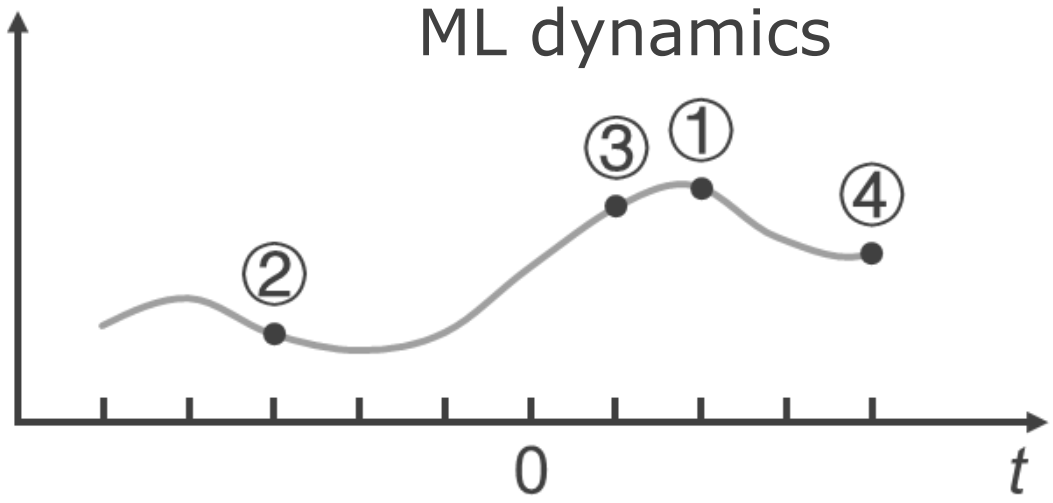
Can we do even better?

dynamics propagation is

- ~~computationally expensive~~
- ~~recursive (iterative)~~





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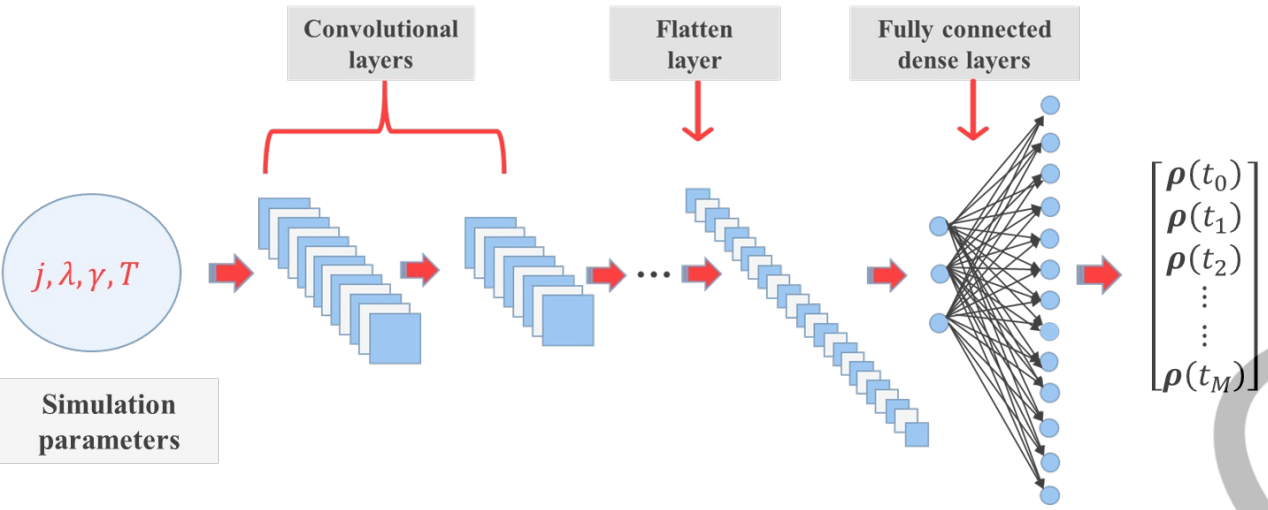
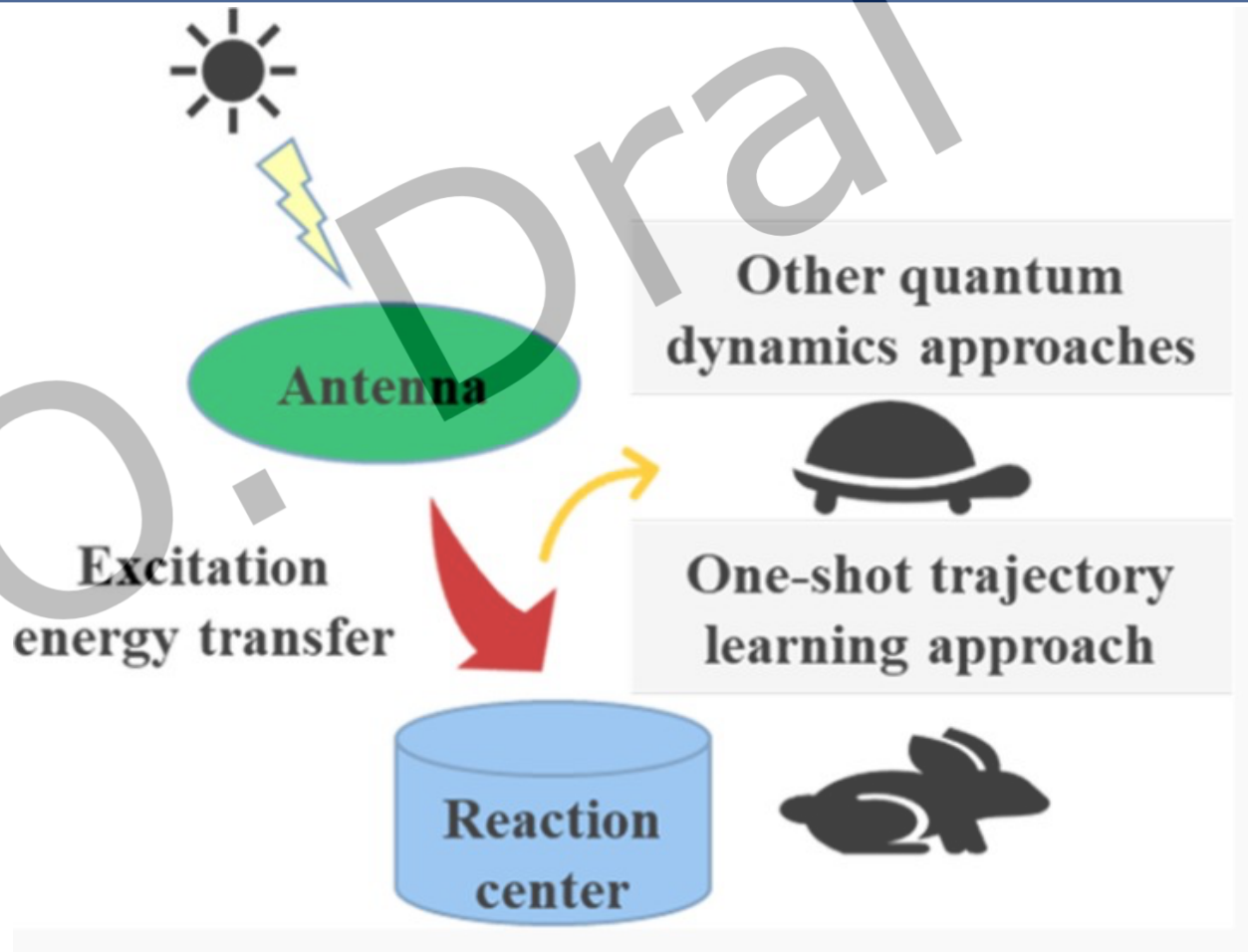
One-Shot Trajectory Learning (OSTL)





- **10 ps long dynamics in just 70 ms**
- good for massive simulation in parameter space

A. Ullah, P. O. Dral. *J. Phys. Chem. Lett.* **2022**, 6037

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2025 – Torun, Poland

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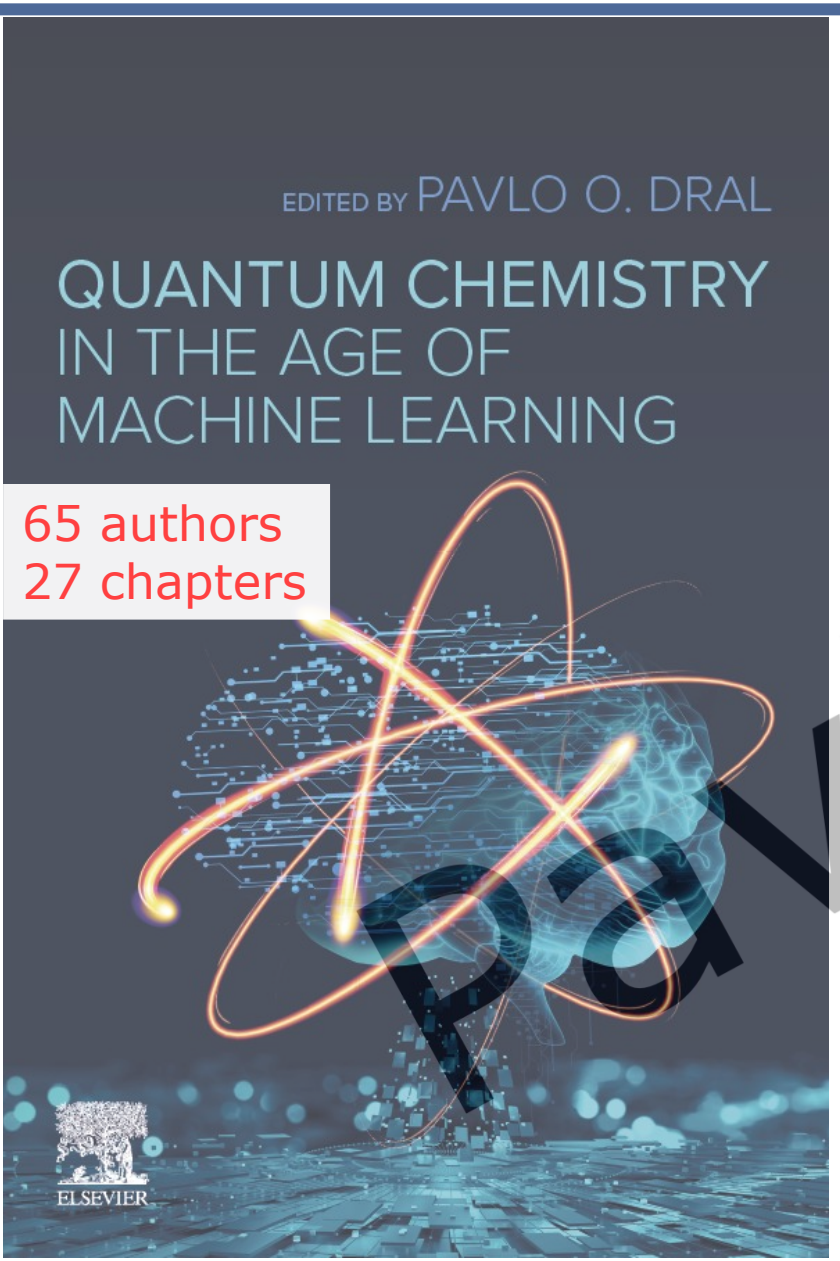
Learning materials



Online course!

https://www.aitomistic.com/en/sub/course

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Xiamen University, China

Nicolaus Copernicus University in Toruń, Poland

Aitomistic, Shenzhen, China

9 September 2026

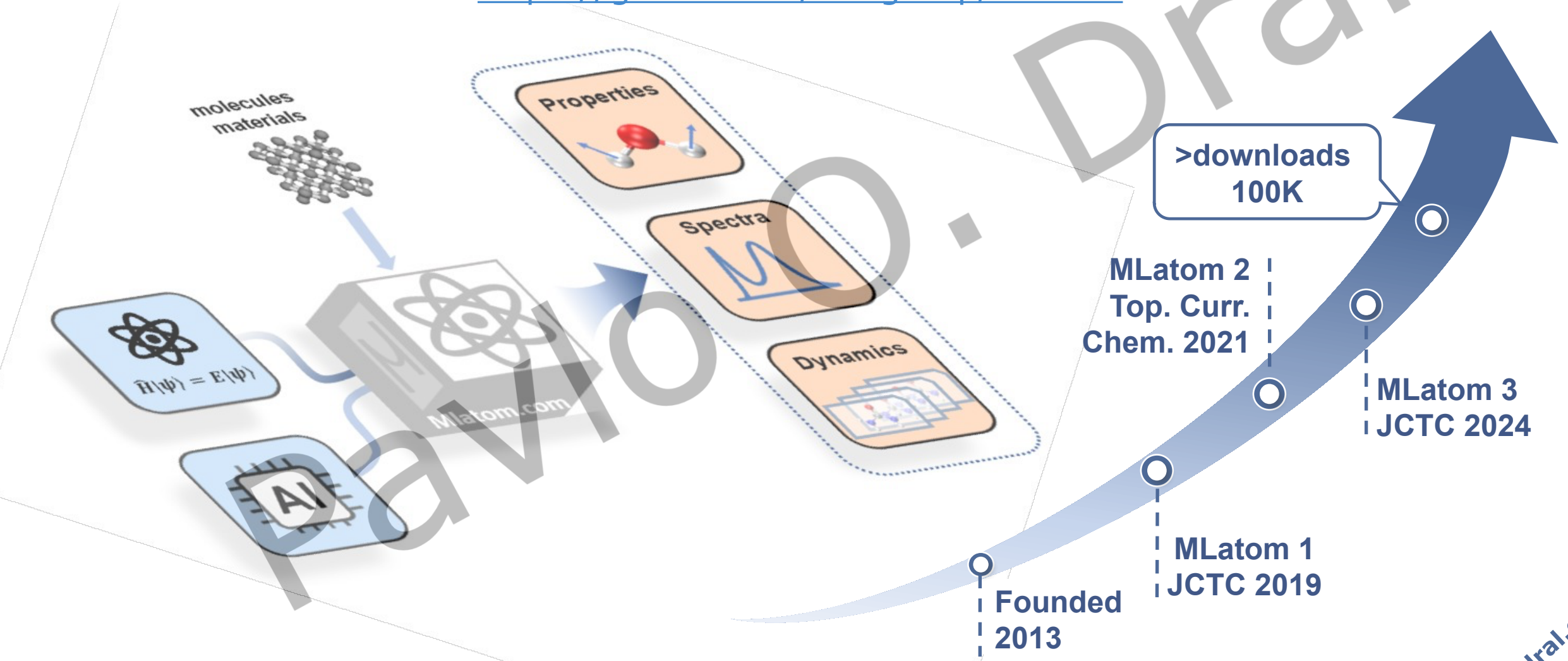
Pavlo O. Dral

dr-dral.com

Our AI ecosystem for computational chemistry

We develop MLatom – an open-source software ecosystem integrating AI and quantum chemistry

https://github.com/dralgroup/mlatom



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MLatom's interfaces

add interface to read "energy" and "gradient" from BDF

#38 opened on Apr 9 by ilcpm • Review required

Quantum chemical programs:

Gaussian

ORCA

PySCF

Turbomole

COLUMBUS

MLQD

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

Semi-empirical quantum chemical programs:

xTB

SPARROW

MNDO

Machine learning programs:

PhysNet

GAP

TORCHANI

SCOML

hyperopt

Dynamics and other atomistic simulation:

ASE

NX newtonx.org

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Aitomistic

Open source (on github, pip install...)

Machine Learning

Simulations

MLatom

>100000 downloads

Quantum Chemistry

Data

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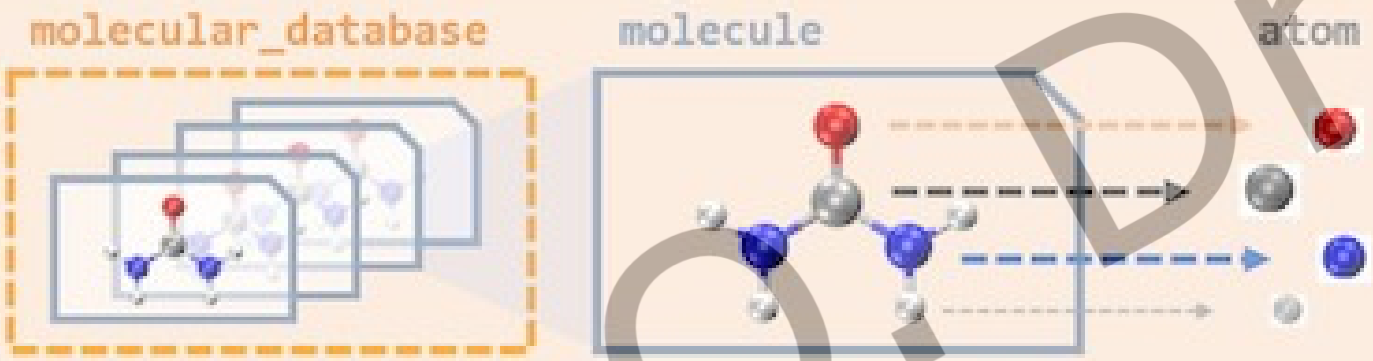
Have it your way...

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



- Python API **V3**

```
import mlatom as ml
```

- Input file

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

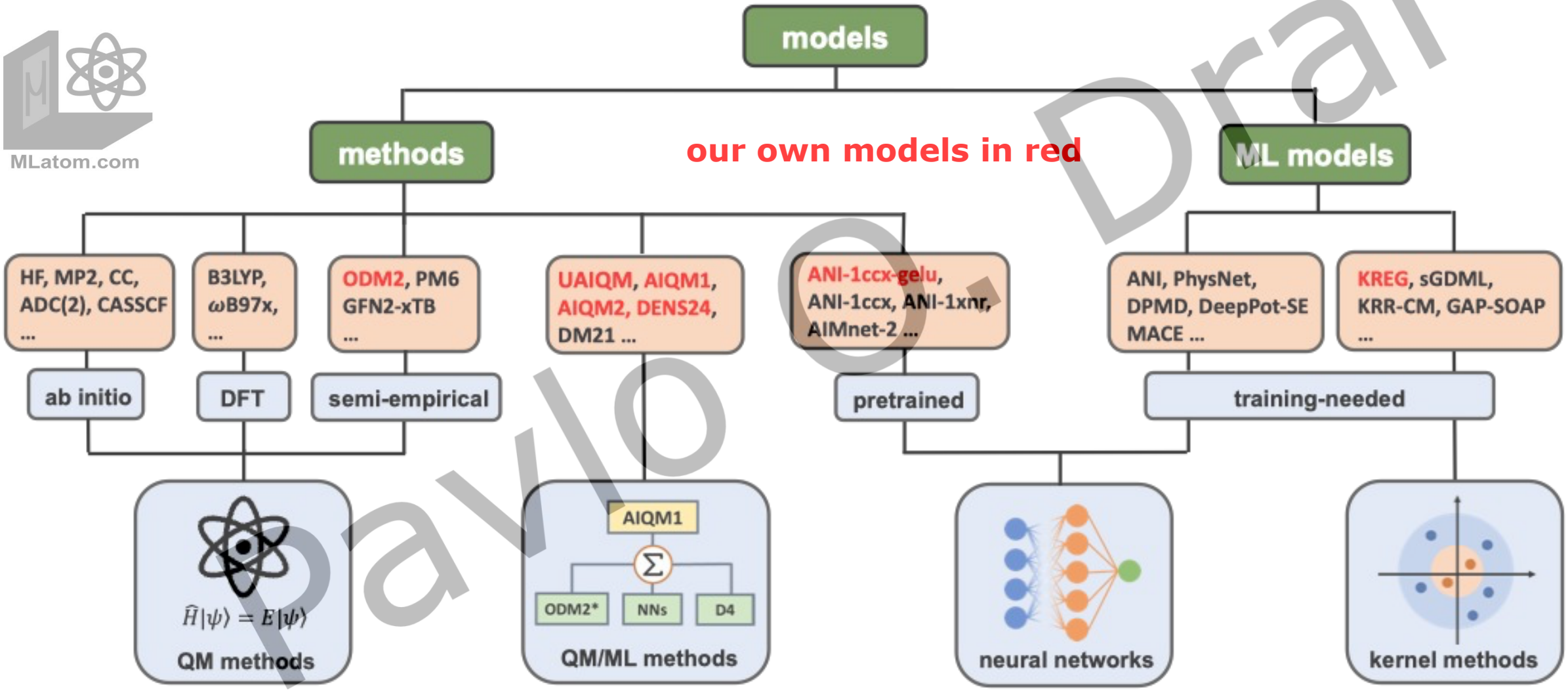
- Command line

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

Pavlo O. Dral

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



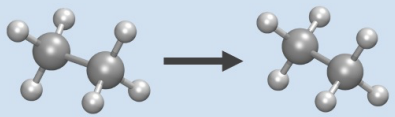
MLatom.com
Pavlo O. Dral

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

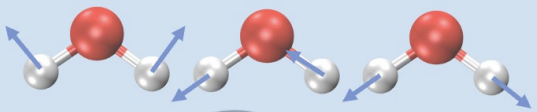
AI-enhanced computational chemistry

Single point calculations — Energies, forces, Hessian matrix…

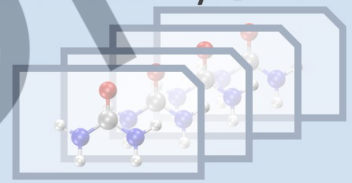
Geometry optimizations



Frequency calculations



Molecular dynamics



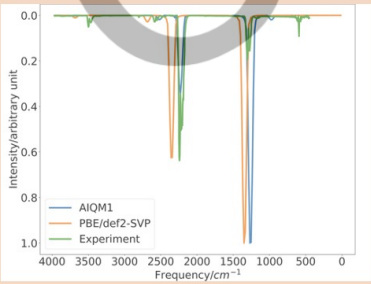
+PIMD coming soon…

Thermochemistry calculations

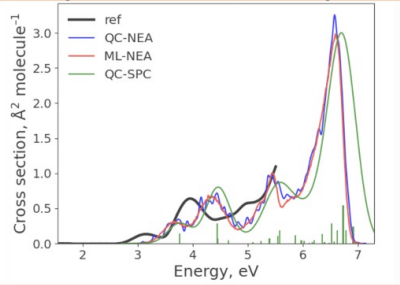
Heat of formation:

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

(Ro)vibrational spectra



One-photon UV/vis spectra



Properties & spectra

Simulations

Quantum dissipative dynamics

Two-photon absorption spectra

MLatom.com

Pavlo O. Dral

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

Local Installation of MLatom

github.com/dralgroup/mlatom

README | Code of conduct | Contributing | Apache-2.0 license | Security

Local installation

The easiest way to run MLatom is online — no installation. To install locally:

```
python3 -m pip install -U mlatom
```

That pulls in the required dependencies automatically (including the PyTorch/TorchANI and geometry-optimization backends the **AIQM2** quick start uses). A few features need one more package — install only what you use:

for	install
PySCF methods: single point, TDDFT, frequencies and thermochemistry, densities, Raman	`pip install pyscf`
AIMNet2 models	`pip install aimnet`
format conversions (SMILES to xyz and back)	`conda install -c conda-forge openbabel`
the ASE interface (ASE optimizers and dynamics) and MACE	`pip install ase`
KREG_API backend (`ml_program='MLatomF'` needs none of this)	`conda install -c conda-forge mkl mkl-service`
MDtrajNet / MLTPA / DMC / hyperparameter search	`pip install e3nn` / `rdkit` / `pyvibdmc` / `hyperopt`

AIQM2 additionally needs the DFT-D4 program, installed via conda:

```
conda install -c conda-forge 'dftd4==3.6.0'   # the version MLatom is tested against
export dftd4bin=$(which dftd4)   # point MLatom at the dftd4 executable
```

See the installation guide for the full dependency list and other methods.

Quick start

Optimize the geometry of a water molecule with **AIQM2** — an AI-enhanced quantum-mechanical method (native to MLatom, CHNO elements) that reaches beyond-DFT accuracy at semi-empirical cost:

```
import mlatom as ml

mol = ml.data.molecule.from_xyz_string('''3

O    0.00000    0.00000    0.11779
H    0.00000    0.75545   -0.47116
H    0.00000   -0.75545   -0.47116
''')
aiqm2 = ml.methods(method='AIQM2')
opt = ml.optimize_geometry(model=aiqm2, initial_molecule=mol).optimized_molecule
print(opt.energy)          # optimized energy in hartree (≈ -76.3838)
```

The same calculation as an input file (`geomopt.inp` , with `init.xyz` holding the geometry):

```
AIQM2               # method
geomopt             # task: geometry optimization
xyzfile=init.xyz    # input geometry
optxyz=opt.xyz      # output geometry
```

```
mlatom geomopt.inp
```

Prefer zero setup? Run these online on the Aitomistic Hub or Aitomistic Lab@XMU (both powered by Protomia) — no installation needed.

https://github.com/dralgroup/mlatom

https://github.com/dralgroup/mlatom-skills

Pavlo O. Dral

```
B3LYP/6-31G*
geomopt
xyz
C
H
H
H
H
'
```

```
GFN2-xTB
geomopt
xyz
C
H
H
H
H
'
```

```
MP2/cc-pVDZ
geomopt
xyzf
C
H
H
H
H
'
```

```
ANI-1ccx
geomopt
xyz
C
H
H
H
H
'
```

```
MLmodelType=ANI MLmodelIn=ani.pt
geomopt
xyz
C
H
H
H
H
'
```

```
UAIQM
geomopt
xyzfile='5

C        0.0000000000        0.0000000000        0.0000000000
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
'
```

Pavlo O. Dral

atom.xmu.edu.cn/course

Courses

Browse available courses and enroll to start learning.

Computational chemistry and AI

Course materials for the part of the course "Computational Chemistry and AI" taught by Prof. Pavlo O. Dral in the Spring semester of 2026

View

atom.xmu.edu.cn/courses/comchem_2026/qc_intro.html#lecture1-ml

Computational chemistry & AI

Search docs

TABLE OF CONTENT

1. Preface
2. Introduction to quantum chemistry and machine learning
   2.1. Slides
   2.2. Quantum chemical levels
   2.3. Finally, your first ML calculations!
   2.4. Homework
   2.5. Further reading
3. Why does DFT work? Improving upon it
4. Universal machine learning models
5. Machine learning basics
6. ML for PES
7. Transfer learning

matter how well you do ML but it if it is trained on a bad QM method, it will also be bad ("garbage in - garbage out").

Without further ado, let's jump into our first ML calculations with Task 1.3 (in in-class exercises, you have 10 min, send answers on WeChat and after everyone finishes, write down the answer on a blackboard):

Exercise ML-basics-1.

Calculate the bond length in H_2 molecule with machine learning (ML) (see instructions below).

Write down:

1. Bond length you obtained.
2. How much time it took to complete the calculations.

The MLatom input file (h2_opt_kreg.inp) is pretty self-explanatory:

```
geomopt                 # Request geometry optimization
MLmodelType=KREG        # with the ML model of the KREG type
MLmodelIn=energies.unf # in energies.unf file
XYZfile='
2

H            0.000          0.000          0.000
H            0.000          0.000          0.800
'
optXYZ=eq_KREG.xyz      # optimized geometry output
```

You also need to upload the file with ML model energies.unf to the same folder as the input file.

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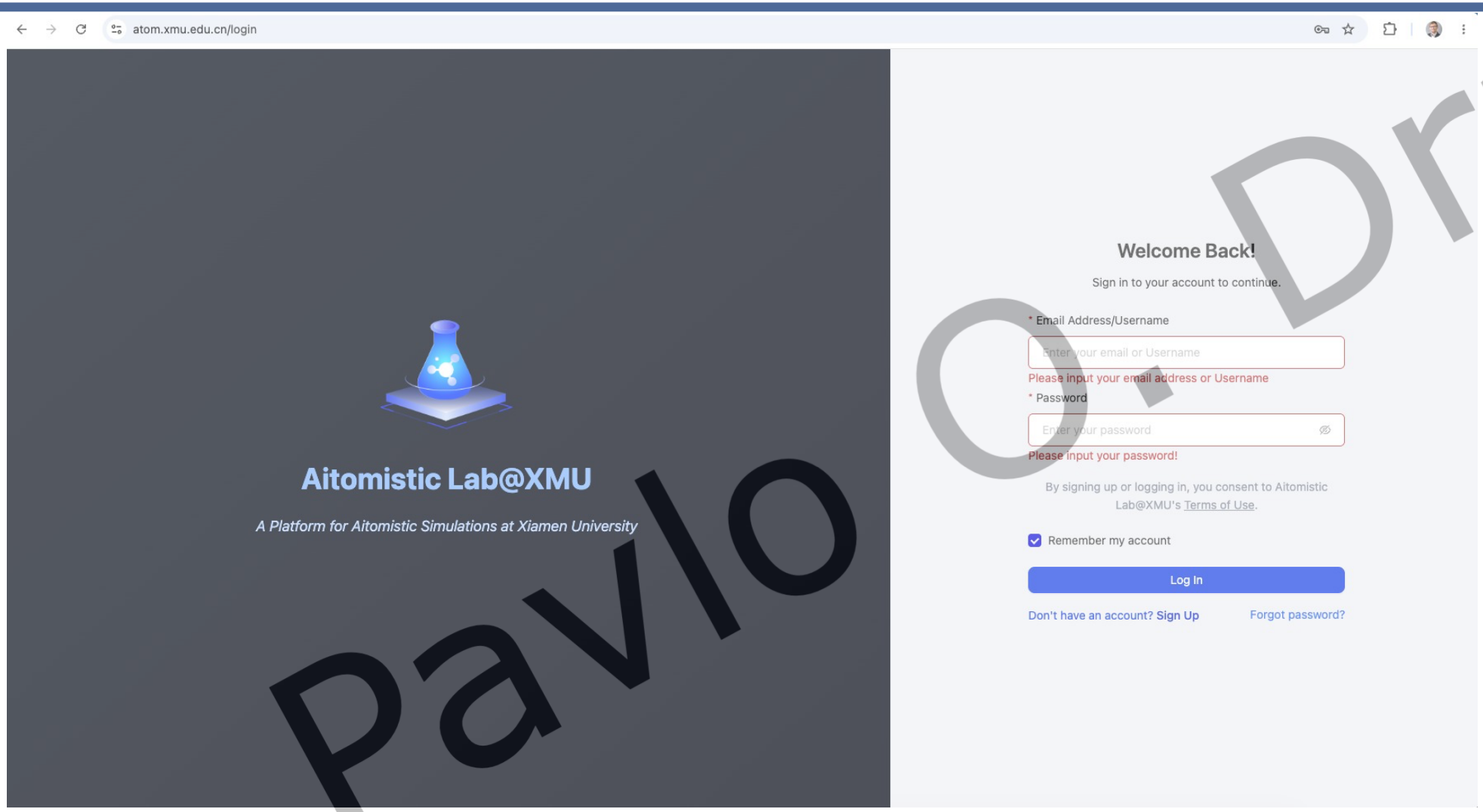
Doing calculations online

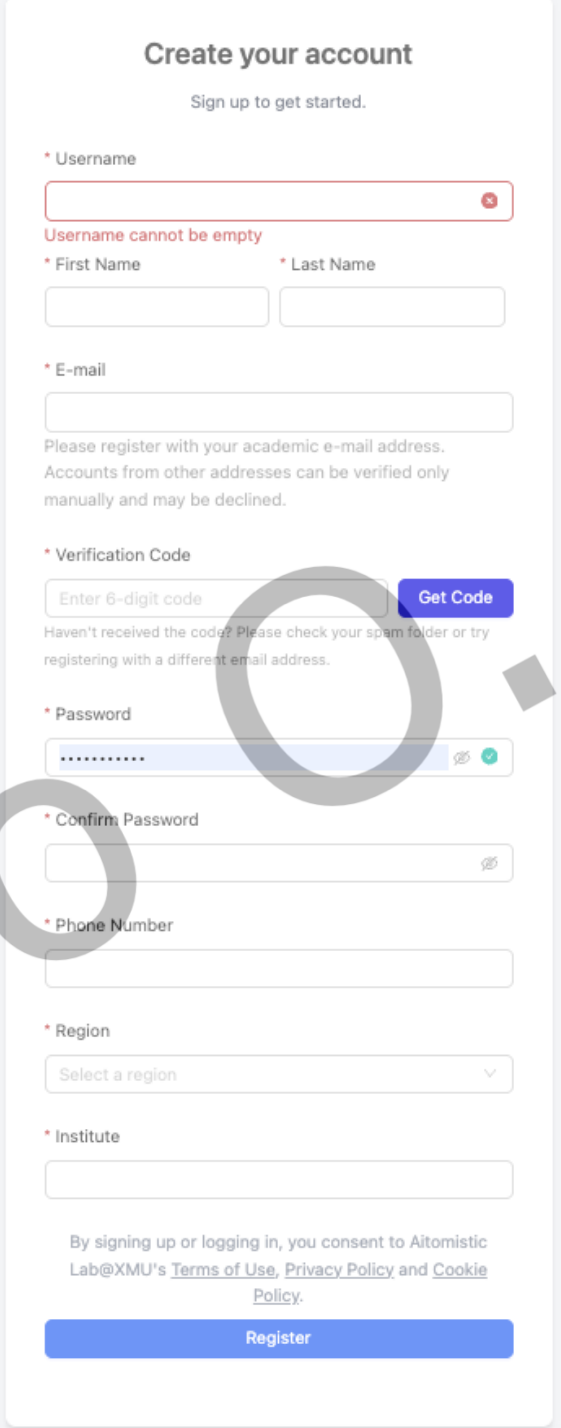


https://atom.xmu.edu.cn (available for free when registered with an academic email)

https://aitomistic.xyz (registration and basic use free for everyone)

Pavlo O. Dral

Aitomistic



https://atom.xmu.edu.cn (available for free when registered with an academic email)

https://aitomistic.xyz (registration and basic use free for everyone)

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Check your email for instructions

You Can Now Use Aitomistic Lab@XMU! Introduction to Aitomistic Lab@XMU with Usage Examples

Dear [redacted],

thank you for registering at Aitomistic Lab@XMU! We have approved your access and you may start using it by logging in to https://atom.xmu.edu.cn.

Note that these resources are made available for academic research and other activities are prohibited. We are happy to provide the computational resources particularly for researchers with limited budget, but please understand that these resources are also limited and shared by many users. Hence, we might need to restrict access to the Lab in case the usage is exceeding what we can afford. If you would need more resources, reserve computational resources for some event (workshop or classes), or want to use the Lab for commercial purposes, please contact us by replying to this email and we will try to find a solution.

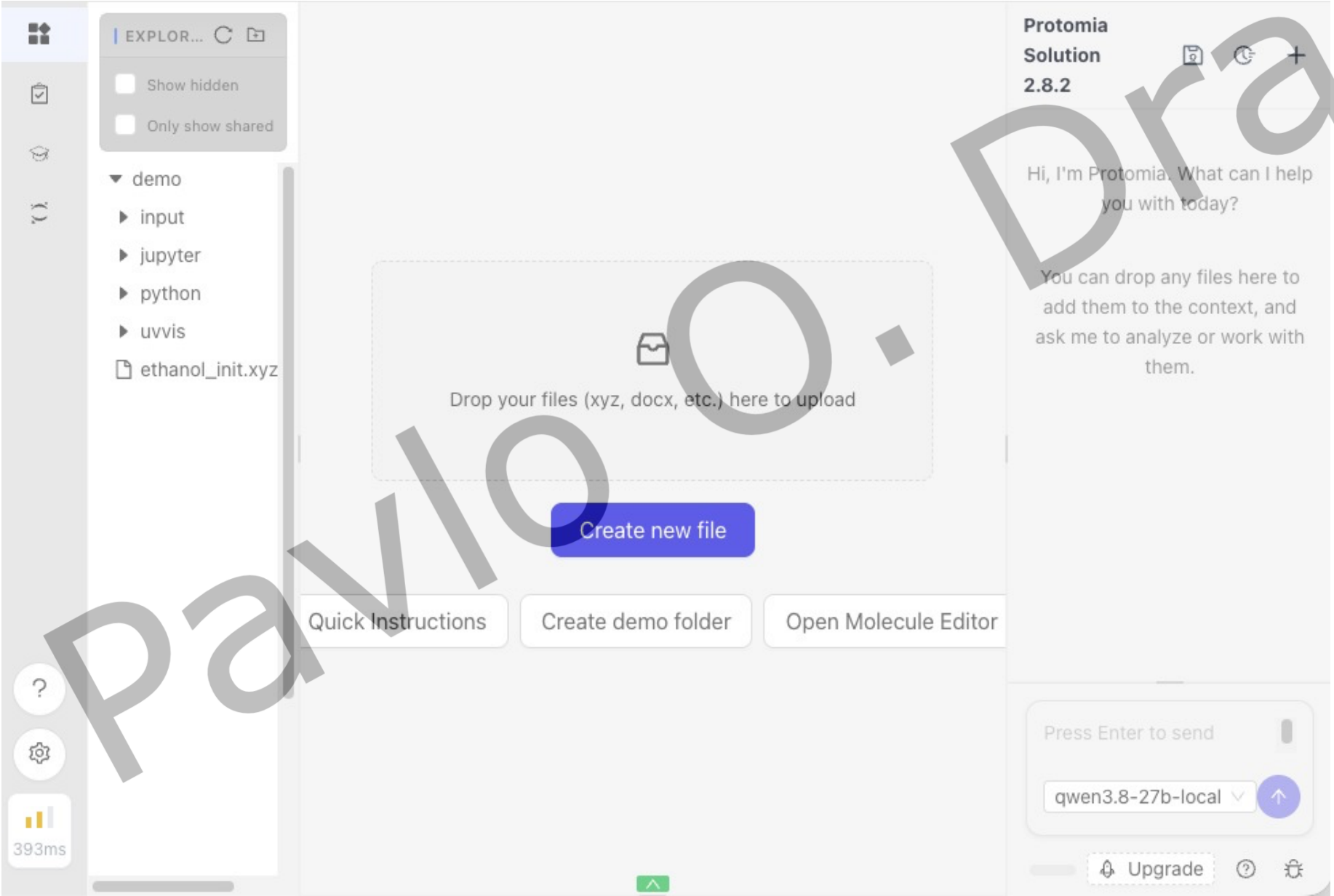
If something does not work, you have feedback and improvement suggestions, we would be happy to learn about them via email or via the Feedback feature inside the Aitomistic Lab.

Also note that the Aitomistic Lab@XMU is provided 'as is', without warranty of any kind, express or implied, including but not limited to the warranties of merchantability, fitness for a particular purpose and noninfringement. In no event shall the authors or copyright holders be liable for any claim, damages or other liability, whether in an action of contract, tort or otherwise, arising from, out of or in connection with the Aitomistic Lab@XMU or the use or other dealings in the Aitomistic Lab@XMU.

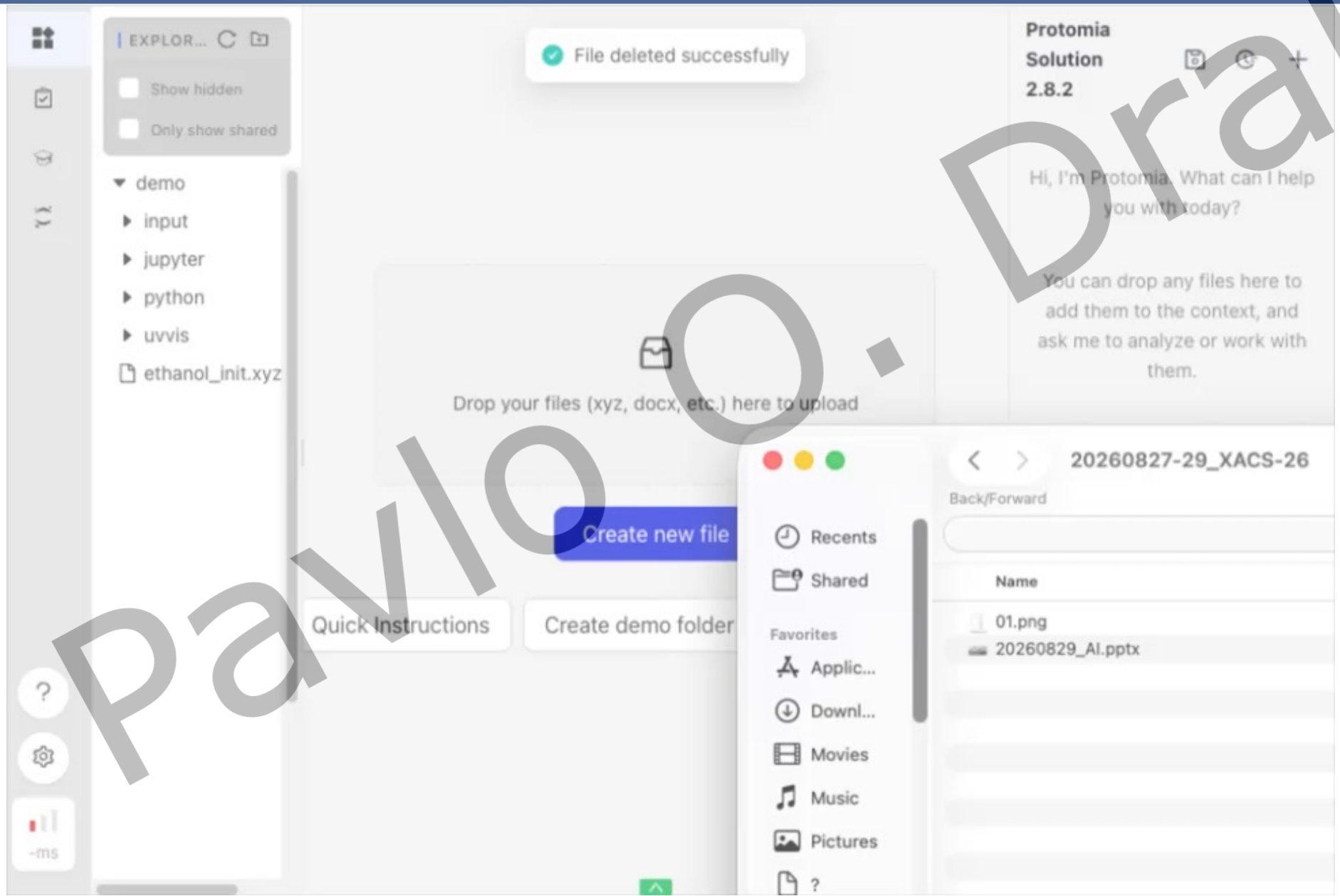
Sincerely yours,
Your Team at Aitomistic Lab@XMU

Introducing Aitomistic Lab@XMU

Pavlo O. Dral


EXPLOR...
Show hidden
Only show shared
demo
input
jupyter
python
uvvis
ethanol_init.xyz
Drop your files (xyz, docx, etc.) here to upload
Create new file
Quick Instructions
Create demo folder
Open Molecule Editor
393ms
Protomia
Solution
2.8.2
Hi, I'm Protomia. What can I help you with today?
You can drop any files here to add them to the context, and ask me to analyze or work with them.
Press Enter to send
qwen3.8-27b-local
Upgrade

Pavlo O. Dral


EXPLOR...
Show hidden
Only show shared
demo
input
jupyter
python
uvvis
ethanol_init.xyz
File deleted successfully
Protomia Solution 2.8.2
Hi, I'm Protomia. What can I help you with today?
You can drop any files here to add them to the context, and ask me to analyze or work with them.
Drop your files (xyz, docx, etc.) here to upload
Create new file
Quick Instructions
Create demo folder
20260827-29_XACS-26
Back/Forward
Recents
Shared
Favorites
Applic...
Downl...
Movies
Music
Pictures
Name
01.png
20260829_AI.pptx

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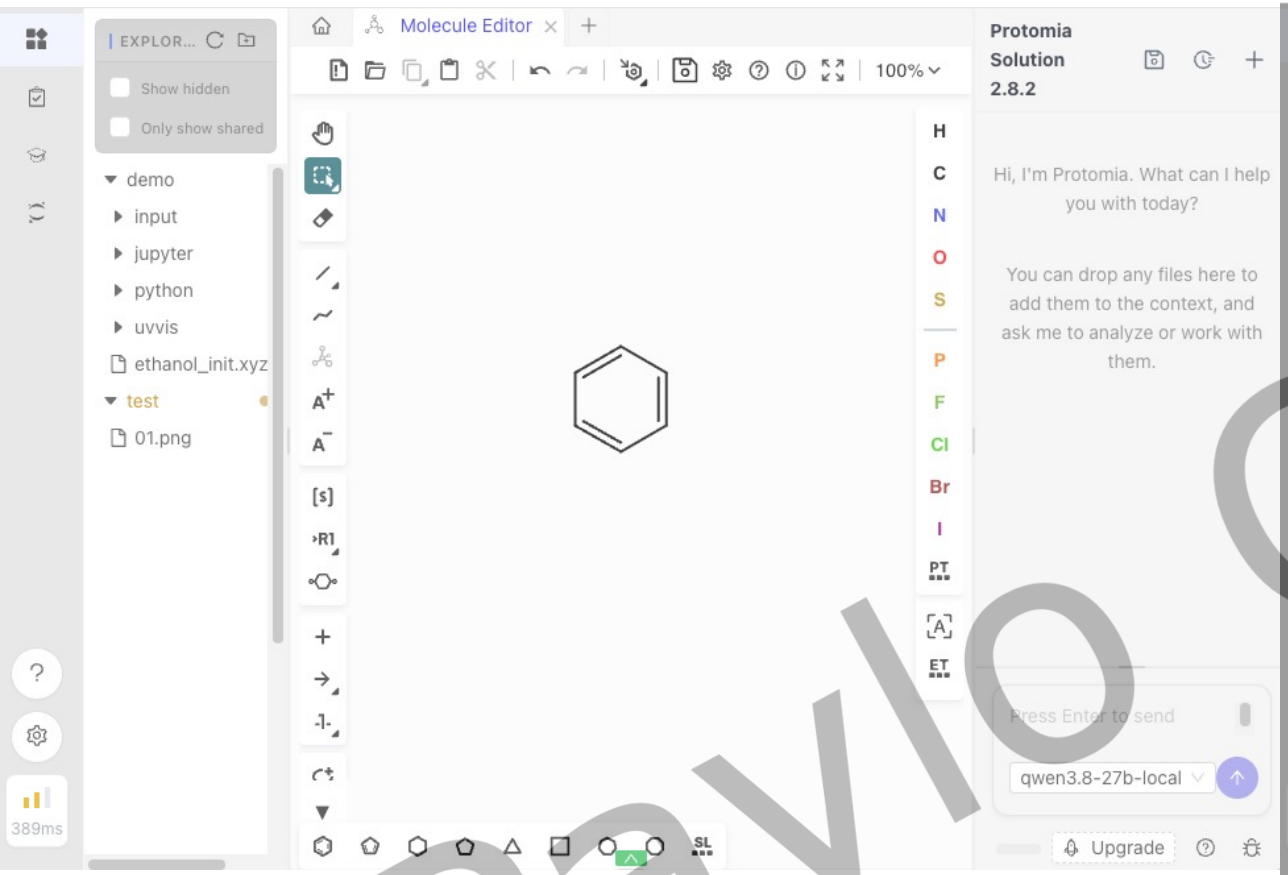
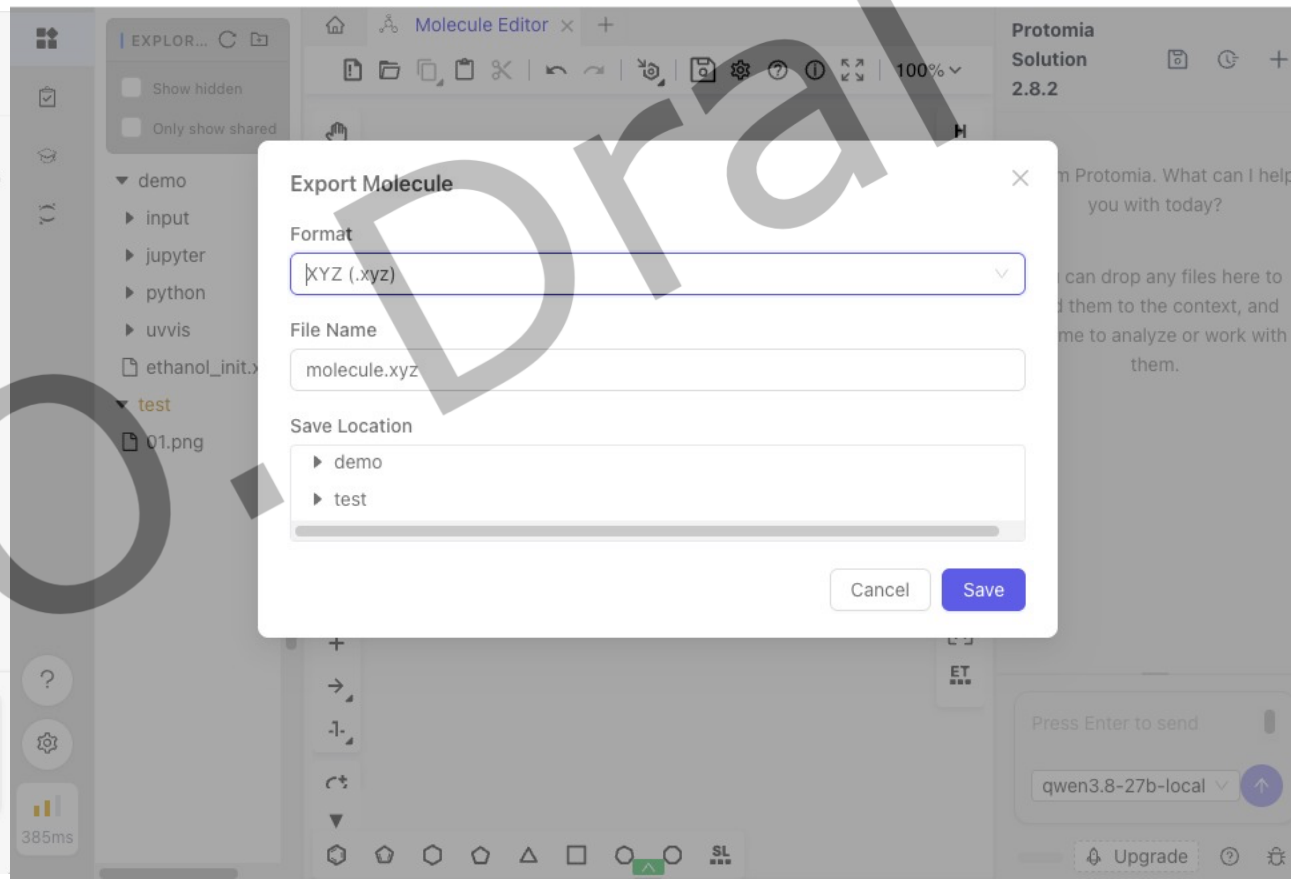

EXPLOR...
Show hidden
Only show shared
demo
input
jupyter
python
uvvis
ethanol_init.xyz
test
01.png
Molecule Editor
100%
Protomia Solution 2.8.2
Hi, I'm Protomia. What can I help you with today?
You can drop any files here to add them to the context, and ask me to analyze or work with them.
Press Enter to send
qwen3.8-27b-local
Upgrade
389ms


Export Molecule
Format
XYZ (.xyz)
File Name
molecule.xyz
Save Location
demo
test
Cancel
Save
385ms

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Aitomi

EXPLORER

- calculations
  - 16ITA
  - 16ITA_dimer
    - core_structure_of_dimer
    - opt_freq_full_structure
      - UAIQM
        - 16ITA.json
        - 16ITA.json.zip
        - 16ITA_crystal.xyz
        - 16ITA_dimer_ini.xyz
        - 16ITA_uaiqm_opted.xyz
        - 2ed9d415-40cf-46fb-b
        - 76de54c7-ccbf-4415-a
        - calc.py
        - dftd4.json
        - dftd4.txt
        - eb08f3a9-0af6-4a04-a
        - eb08f3a9-0af6-4a04-a
        - example.sh
        - freq.log
        - gaussian.com
        - model.json
        - model_predict_kwargs
    - opt_freq_model
    - uvvis

59ms

16ITA_dimer_ini.xyz | 16ITA_uaiqm_opted.xyz | AITOMIA

1 2

```
714

C    2.2112054758775    3.5197793043290    -2.6493395676902
C    2.3333751994675    4.7066975749135    -3.3700576203373
C    2.2640290150525    5.9136671677824    -2.6737718246351
H    2.3412011859445    6.8389174713286    -3.2300126972531
C    2.0977040351767    5.9309931689067    -1.2932445696169
H    2.0408275352385    6.8729871278169    -0.7660259784736
C    1.9896957011252    4.7352491104490    -0.5900502224319
H    1.8504990036569    4.7503980176509     0.4860094406428
C    2.0390377502618    3.5099159499065    -1.2586865861668
C    1.9102512919706    2.2048200652166    -0.4942902744449
H    1.9246634197864    1.3829144679854    -1.2130082792365
C    3.1070721463076    1.9816909817246     0.4331621671269
H    4.0340826493530    1.9950606698427    -0.1458940028188
H    3.1742041911812    2.7558987735340     1.2004980915698
H    3.0367451126373    1.0130664111894     0.9354549480634
C    0.5645362113050    2.1333103852210     0.2300612321852
H   -0.2543357346174    2.2048710966892    -0.4928895210576
H    0.4639530906585    1.1884602005229     0.7723740268585
H    0.4609182286033    2.9544875537983     0.9396898449164
C    2.5132061188163    4.6806333070713    -4.8845438326538
H    2.9952651007218    3.7144102646041    -5.0947189136245
C    1.1610324792186    4.6573806039098    -5.6201528065277
H    0.5519540104443    3.8158594339043    -5.2880360832700
H    0.5985391790111    5.5701700636147    -5.4170329076792
H    1.3121438634266    4.5846008946392    -6.6971127200995
C    3.4370192949536    5.7059312080626    -5.4082601637649
H    4.2740641529375    6.0444844539798    -4.8094897315349
H    3.3528097176930    6.0296102641114    -6.4397312829619
C    3.5424696493984    1.6256248254038    -3.3404468227055
```

TERMINAL OUTPUT

```
(base) dral@login:~$
```

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Jupyter Lab

No Jupyter instances are currently running.

Start a new instance by launching a new job.

* CPU Number: 1

* GPU Number: 0

Partition: Default

Node: Select a machine

Launch

89ms

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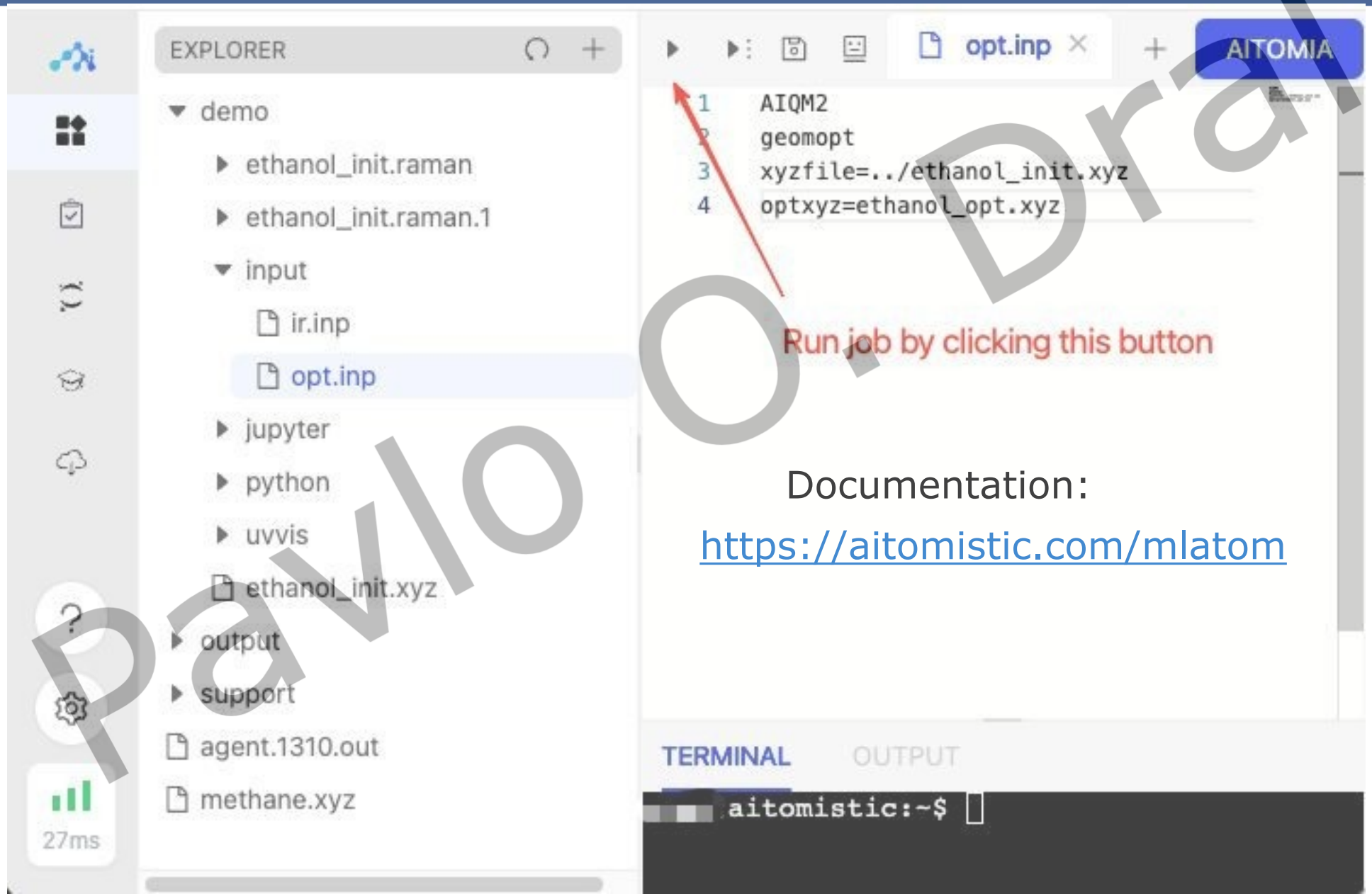
MLatom Use



Documentation:

https://aitomistic.com/mlatom

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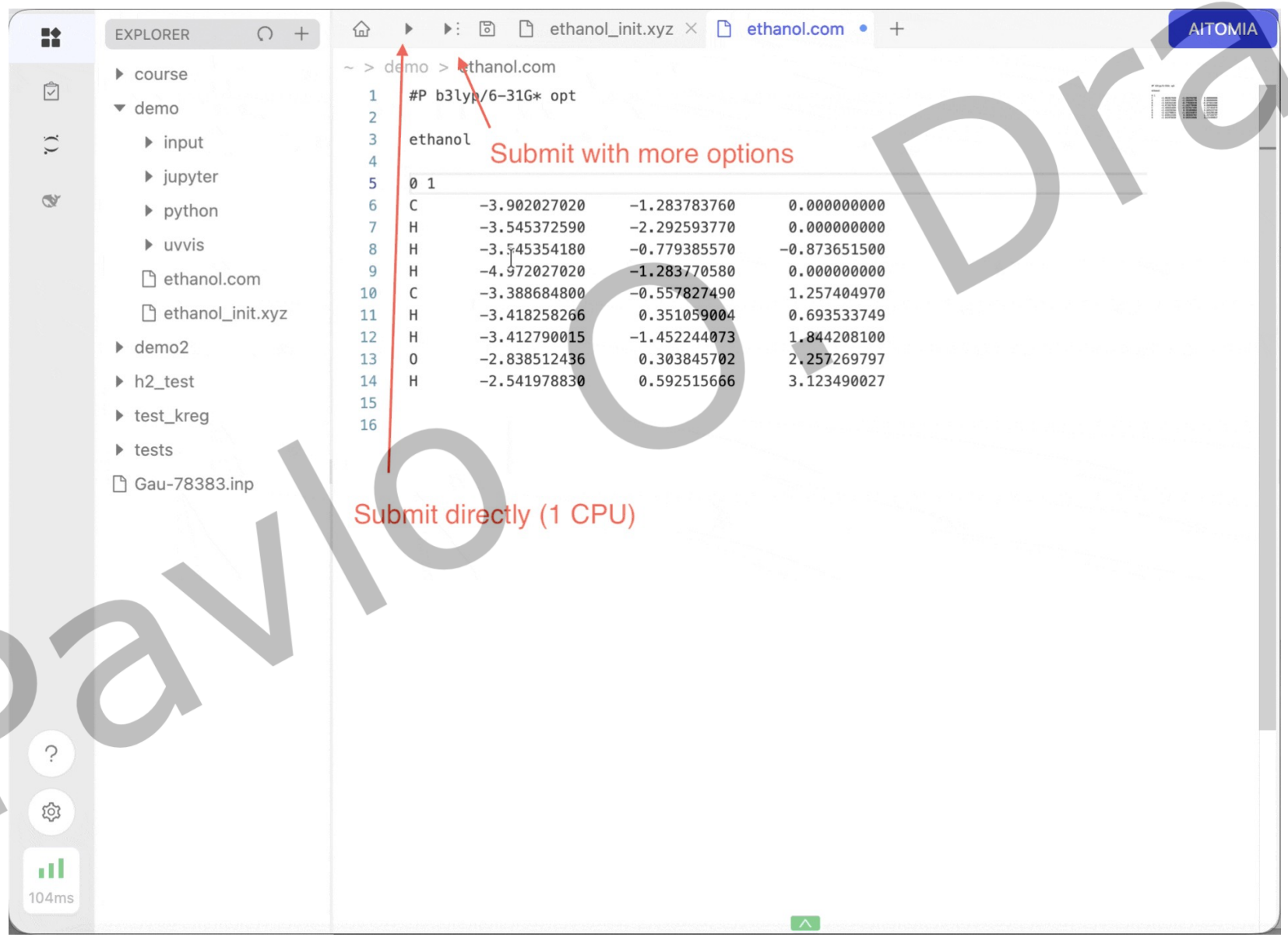
Only for Xiamen University Users



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Job Name: Job Name Start Time: Select date End Time: Select date State: Search

Job list

Job Name	CPU Cores	Partition	Node List	Time Start	Time End	State	Actions
jupyter_slurm.sh	1	cpu	b006	2025-08-22 10:36:52	2025-08-22 18:37:18	TIMEOUT	
jupyter_slurm.sh	1	cpu	b006	2025-08-21 20:10:31	2025-08-22 04:10:47	TIMEOUT	
opt.py	1	cpu	b006	2025-08-19 11:16:21	2025-08-19 11:16:34	FAILED	
opt.py	1	cpu	b006	2025-08-19 11:10:24	2025-08-19 11:11:07	FAILED	
jupyter_slurm.sh	1	cpu	b006	2025-08-14 17:33:23	2025-08-15 01:33:32	TIMEOUT	
jupyter_slurm.sh	1	cpu	b002	2025-08-07 14:37:20	2025-08-07 22:37:45	TIMEOUT	
jupyter_slurm.sh	1	cpu	b006	2025-08-05 10:28:51	2025-08-05 18:29:10	TIMEOUT	
ir.inp	1	cpu	b002	2025-07-24 22:16:59	2025-07-24 22:17:35	COMPLETE	
mol1.inp	1	cpu	b002	2025-07-24 22:16:42	2025-07-24 22:22:09	COMPLETE	
ir.inp	1	cpu	b004	2025-07-21 19:48:31	2025-07-21 19:49:02	COMPLETE	

< 1 2 3 4 5 ... 16 >

44ms

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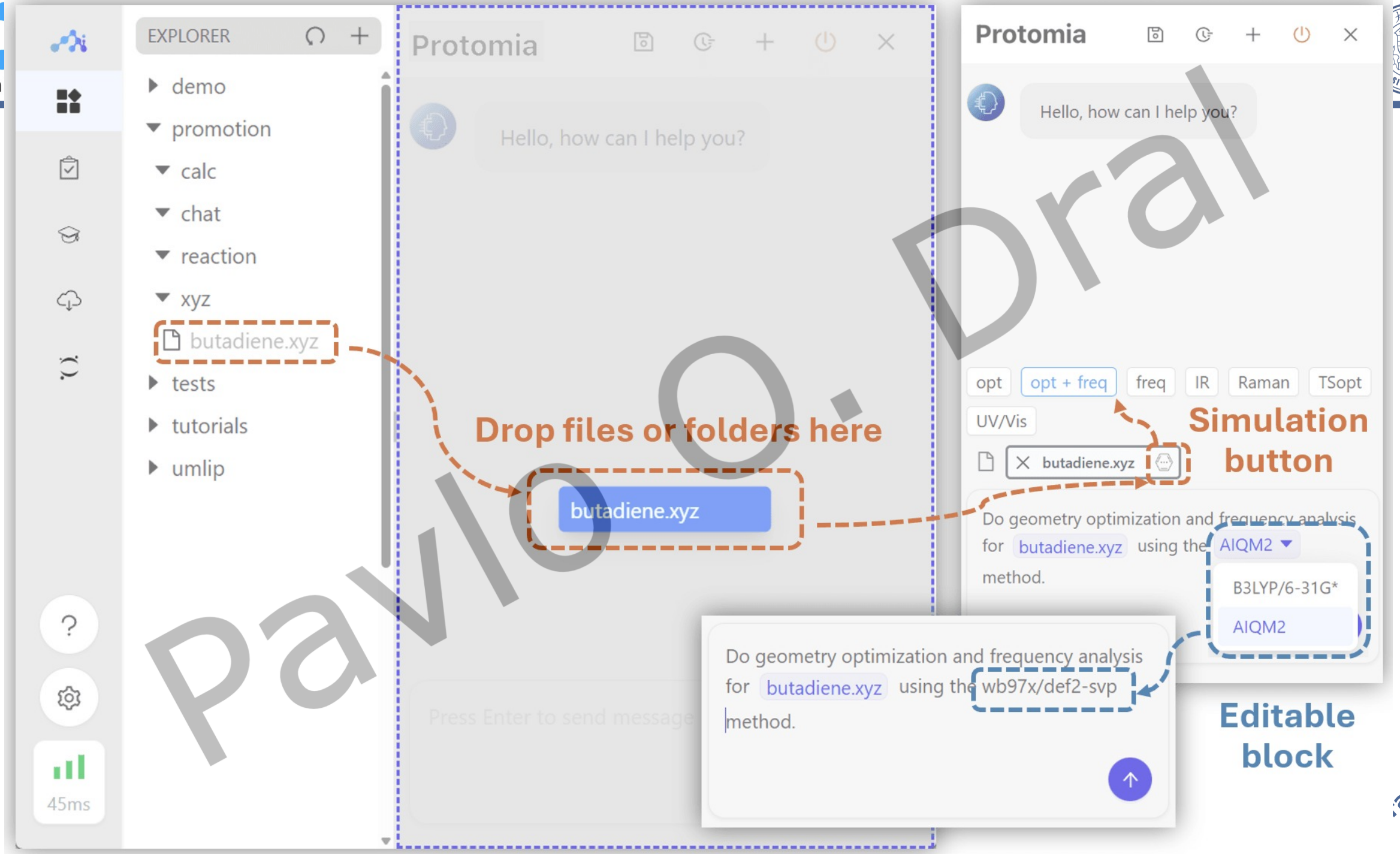
EXPLORER
demo
promotion
calc
chat
reaction
xyz
butadiene.xyz
tests
tutorials
umlip
45ms
Protomia
Hello, how can I help you?
Drop files or folders here
butadiene.xyz
Press Enter to send message
Protomia
Hello, how can I help you?
opt
opt + freq
freq
IR
Raman
TSopt
UV/Vis
butadiene.xyz
Simulation button
Do geometry optimization and frequency analysis for butadiene.xyz using the AIQM2 method.
B3LYP/6-31G*
AIQM2
Do geometry optimization and frequency analysis for butadiene.xyz using the wb97x/def2-svp method.
Editable block

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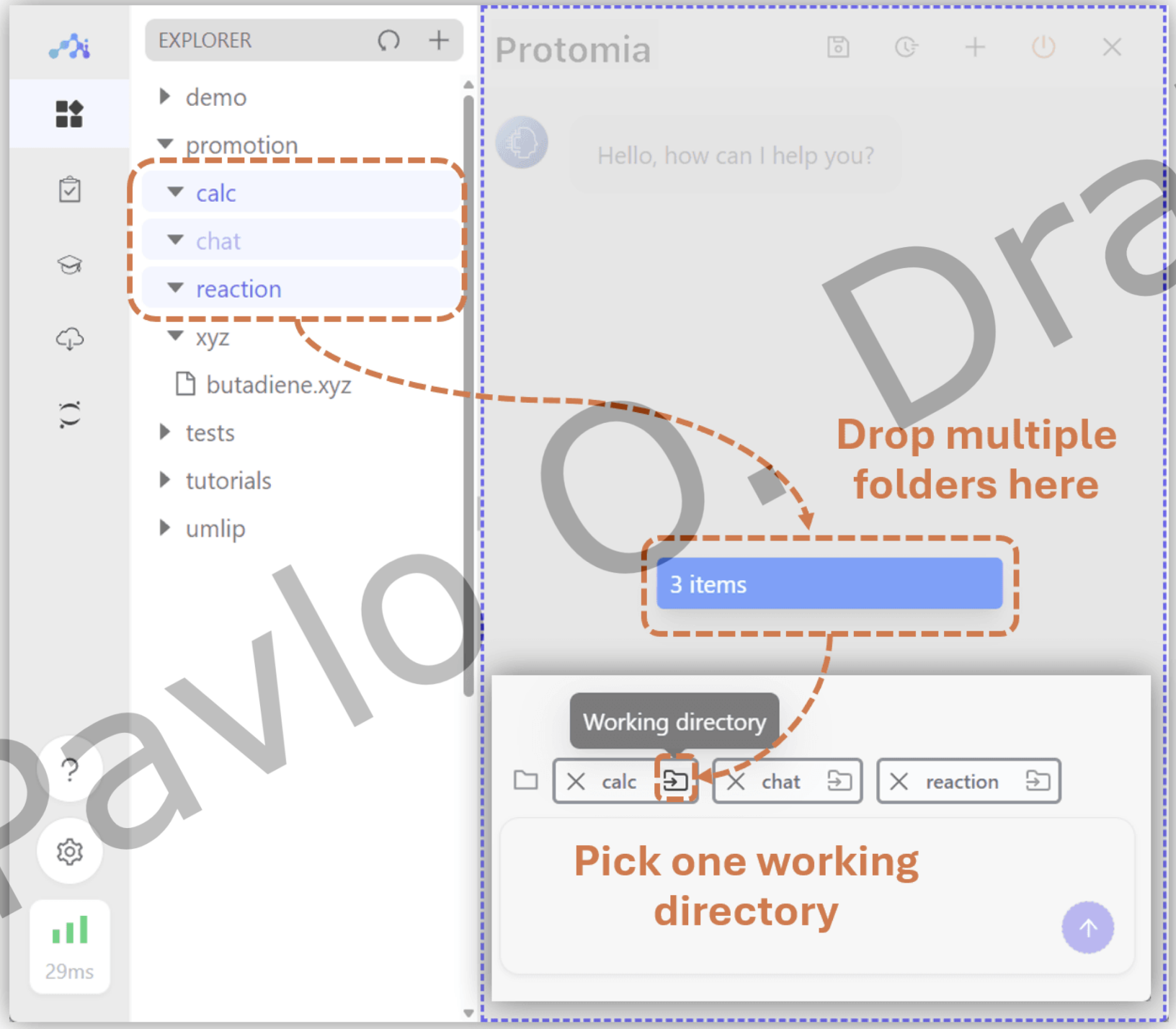
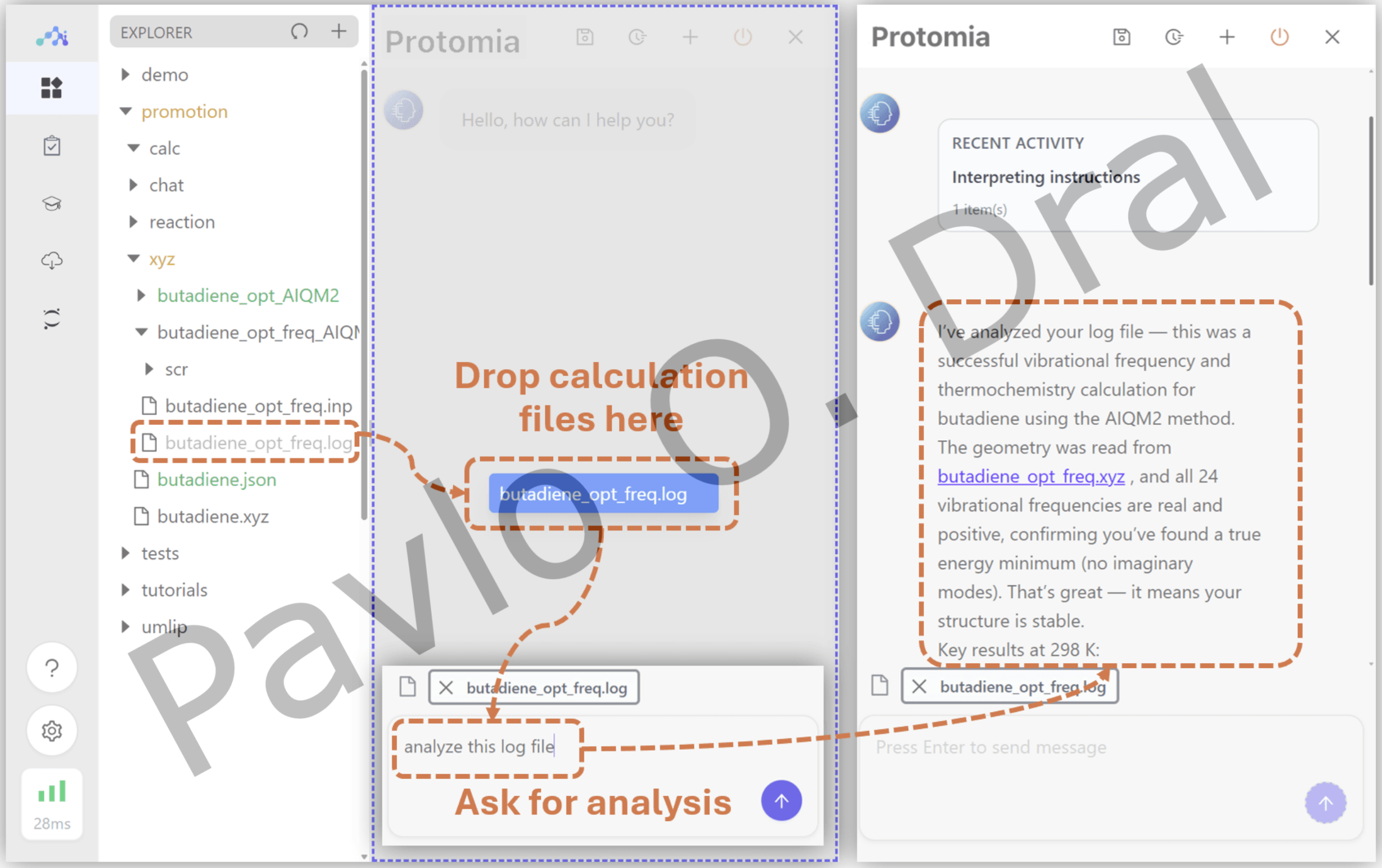

EXPLORER
demo
promotion
calc
chat
reaction
xyz
butadiene.xyz
tests
tutorials
umlip
29ms
Protomia
Hello, how can I help you?
Drop multiple folders here
3 items
Working directory
calc
chat
reaction
Pick one working directory

Pavlo O. Dral


EXPLORER
demo
promotion
calc
chat
reaction
xyz
butadiene_opt_AIQM2
butadiene_opt_freq_AIQM
scr
butadiene_opt_freq.inp
butadiene_opt_freq.log
butadiene.json
butadiene.xyz
tests
tutorials
umlip
28ms
Protomia
Hello, how can I help you?
Drop calculation files here
butadiene_opt_freq.log
butadiene_opt_freq.log
analyze this log file
Ask for analysis
Protomia
RECENT ACTIVITY
Interpreting instructions
1 item(s)
I've analyzed your log file — this was a successful vibrational frequency and thermochemistry calculation for butadiene using the AIQM2 method. The geometry was read from butadiene_opt_freq.xyz , and all 24 vibrational frequencies are real and positive, confirming you've found a true energy minimum (no imaginary modes). That's great — it means your structure is stable.
Key results at 298 K:
butadiene_opt_freq.log
Press Enter to send message

Pavlo O. Dral

Aitomistic

Protomia

Ask about AIQM2

what is AIQM2 and how to use it?

AIQM2 is the second-generation AI-enhanced quantum mechanics method designed for high-speed, chemically accurate simulations of organic reactions — including transition state searches, geometry optimizations, frequency calculations, and reactive dynamics. It combines machine learning with semi-empirical quantum mechanics (using GFN2-xTB as its baseline) to deliver accuracy competitive with DFT at a fraction of the computational cost. AIQM2 also supports property predictions like dipole moments for IR spectrum generation.

To use AIQM2 in MLatom, input file or Python script.

Introduction

Example 1: Input File for Single Point Energy + Geometry Optimization

```
AIQM2
xyzfile=ts.xyz
geomopt
ts=True
optxyz=ts_opt.xyz
```

Example usage

+ promotion

Press Enter to send message

Protomia

Example 2: Frequency Calculation & IR Spectrum (Input File)

After geometry optimization, calculate frequencies and generate IR spectrum:

```
ir
AIQM2
xyzfile=opt.xyz
```

Example usage

Frequencies are automatically scaled by 0.962 for better agreement with experiment.

'acetone', etc.).

Sources:

- http://mlatom.com/docs/tutorial_aiqm2.rst.html (tutorial_aiqm2.rst)
- http://mlatom.com/docs/tutorial_aiqm2.html (Explore Diels-Alder reactions with AIQM2)
- http://mlatom.com/docs/tutorial_ts.html (Choosing the method or model)
- http://mlatom.com/docs/tutorial_ts.rst.html (tutorial_ts.rst)
- http://mlatom.com/docs/tutorial_uaiqm.rst.html (tutorial_uaiqm.rst)

Sources and further reading

+ promotion

Press Enter to send message

Pavlo O. Dral

Aitomistic

Protomia

Chat History

Check chat history

what is AIQM2 and how to use it
3 messages 2026-03-19 16:52:33

analyze this log file
3 messages 2026-03-17 21:32:27

analyze this log file
3 messages 2026-03-17 21:29:26

Do geometry optimization and frequency analysis f...
20 messages 2026-03-17 21:23:29

what's the reaction energy for DA reaction between ...
28 messages 2026-03-11 10:04:13

for Diels-Alder reaction between ethylene and 1,3-b...
32 messages 2026-03-11 09:55:42

Do geometry optimization and frequency analysis f...
16 messages 2026-03-11 09:42:34

Restart from previous chat

+ promotion

Press Enter to send message

34ms

Protomia

what is AIQM2 and how to use it?

RECENT ACTIVITY

Interpreting instructions

1 item(s)

AIQM2 is the second-generation AI-enhanced quantum mechanics method designed for high-speed, chemically accurate simulations of organic reactions — including transition state searches, geometry optimizations, frequency calculations, and reactive dynamics. It combines machine learning with semi-

+ promotion

Press Enter to send message

Pavlo O. Dral

Protomia

Select Folder to Save Conversation

File name: what_is_AIQM2_and_how_to_use_it.md

Select a folder to save the conversation:

Current Selected Path:
/aitomistic/hub/home/chenyxx/promotion/chat

- demo
- promotion
  - calc
  - chat
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what_is_AIQM2_and_how_to_use_it.md

Protomia

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Wrap what_is_AIQM2_and_how_to_use_it.md

```
# what is AIQM2 and how to use it

**Export Date:** 2026/3/20 15:02:30

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## User

what is AIQM2 and how to use it?


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## Assistant

Interpreting instructions


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## Assistant

AIQM2 is the second-generation AI-enhanced quantum
mechanics method designed for high-speed, chemically
accurate simulations of organic reactions — including
transition state searches, geometry optimizations,
frequency calculations, and reactive dynamics. It combines
machine learning with semi-empirical quantum mechanics
(using GFN2-xTB as its baseline) to deliver accuracy
competitive with DFT at a fraction of the computational
```

Pavlo O. Dral

Protomia helps to develop Protomia

25 Apr 2026 20:56	Protomia (Pavlo O. Dral)
25 Apr 2026 18:20	Pavlo O. Dral
25 Apr 2026 18:14	Pavlo O. Dral
25 Apr 2026 17:21	Protomia (Pavlo O. Dral)
25 Apr 2026 15:20	Protomia (Pavlo O. Dral)
25 Apr 2026 15:17	Protomia (Pavlo O. Dral)
25 Apr 2026 15:14	[redacted]
25 Apr 2026 14:19	Protomia (Pavlo O. Dral)
25 Apr 2026 14:19	Protomia (Pavlo O. Dral)
25 Apr 2026 12:38	Pavlo O. Dral
25 Apr 2026 09:44	Protomia (Pavlo O. Dral)
25 Apr 2026 09:31	Pavlo O. Dral
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24 Apr 2026 23:49	Protomia (Pavlo O. Dral)
24 Apr 2026 23:36	Protomia (Pavlo O. Dral)

Pavlo O. Dral

Aitomistic

Protomia Solution 2.8.2

Show me the electrostatic-potential (ESP) map for water using HF/STO-3G via PySCF — render the 3D ESP-coloured surface as a .png.

ESP_PYSCF_164807

copy

Ran 2 actions

I'll run the HF/STO-3G ESP calculation for water, which will also render the ESP-coloured surface automatically.

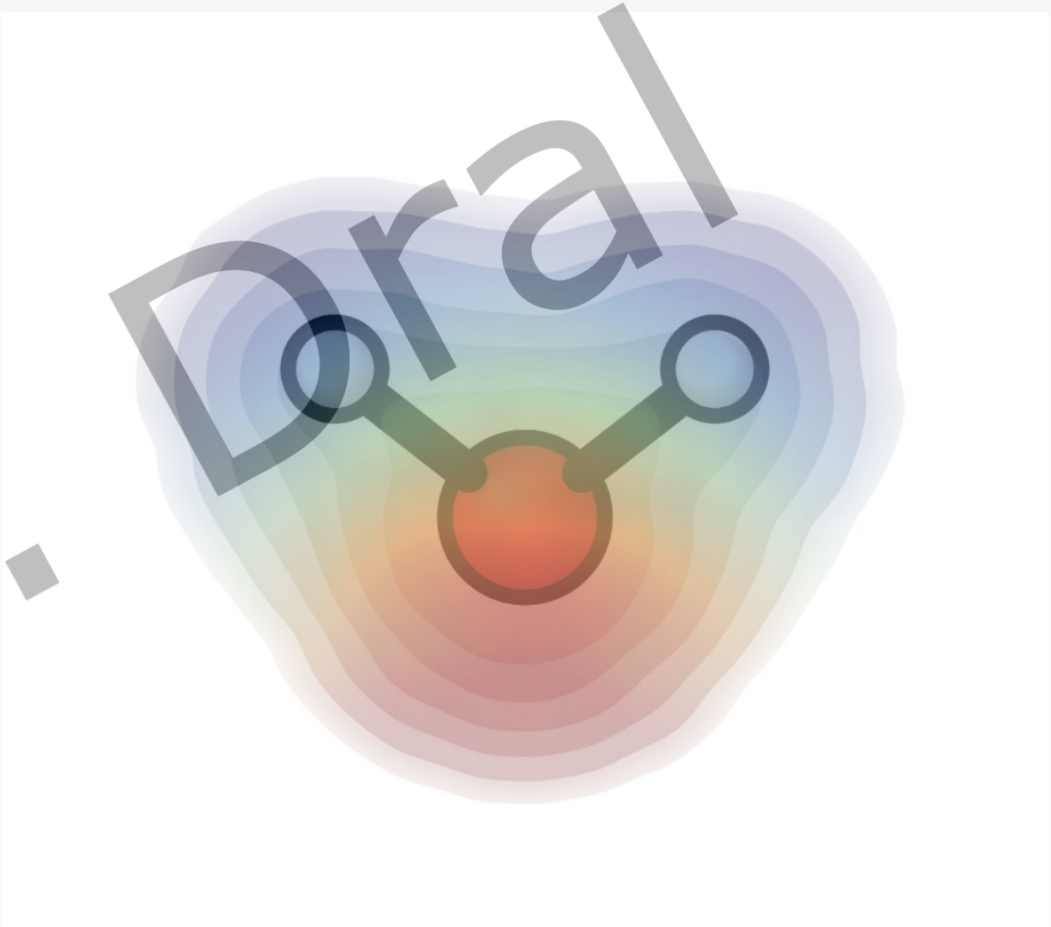
Ran 1 action

The HF/STO-3G single-point for water has been submitted to the compute cluster (job 183770) — from the resulting wavefunction, the ESP grid will be generated and the ESP-coloured surface rendered to a PNG automatically.

It's a tiny system so it should be quick. I'll report back with the rendered surface and the energy once it finishes — feel free to keep chatting in the meantime.

The HF/STO-3G calculation for water is done — here's the ESP map rendered from the resulting wavefunction:

Protomia Solution 2.8.2



Key results (HF/STO-3G, ground state):

- **Total electronic energy: −74.964449 Hartree**
- HOMO: −10.637 eV
- LUMO: 16.190 eV
- HOMO–LUMO gap: 26.827 eV

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Aitomistic

Protomia Solution 2.8.2

Show me the HOMO surface picture (3D rendered orbital, .png) for water using HF/STO-3G via PySCF.

HOMOLUMO_VIZ_164807

copy

Ran 2 actions

I'll run an HF/STO-3G single-point on water to generate wavefunctions and render the HOMO orbital surface automatically.

Ran 1 action

The water HOMO visualization job has been submitted to the cluster (Slurm job 183766) — it's running an HF/STO-3G single-point calculation, after which the HOMO (and LUMO) orbital surface is rendered to a PNG automatically.

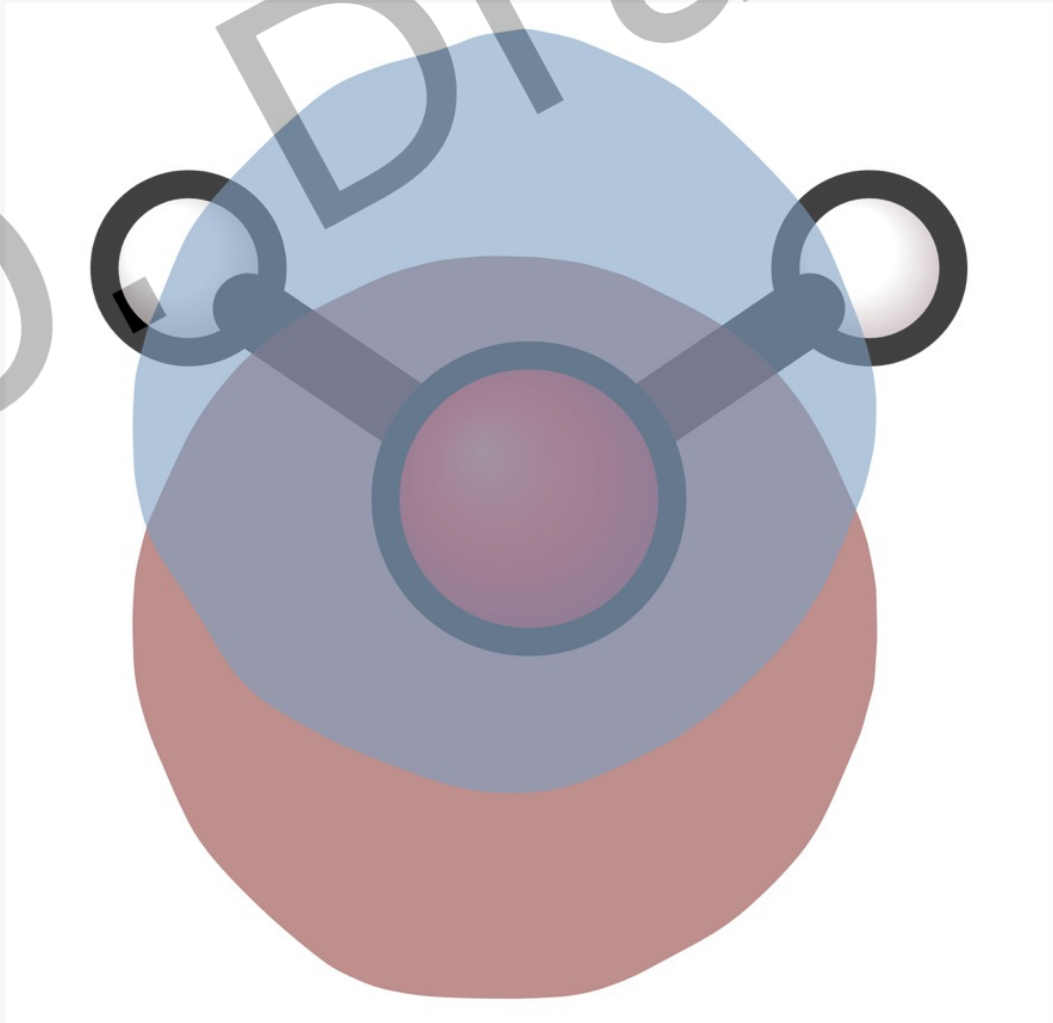
As soon as it finishes — typically a couple of minutes for a small molecule like this — I'll hand back the rendered HOMO surface picture right here in chat. Feel free to keep chatting in the meantime; I'll report the result the moment it's ready.

The water calculation finished — here's your HOMO surface picture! 🎉

Below is the 3D-rendered HOMO isosurface from the HF/STO-3G calculation on water (and the LUMO as a bonus). You can see the

Protomia Solution 2.8.2

Below is the 3D-rendered HOMO isosurface from the HF/STO-3G calculation on water (and the LUMO as a bonus). You can see the classic lone-pair-shaped orbital on the oxygen, which is exactly what you expect as the HOMO of H_2O.



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Protomia Solution 2.8.2

Compute the UV-Vis absorption spectrum of triphenylamine: optimize the geometry with AIQM3, then run OMNI-P2x for the excited states.

OMNIP2X_164807

Ran 2 actions

I'll set up a multi-stage calculation: AIQM3 geometry optimization first, then an OMNI-P2x excited-state (UV-Vis) single point on the optimized geometry, with everything saved to your working folder.

Ran 1 action

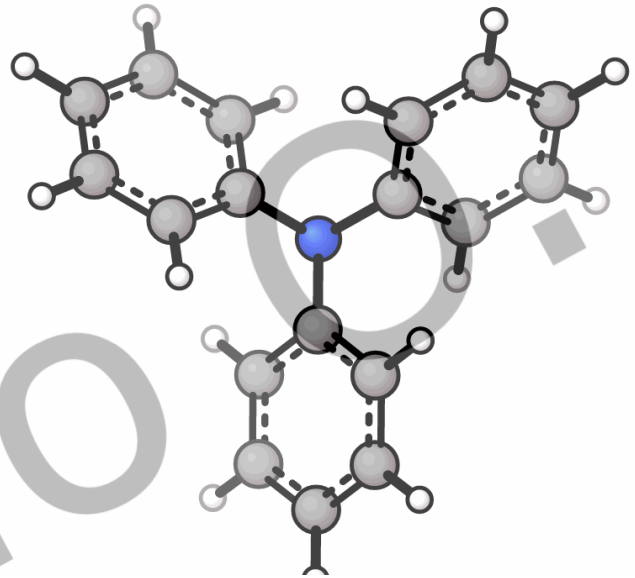
Your calculation is submitted and running on the cluster. Here's the plan that's queued:

1. **Stage 1 — Geometry optimization** of triphenylamine with **AIQM3**
2. **Stage 2 — Excited states (UV-Vis)** with **OMNI-P2x** on the optimized geometry

Protomia Solution 2.8.2

Files in your working folder:

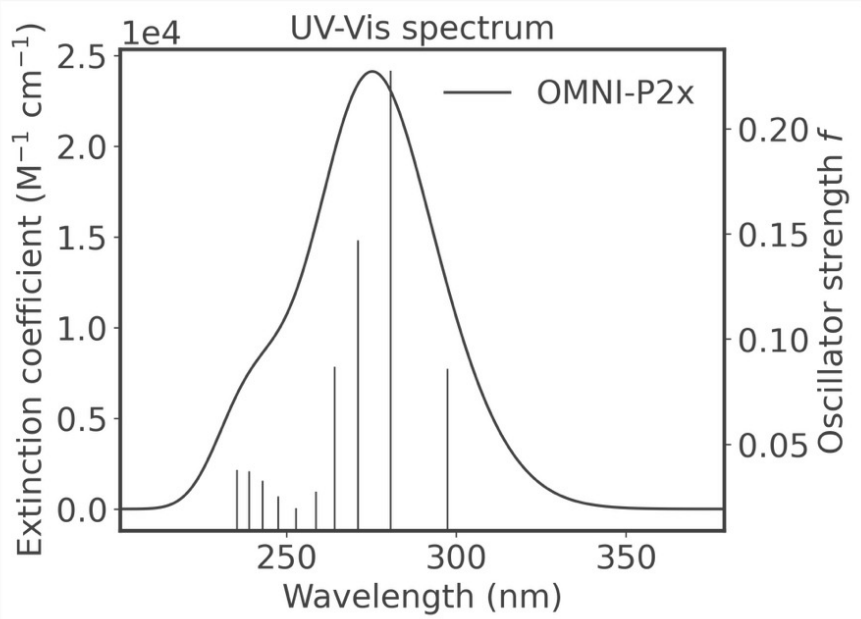
- Result bundle: triphenylamine_opt_AIQM3_9040fbb9
- Optimized geometry: triphenylamine_opt_AIQM3.xyz
- Structure rotation:



Protomia Solution 2.8.2

S_2	4.4181	280.6	0.227
S_3	4.5736	271.1	0.147
S_4	4.6934	264.2	0.087
S_5	4.7945	258.6	0.027

Spectrum:



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Aitomistic

H3_umbrella_inversion_tsopt_AIQM3.xyz | NH3_umbrella_inversion_tsopt_AIQM3.xyz

Charge 0 Mult 1

Protomia Solution 2.6.0

keep chatting in the meantime!

The NEB search and transition-state refinement have finished! Here are the key results for the ammonia umbrella-inversion TS:

Transition-state geometry (AIQM3 optimized):

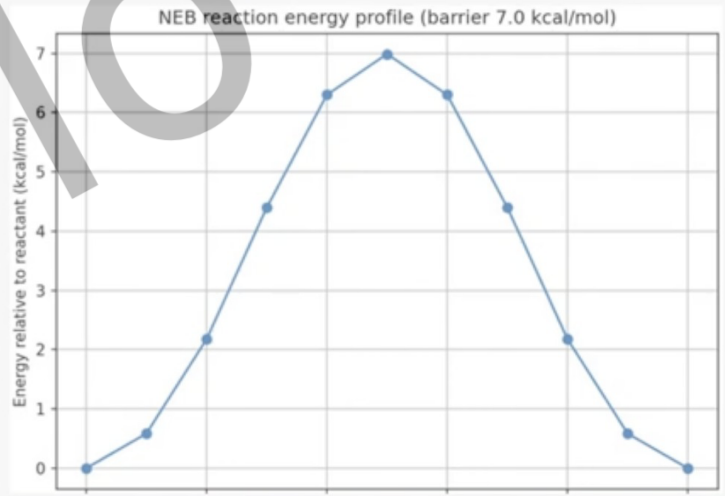
- Total electronic energy: **−56.4985 Hartree**
- The TS is confirmed with exactly **one imaginary frequency: −871.1 cm⁻¹**
- Forward barrier from reactant: **6.1 kcal/mol**
- Dipole moment: **0.0 D** (planar D_3h symmetry at the saddle point)

Optimized TS structure: NH3_umbrella_inversion_tsopt_AIQM3.xyz

TS Verification:

```
Imaginary frequencies: 1 (-871.1i cm⁻¹)  ✓
Normal mode match: umbrella inversion (H atoms move through the N plane)  ✓
Verdict: VALID TS
```

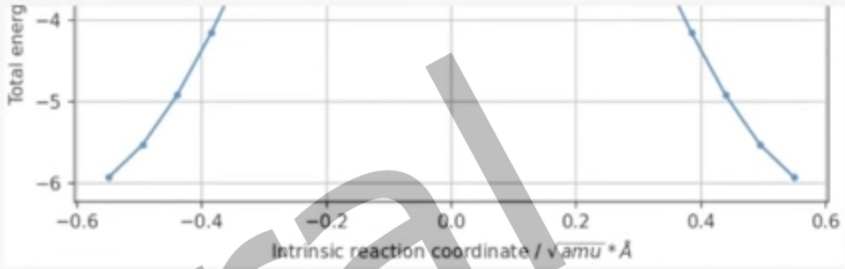
NEB energy profile (reactant → TS → product):



+ NH3_umbrella_inversion_tsop...

Press Enter to send message

Protomia Solution 2.6.0



The IRC confirms that the transition state connects the two pyramidal minima (reactant and product) through the planar D_3h saddle point, exactly as expected for the ammonia umbrella inversion.

IRC trajectory files:

- Full path (both directions): NH3_umbrella_inversion_irc_full.xyz
- Backward (toward reactant): backward.xyz
- Forward (toward product): forward.xyz

Full IRC bundle: NH3_umbrella_inversion_irc_AIQM3_bundle

Summary of the complete characterization:

Property	Value
TS energy	−56.4985 Hartree
Imaginary frequency	−871.1 cm⁻¹
Forward barrier	6.1 kcal/mol
TS symmetry	Planar D_3h (dipole = 0.0 D)
IRC connectivity	Reactant ↔ TS ↔ Product ✓

The umbrella inversion of NH_3 is now fully characterized: the NEB located the planar transition state, the frequency calculation confirmed it is a first-order saddle point with the correct umbrella-inversion normal mode, and the IRC verified that it smoothly connects the two equivalent pyramidal minima.

copy

+ NH3_umbrella_inversion_irc_...

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