QHFlow

: Accelerating DFT with Equivariant Flow Matching

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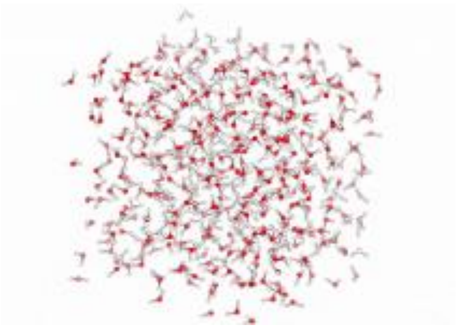
NVIDIA BioNeMo Reading group | Oct. 30. 2025

NeurIPS 2025 spotlight

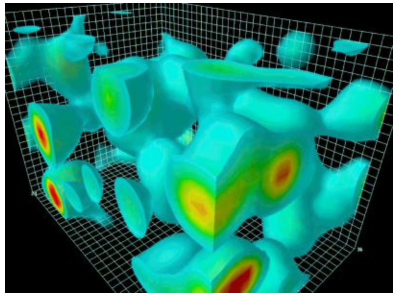
KAIST POSTECH POHANG UNIVERSITY OF SCIENCE AND TECHNOLOGY

Atomistic interaction modeling for materials

Atomistic Interaction Modeling



Molecular Dynamics



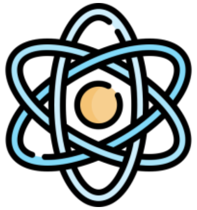
Wavefunction

Example

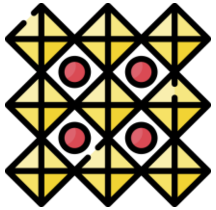
Classical Force Field
Machine Learning Force Field (MLFF)
Machine Learning Interatomic Potential (MLIP)
Density Functional Theory (DFT)
Wavefunction based method (QVMC, CCSD)
...

Material Understanding

Chemical Reaction

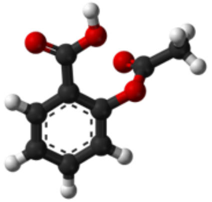


Quantum Effects



Solid State Effects

Material Discovery

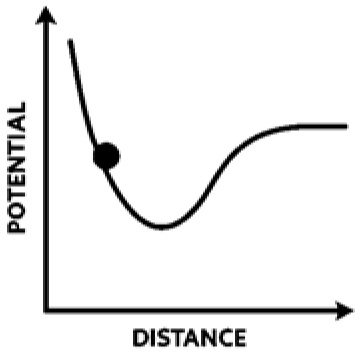


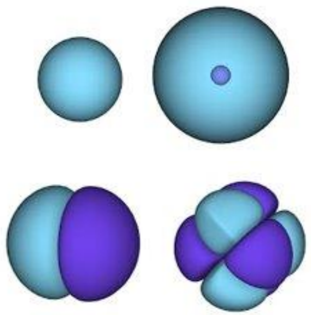
Molecule

Drug

Battery cathode

Our interests: DFT





	Classical Efficiency	Balanced	Quantum Accuracy
Level of Theory	*(classical) Interatomic potential*	*Electron density*	*Wavefunction*
Speed	Fastest	Speed	Slowest
Accuracy Fidelity	Low Poor quantum interaction	Accuracy	High Accurate quantum interaction
Examples	Classical Force Field	***Density Functional Theory***	QVMC, CCSD(S)

Our interests: DFT

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	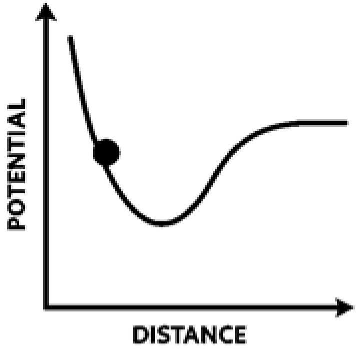	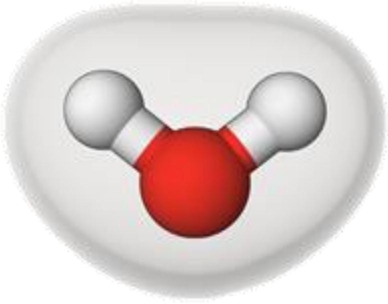	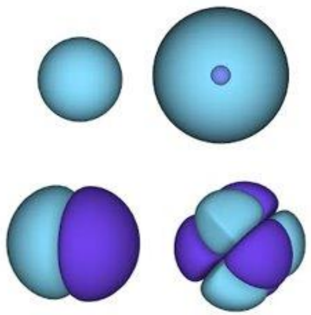
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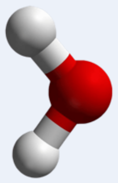
Accuracy **Fidelity**	Low Poor quantum interaction		High Accurate quantum interaction
Examples	Classical Force Field	***Density Functional Theory***	QVMC, CCSD(S)

DFT is a common standard in computational chemistry for both industry and academia

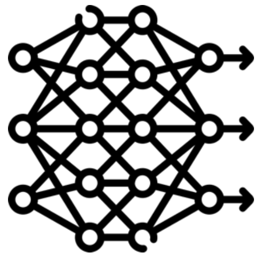
Our goal: ML-DFT

Goal 1: Fast Prediction

(One-shot approximation)



Molecule



Neural Network

Total energy / Force
HOMO/LUMO levels
Band structure
Wavefunction
…

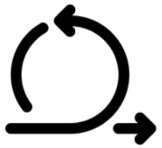
Quantum Property
With ML output

Fast Prediction

ML Output

Goal 2: DFT Acceleration

(With DFT calculation)



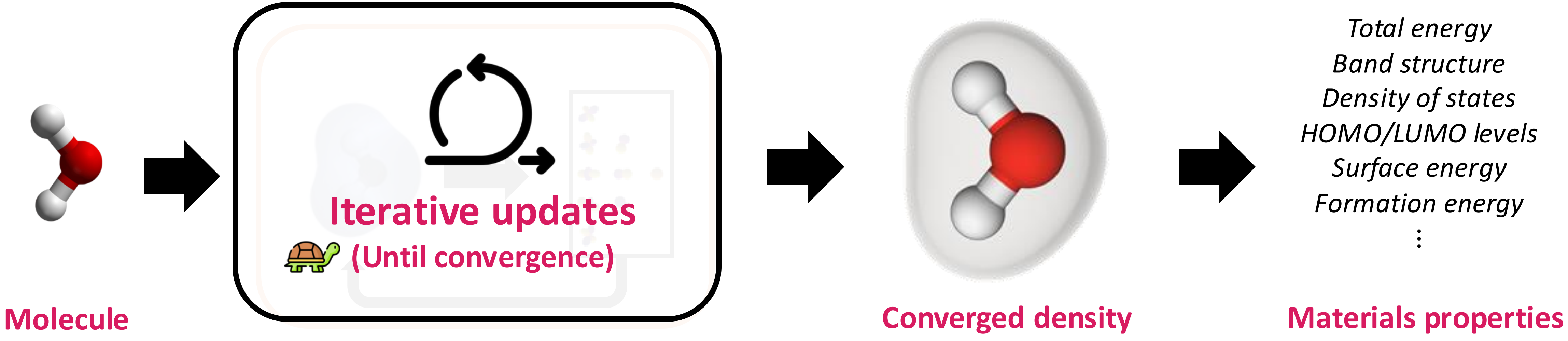
Accelerating DFT

Total energy / Force
HOMO/LUMO levels
Band structure
Wavefunction
…

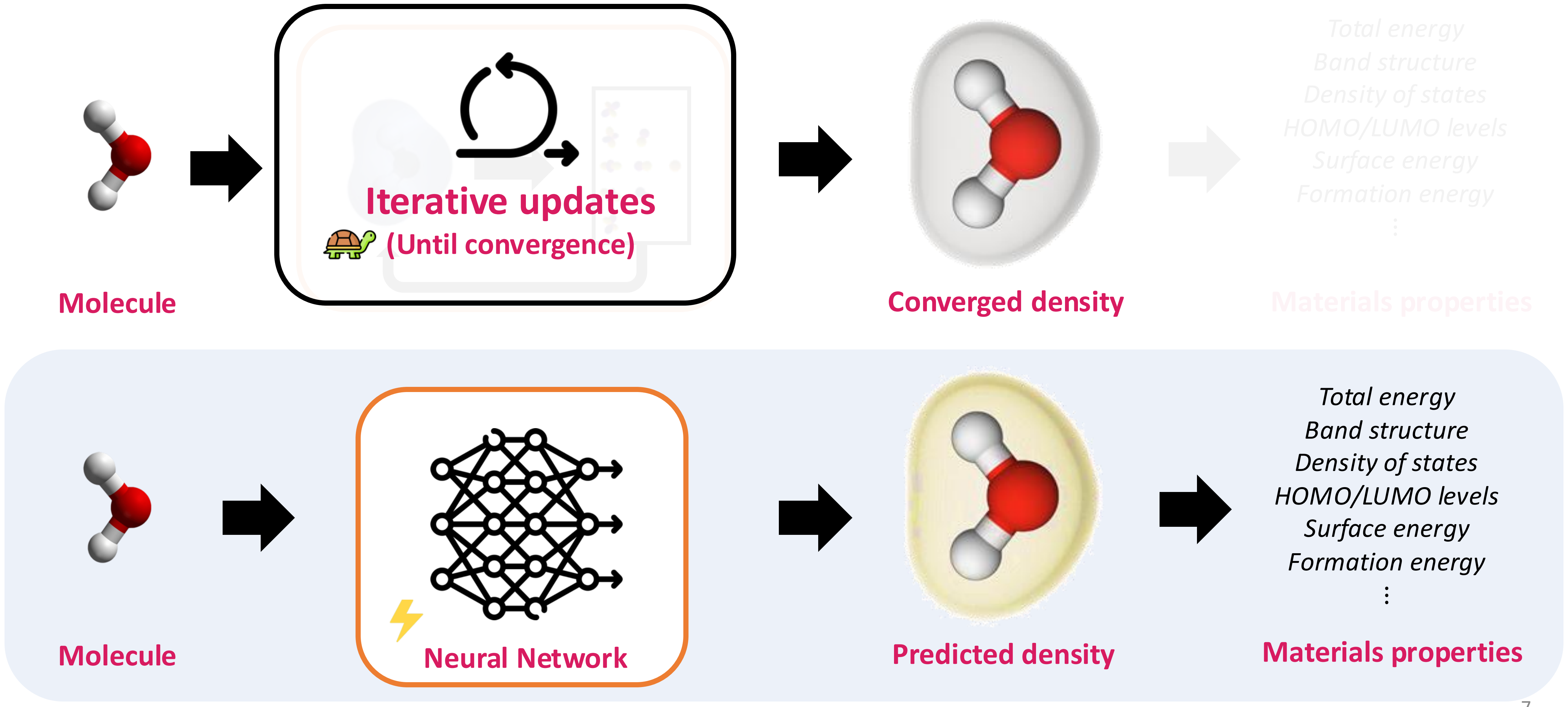
Quantum Property
With DFT output

DFT-level Accuracy

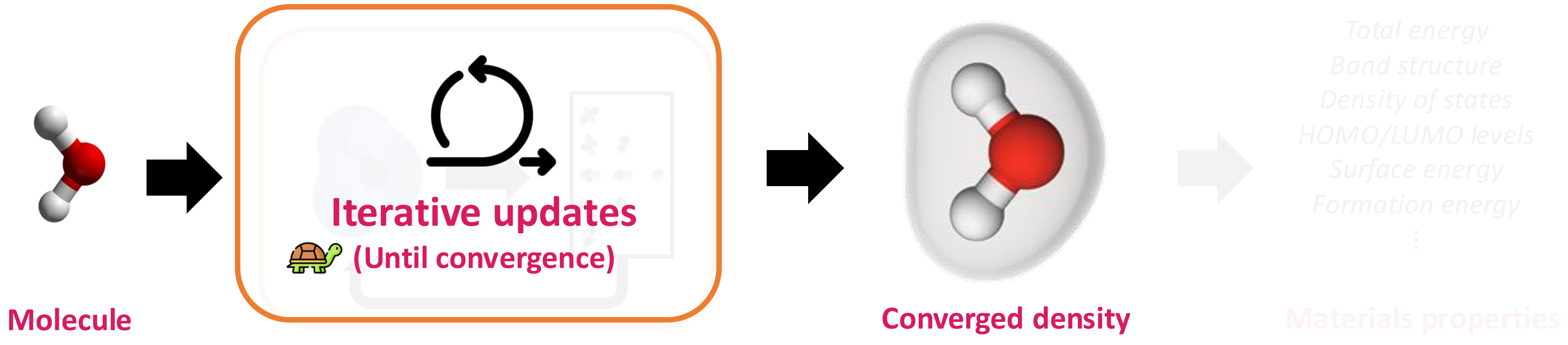
What is DFT?


Iterative updates
(Until convergence)
Molecule
Converged density
Total energy
Band structure
Density of states
HOMO/LUMO levels
Surface energy
Formation energy
⋮
Materials properties

Our goal: (1) DFT Approximation



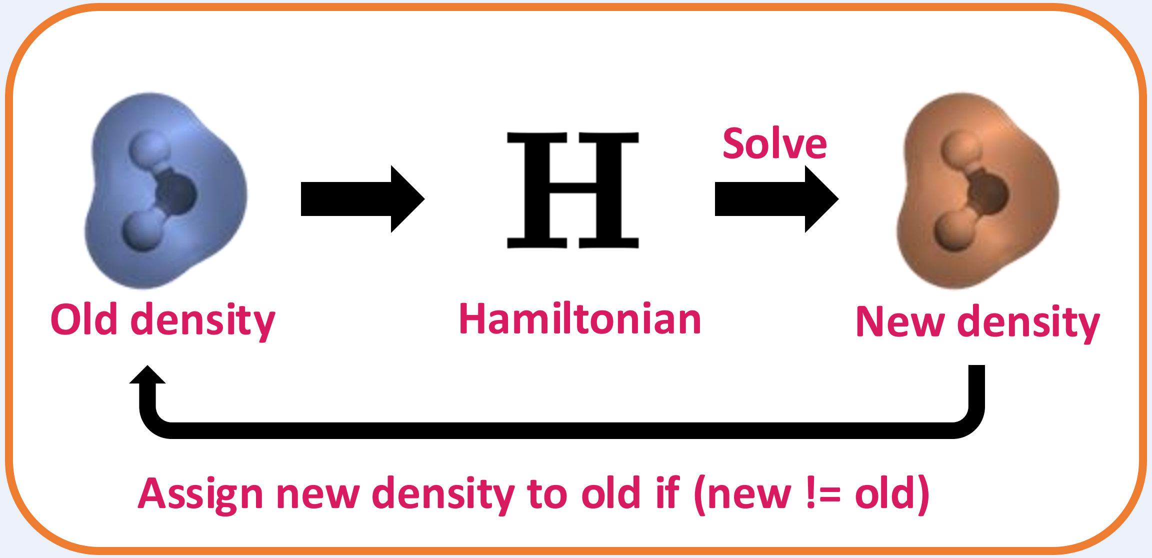
Our goal: (2) DFT Acceleration



Self-Consistent Field

(=Iterative updates, SCF)

Good initial density is needed



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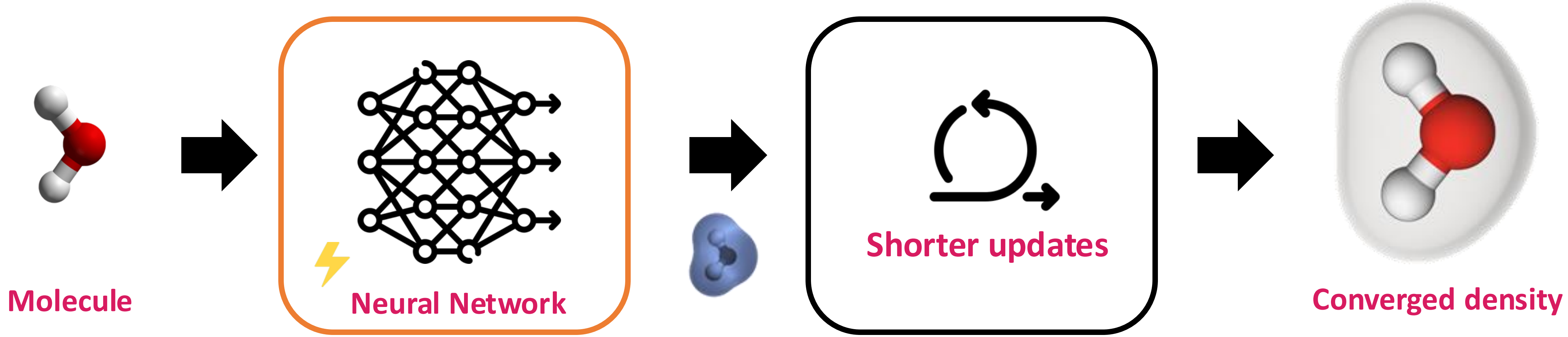

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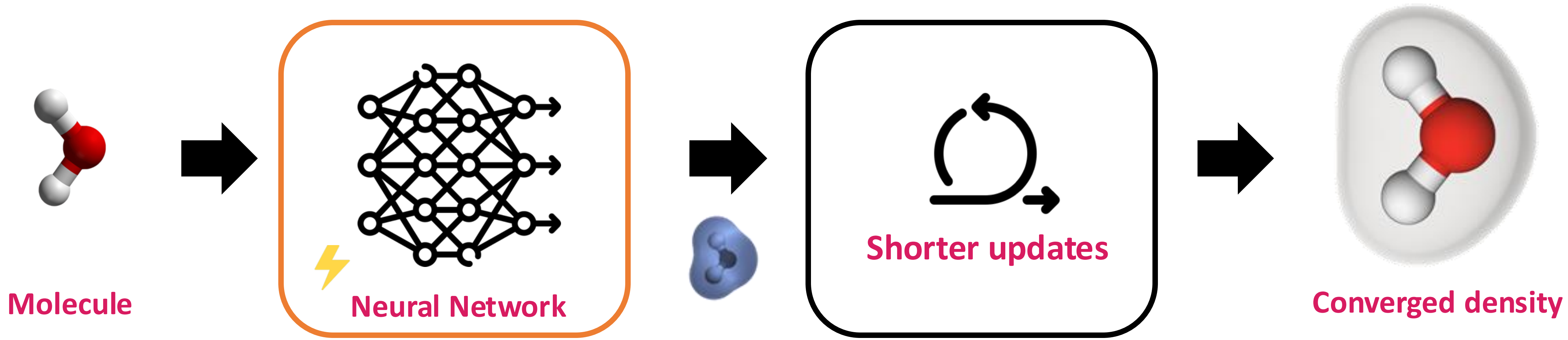
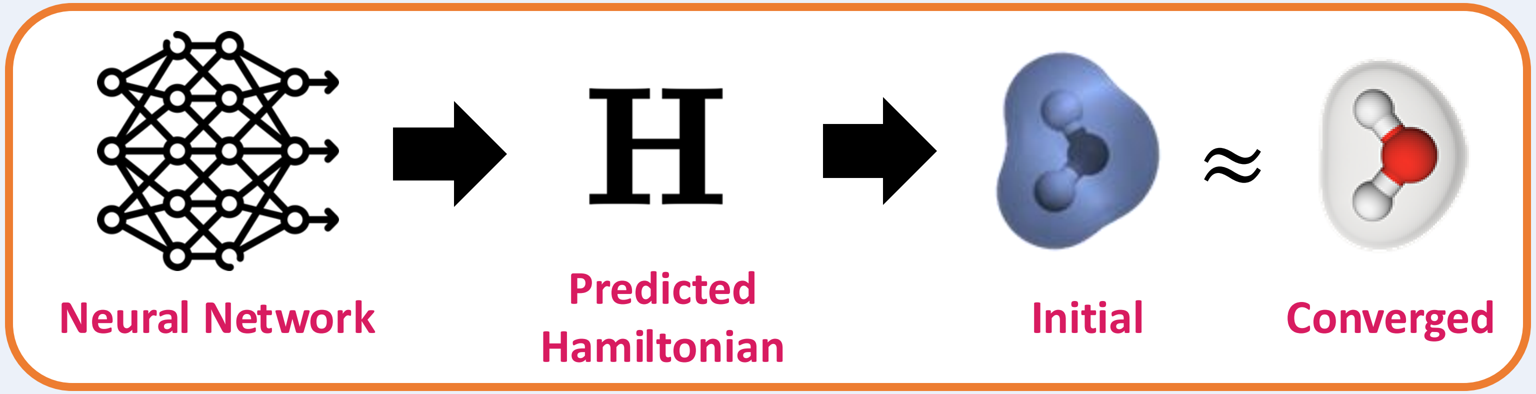
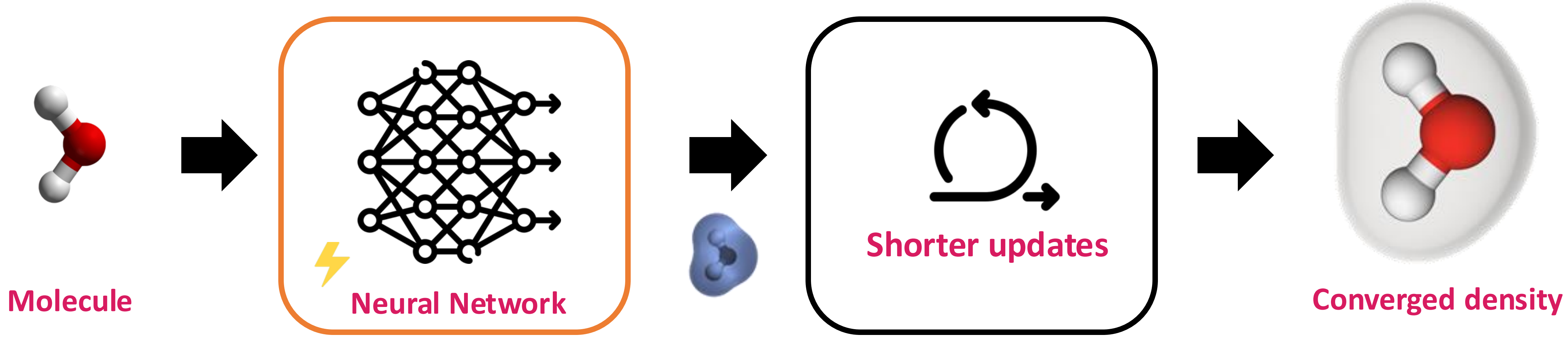
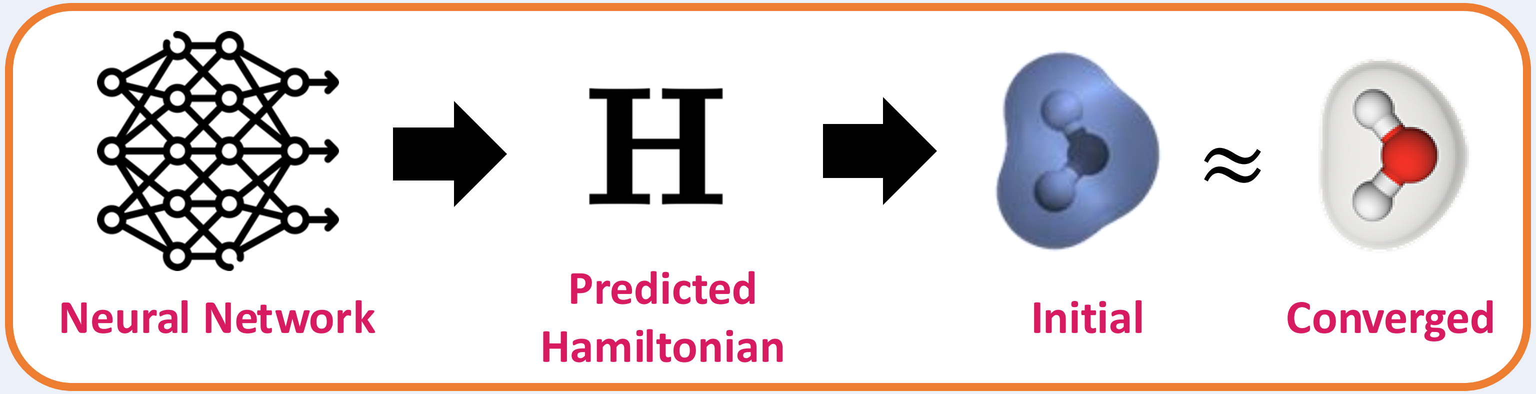




Spoiler: with ML acceleration..

Our goal: (2) DFT Acceleration





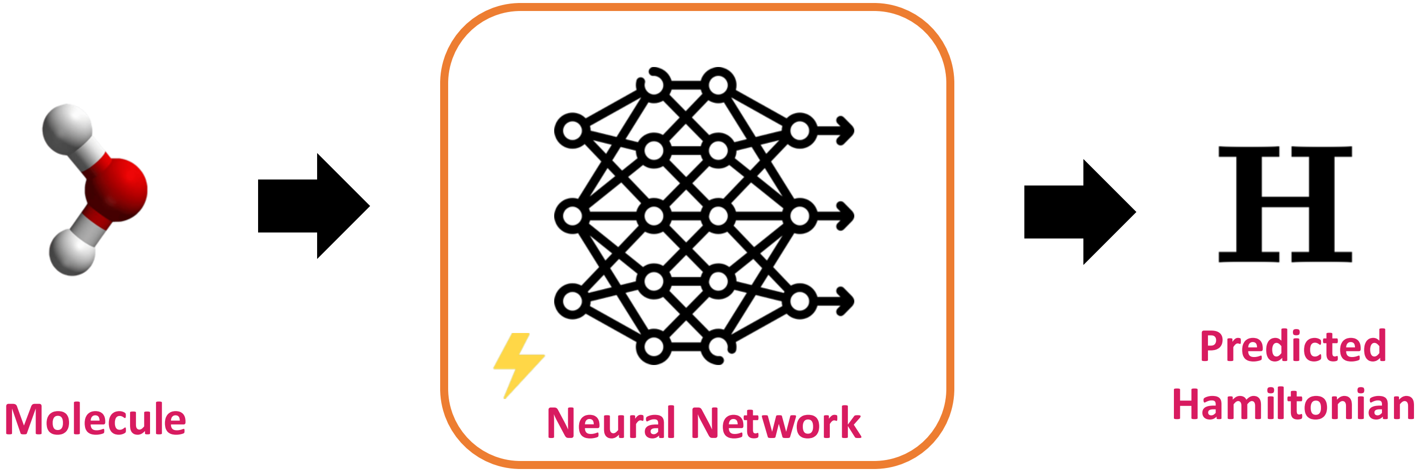
Spoiler: with ML acceleration..

-70% steps

-50% total time

(vs. conventional density initialization)

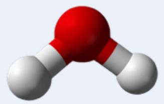
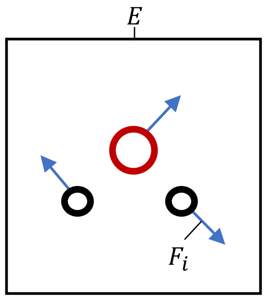
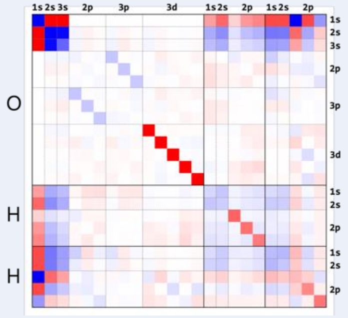
Our objective



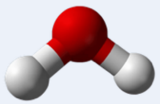
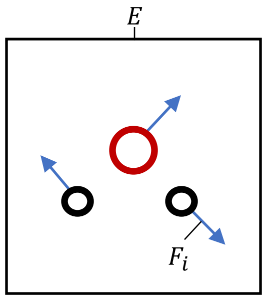
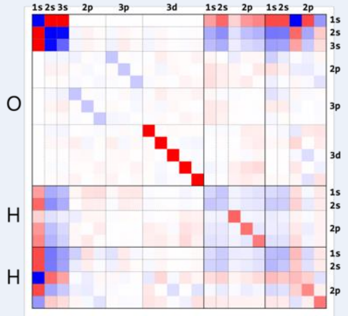
Objective (as ML task):

Predict the Hamiltonian matrix from atomic geometry without SCF iterations

ML-DFT vs. MLFF / MLIP

Input 	MLFF / MLIP *NequIP, Equiformer*	ML-DFT *QHNet, QHFlow*
Output format		
Prediction Target	*Energy / Force*	***DFT Hamiltonian matrix***
Available Properties	Energy, Force, Stress (+ Scalar properties)	**All DFT properties** Energy, Force, Stress, Electron density Wavefunction, DOS, etc.
Correctability	No	Yes
Energy Error (MD17)	1 Equiformer=1	1/50 QHFlow / Equiformer

ML-DFT vs. MLFF / MLIP

	MLFF / MLIP *NequIP, Equiformer*	ML-DFT *QHNet, QHFlow*
Input 		
Output format		
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Schrödinger Equation

The **Hamiltonian** of interest stems from the ***Schrödinger Equation***

$$\hat{H}\psi = E\psi$$

This equation is the **master equation of chemistry** (Quantum mechanics)

$\hat{H}$: ***Hamiltonian operator*** of the system

E : ***Total energy*** of the system

ψ : ***Wavefunction***

By solving the equation, we can get all information about the material!

However, ***directly solving it is extremely hard*** - $O(N!)$ (Full Configuration Interaction)

Griffiths, David J., and Darrell F. Schroeter. Introduction to quantum mechanics. Cambridge university press, 2018.

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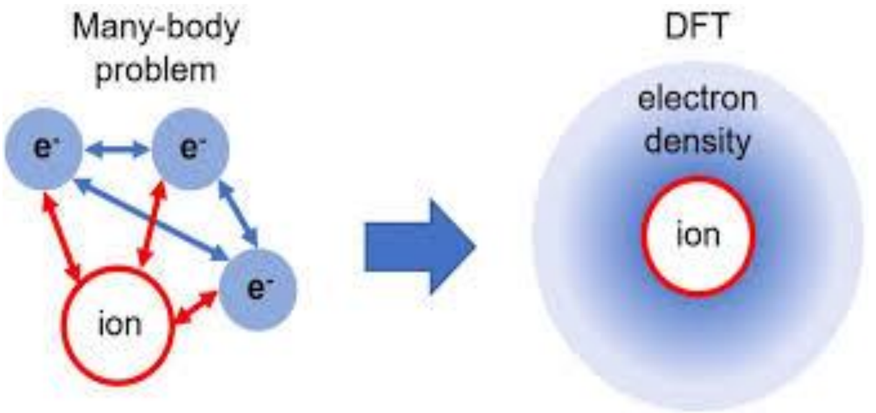
Kohn-Sham (KS) Density Functional Theory

(Kohn-Sham) DFT is a practical approximation of the **Schrödinger Equation**

Main idea: Reformulate ***many-body interaction*** to ***functional of the density*** ρ



Schematic of the DFT assumption

Advantage: make the complex problem into ***small independent problem***

$$\hat{H}\psi = E\psi$$

Original Schrödinger Equation

$$(\hat{H}_{\mathrm{KS}}[\rho]\phi_i)(r) = \phi_i(r), \quad \rho(r) = \sum_i |\phi_i(r)|^2$$

Kohn-Sham DFT formulation

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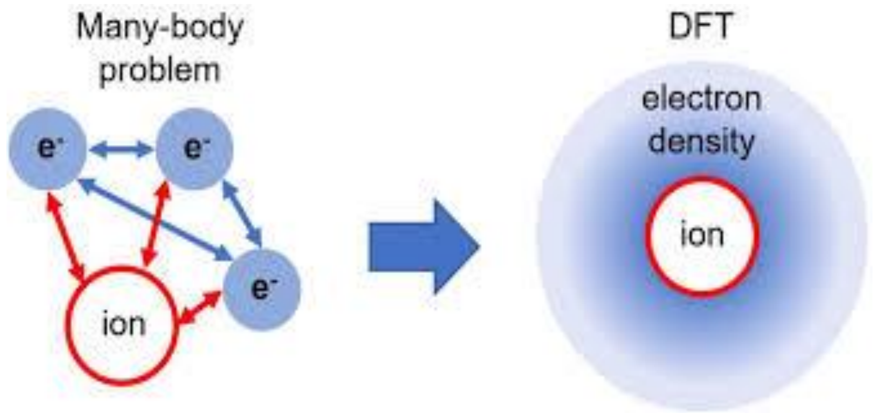

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Kohn-Sham DFT formulation

DFT in matrix formulation

KS-DFT equation can be converted into **the matrix form**

Also known as the **Roothaan-Hall DFT** (*RH-DFT*):

$$\mathbf{HC} = \mathbf{SC}\epsilon \qquad \text{RH-equation}$$

$\mathbf{H}$: ***Hamiltonian matrix*** *(or called Fock matrix* $\boldsymbol{F}$*)*

$\mathbf{C}$: *Density coefficient matrix*

$\mathbf{S}$: *Overlap matrix*

ϵ :*Diagonal orbital energy matrix*

With RH-DFT, we can handle the **density function** ρ as the coefficient matrix $\mathbf{C}$

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DFT in matrix formation

$$\mathbf{HC} = \mathbf{SC}\epsilon$$

$\mathbf{S}$ is fixed when the system is given, easy to calculate (it depends on orbital basis set)

$\mathbf{C}$, $\boldsymbol{\epsilon}$ can be obtained when $\mathbf{H}$, $\mathbf{S}$ are known

If we know the $\mathbf{H}$, then we can get electron density from obtained $\boldsymbol{C}$

(Note) $\boldsymbol{C}$ is not uniquely determined due to gauge freedom, so not a good target for supervised learning

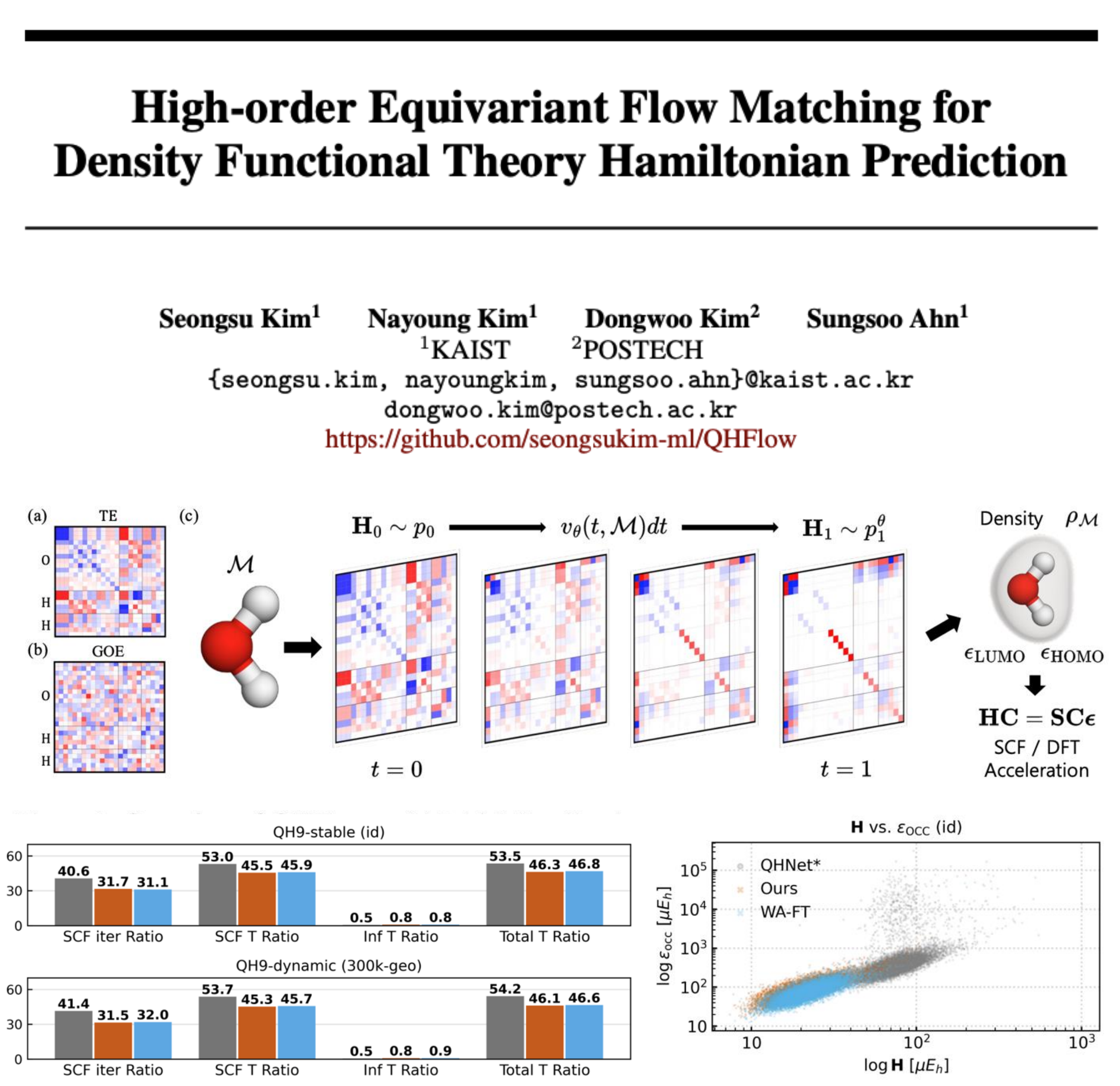
From $\mathbf{H}$, $\mathbf{C}$, and $\boldsymbol{\epsilon}$, we can calculate the *HOMO/LUMO*, *Energy*, *Force*, etc..

We introduce **QHFlow**,

a **Hamiltonian prediction** framework

high-order **equivariant flow matching** with

invariant tensor-expansion priors



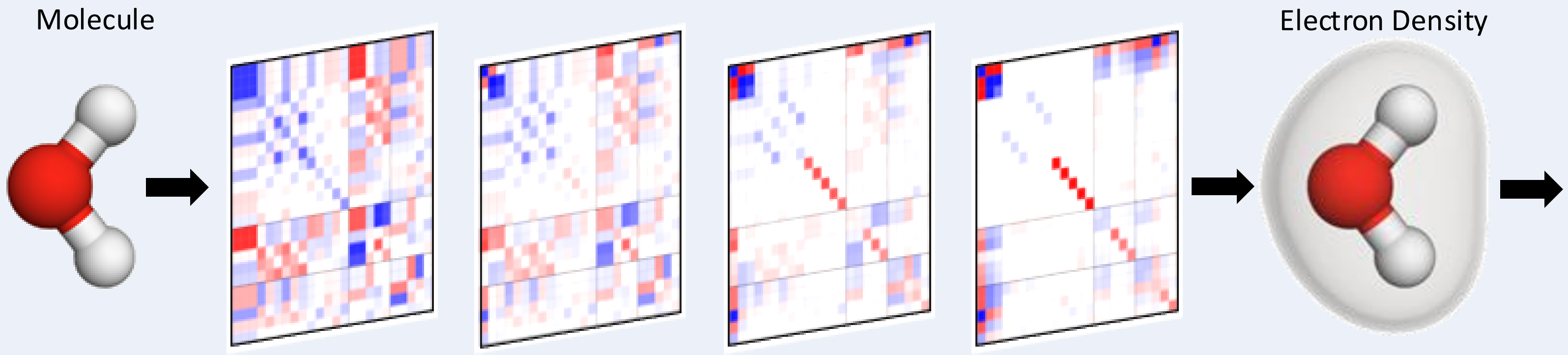
QHFlow significantly improves DFT (SCF) performance

- Reduces the **Hamiltonian error UP TO 73%**
- Reduces the **SCF iteration steps UP TO 68%**
- Reduces the **total DFT (SCF) time UP TO 54%**

https://arxiv.org/pdf/2505.18817
https://github.com/seongsukim-ml/QHFlow

Overview of QHFlow

Symmetry-Preserving Flow Matching Framework



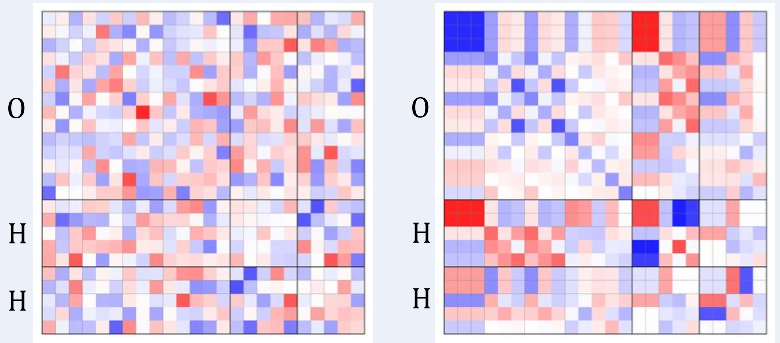
$$\mathbf{HC} = \mathbf{SC}\epsilon$$

SCF / DFT Acceleration

ϵ_{LUMO} ϵ_{HOMO}

Quantum Properties

High-order equivariant Prior



Gaussian noise based

Equivariant operated based

Physics Informed Finetuning

$$Loss_{\mathrm{FT}} = ||\tilde{\epsilon}_\theta - \epsilon||$$

DFT identity $\epsilon = \mathbf{C}^\top \mathbf{H}\mathbf{C}$

Approximated Energy $\tilde{\epsilon}_\theta = \mathbf{C}^\top \mathbf{H}_\theta \mathbf{C}$

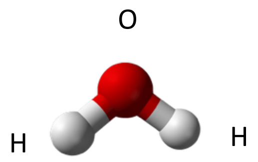
Problem setting

Objective: predict the Hamiltonian matrix $\mathbf{H}$

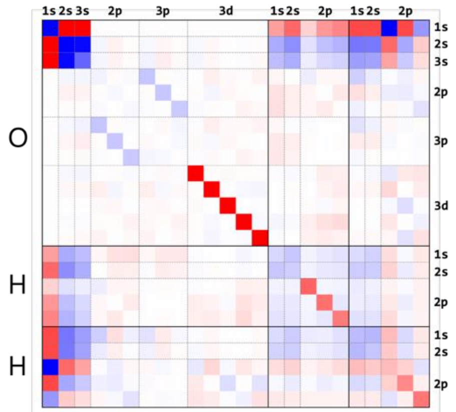
Input: (1) Molecular geometry $\mathcal{M}$ (atomic numbers Z, atomic positions X)

(2) Conventional Hamiltonian initial guess matrix $\mathbf{H}_{\mathrm{init}}$

$$\mathbf{H}_{\mathrm{pred}} = f_\theta(\mathcal{M}, \mathbf{H}_{\mathrm{init}}) + \mathbf{H}_{\mathrm{init}}$$

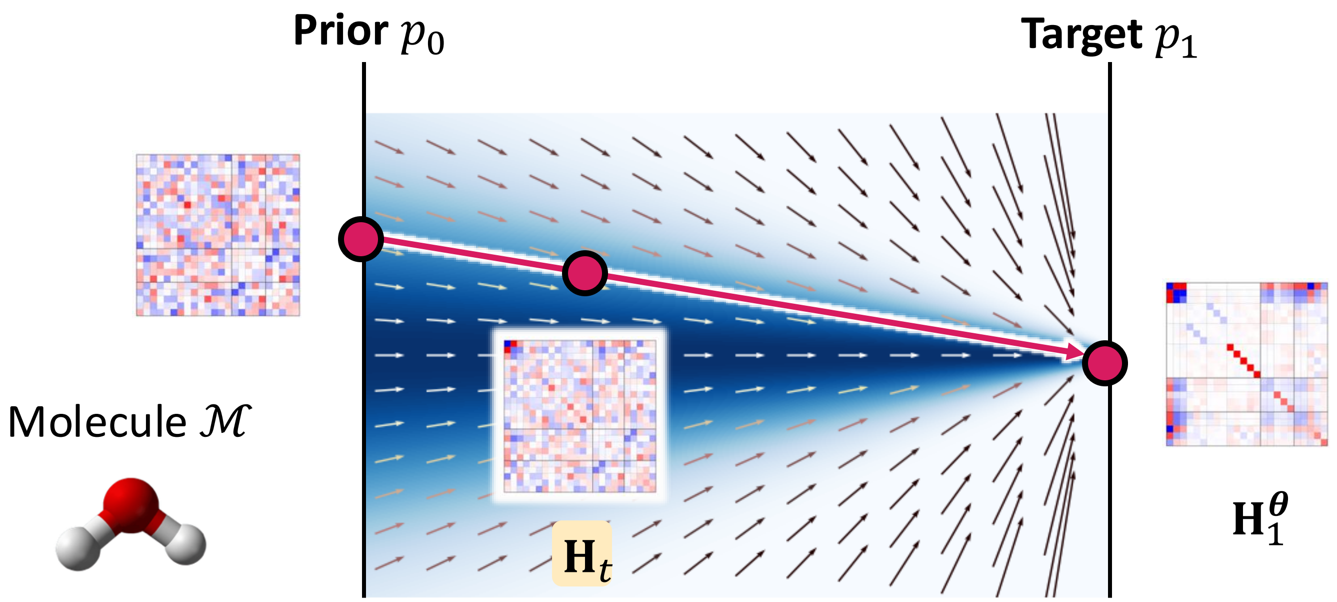


Example of $\mathcal{M}$ (H_2O)



Example of Hamiltonian matrix $\mathbf{H}$ (H_2O)

Our method: Molecule conditioned flow matching



Insight: Learning the end point prediction $\mathbf{H}_1^{\boldsymbol{\theta}}$ from middle point $\mathbf{H}_t$

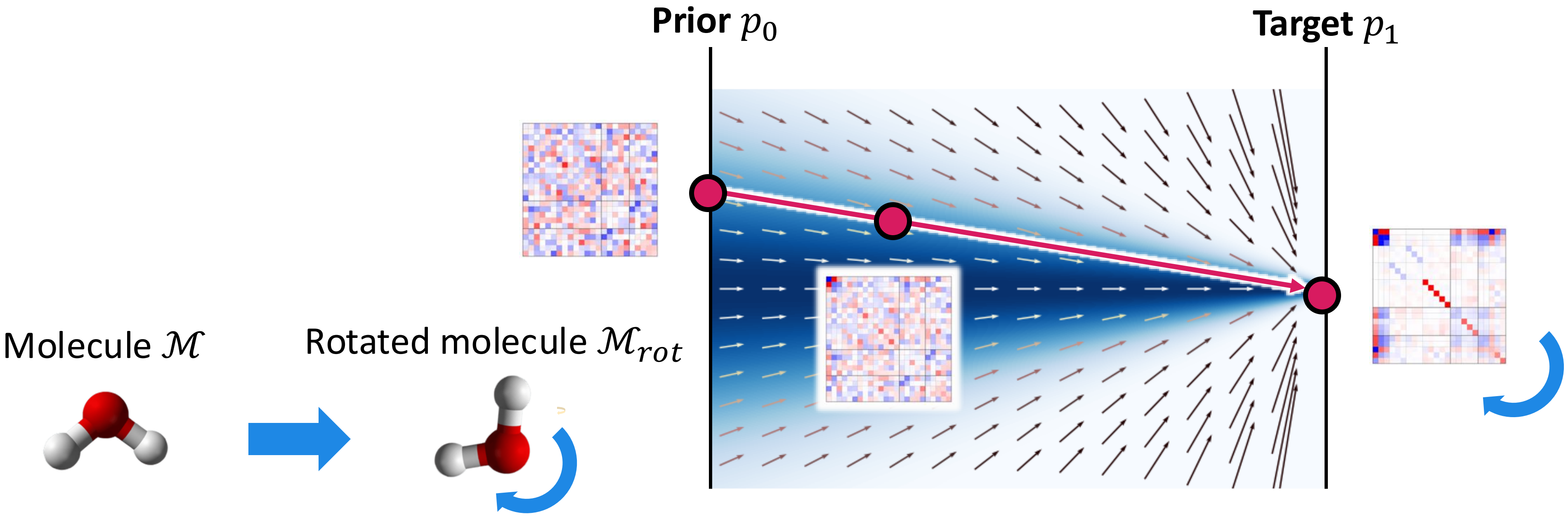
Vector field:

$$v_t^{\theta} = \frac{\mathbf{H}_1^{\boldsymbol{\theta}} - \mathbf{H}_t}{1-t}$$

Objective function:

$$\mathcal{L}_{\mathrm{CFM}} = \mathbb{E}_{(\mathbf{H},\mathcal{M})\sim\mathcal{A},t\sim\mathcal{U}(0,1),\mathbf{H}_t\sim p_t(\cdot|\mathbf{H})}\left[\frac{1}{(1-t)^2}\left\|\mathbf{H}_1^{\theta}(\mathbf{H}_t,\mathcal{M}) - \mathbf{H}_{1,\mathcal{M}}\right\|_2^2\right]$$

Our method: Equivariant flow matching

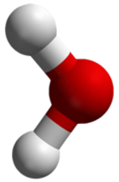


Preserving ***symmetry*** with flow matching ➔ Equivariant flow matching

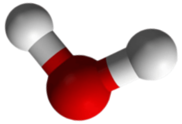
Equivariant property of Hamiltonian (Symmetry)

Just like **forces, Hamiltonian matrix** rotates along with the system

Position P

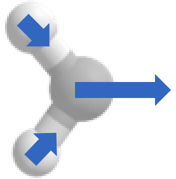


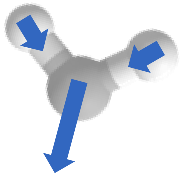
Rotation



$$\mathrm{P} \xrightarrow{R} \mathbf{R}\mathrm{P}$$

Force F





$$F \xrightarrow{R} \mathbf{R}\mathrm{F}$$

Hamiltonian H

?

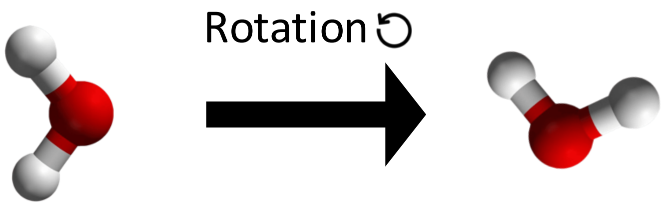
$$H \xrightarrow{R} \mathbf{D}(\mathbf{R})^{\mathrm{T}} H \mathbf{D}(\mathbf{R})$$

$\mathbf{D}(\mathbf{R})$ plays a role of high-order rotation

Equivariant property of Hamiltonian (Symmetry)

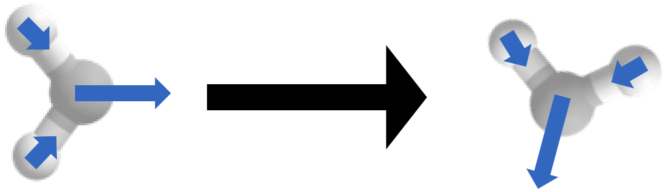
Just like **forces, Hamiltonian matrix** rotates along with the system

Position P



$$\mathrm{P} \xrightarrow{R} \mathbf{R}\mathrm{P}$$

Force F



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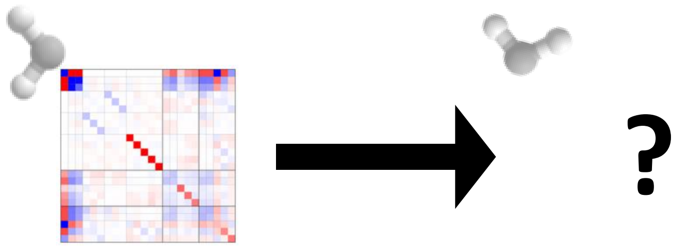
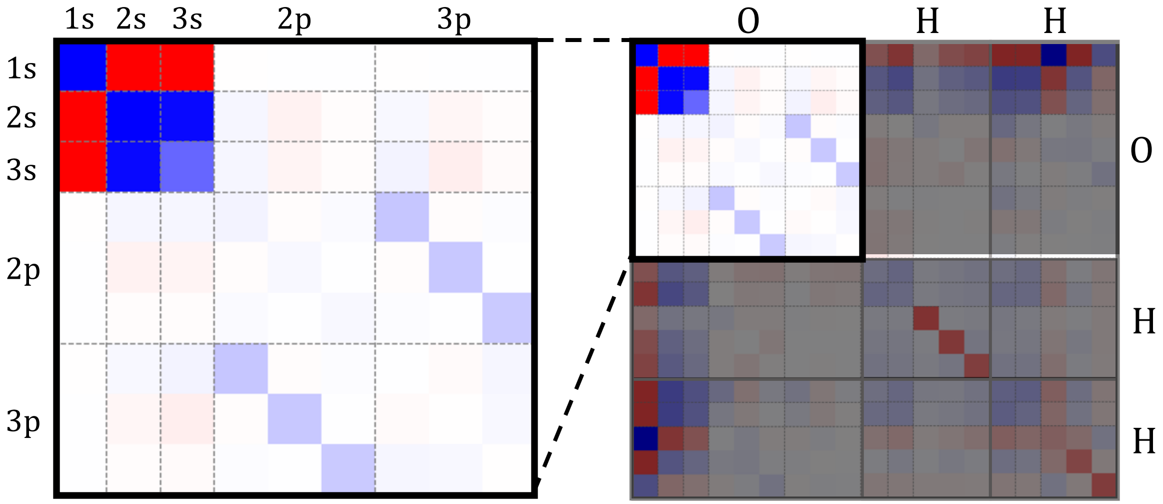
Hamiltonian H



$$H \xrightarrow{R} \boldsymbol{D}^{\top} H \boldsymbol{D}$$

$\boldsymbol{D} \coloneqq \boldsymbol{D}(\mathbf{R})$ plays a role of high-order rotation

Equivariance of Hamiltonian

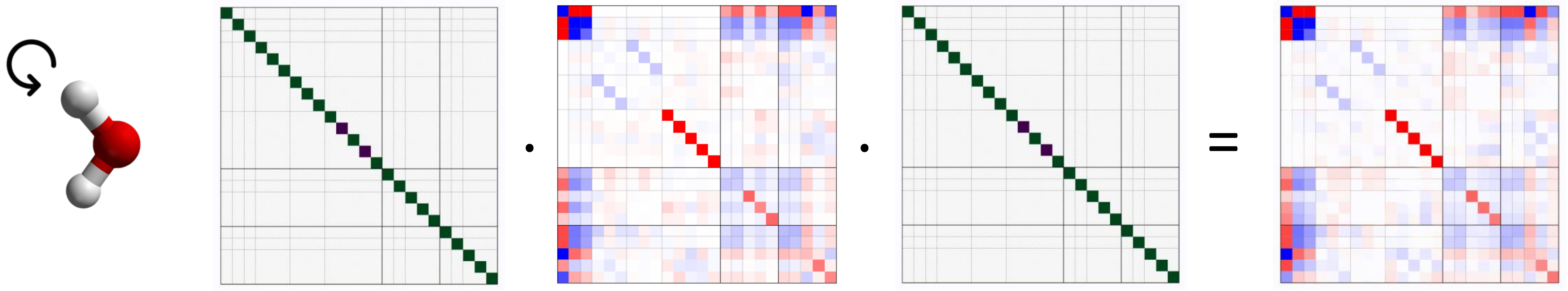


Atomic block matrix *Full Hamiltonian matrix*

Hamiltonian matrix has **high-order equivariant structure**

Each block matrix needs a special type of rotation matrix!
Wigner D-matrix

Equivariance of Hamiltonian



Wigner D-matrix Wigner D-matrix

$$\mathbf{D}^T H\mathbf{D} = \mathbf{H}_{\mathrm{rot}}$$

Applying **a special rotation matrix** for rotation of the Hamiltonian matrix
(Wigner D-matrix)

Equivariant flow matching for Hamiltonian

Rotated Hamiltonian has the same probability for any Hamiltonian, that is

$$p_t(\boldsymbol{R} \cdot \mathbf{H}) = p_t(\mathbf{H})$$

Following *Song et al*, this property can be satisfied by

(1) Rotation invariant prior distribution $(t = 0)$

$$p_0(\boldsymbol{R} \cdot \mathbf{H}) = p_0(\mathbf{H})$$

(2) Rotation equivariant vector field

$$v_t(\boldsymbol{R} \cdot \mathbf{H} | \boldsymbol{R}\mathcal{M}) = \boldsymbol{R} \cdot v_t(\mathbf{H} | \mathcal{M})$$

Yuxuan Song, Jingjing Gong, Minkai Xu, Ziyao Cao, Yanyan Lan, Stefano Ermon, Hao Zhou, and Wei-Ying Ma. Equivariant flow matching with hybrid probability transport for 3d molecule generation. Advances in Neural Information Processing Systems, 2023

Our method: Invariant prior design

Two types of prior satisfying the invariance:

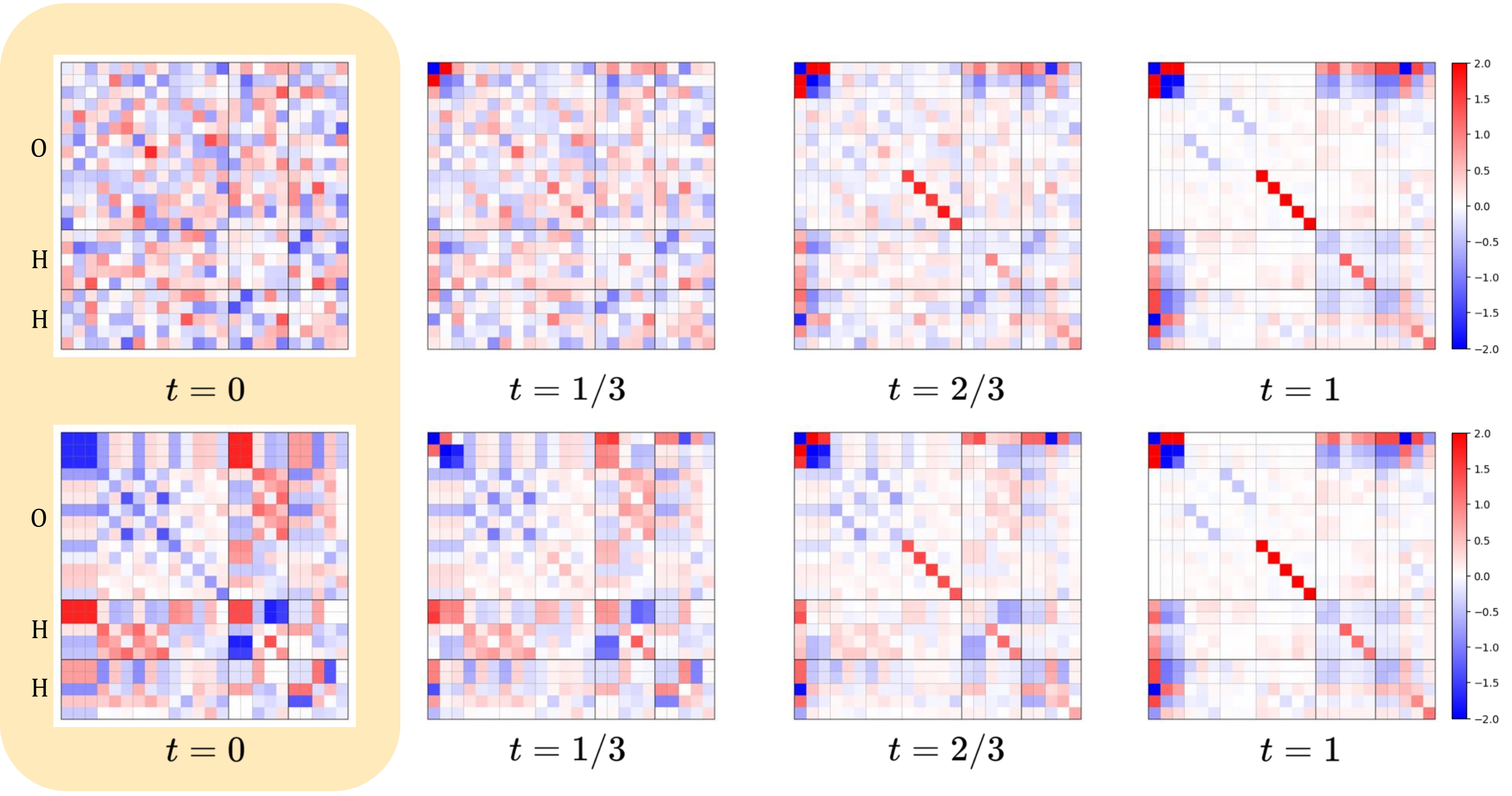
$$p_0(\boldsymbol{R} \cdot \mathbf{H} | \boldsymbol{R}\mathcal{M}) = p_0(\mathbf{H} | \mathcal{M})$$

GOE

Gaussian Orthogonal Ensemble

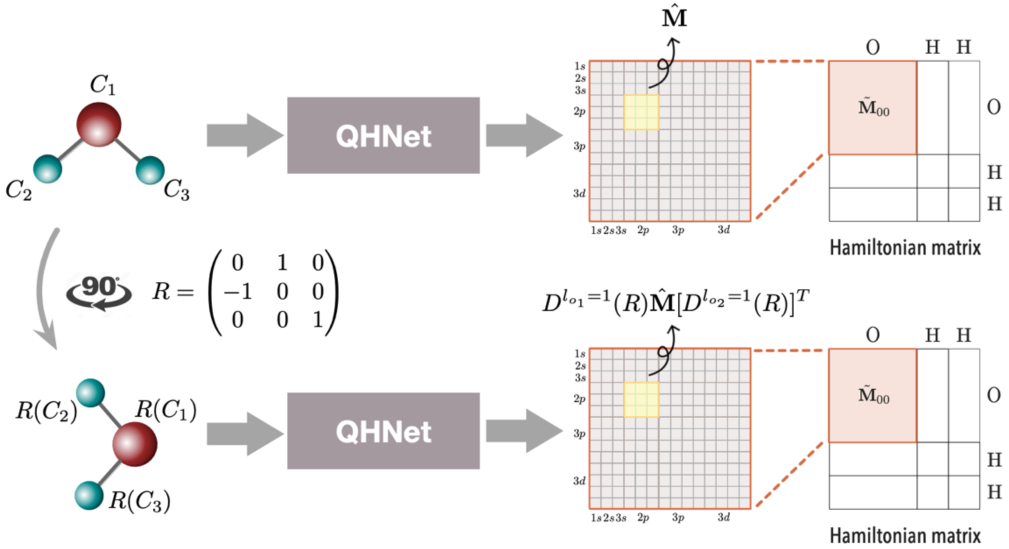
TE

Tensor Expansion

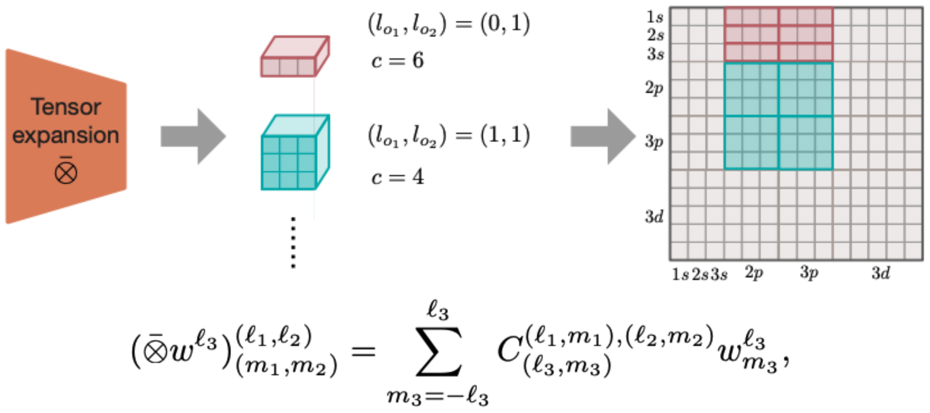


Equivariant vector field

Using rotation equivariant Hamiltonian prediction architecture (QHNet ,*Yu et al, 2023*)



QHNet



Tensor Expansion

Modified the architecture to introduce two additional inputs:

- t: **Time conditioning** for flow matching
- $\mathbf{H}_t$: the **current Hamiltonian** matrix

Haiyang Yu, Zhao Xu, Xiaofeng Qian, Xiaoning Qian, and Shuiwang Ji. Efficient and equivariant graph networks for predicting quantum hamiltonian. In International Conference on Machine Learning, 2023

Our method: Physics-informed finetuning

- **Approximated orbital energies $\tilde{\boldsymbol{\epsilon}}$** (from *Li et al*)

$$\tilde{\boldsymbol{\epsilon}}_\theta = \mathbf{C}^\top \mathbf{H}_\theta \mathbf{C}$$

- **Ground-truth orbital energies $\boldsymbol{\epsilon}$**

$$\boldsymbol{\epsilon} = \mathbf{C}^\top \mathbf{H} \mathbf{C}$$

- Our finetuning aligns these two values

$$Loss_{\mathrm{FT}} = ||\tilde{\boldsymbol{\epsilon}}_\theta - \boldsymbol{\epsilon}||$$

$$Total\ Loss = Loss_{flow} + Loss_{FT}$$

$$\mathbf{HC} = \mathbf{SC}\boldsymbol{\epsilon}$$

RH-DFT equation

$$\mathbf{C}^\top \mathbf{SC} = \mathbf{I}$$

Identity property

$$\mathbf{C}^\top \mathbf{HC} = \boldsymbol{\epsilon}$$

Orbital energy

Li, Yunyang, et al. "Enhancing the Scalability and Applicability of Kohn-Sham Hamiltonians for Molecular Systems." *The Thirteenth International Conference on Learning Representations*.

Experiment

DFT Approximation – MD17

- Molecular dynamics trajectory for four small molecules
  - **Same chemical formula** Z with ***different atomic positions*** X

$$\mathbf{HC} = \mathbf{SC}\boldsymbol{\epsilon}$$

H: Hamiltonian MAE
ϵ_{occ}: occupied energy MAE
$\mathcal{S}_c$: Similarity score of the coefficients

	Model	Water (3 atoms)			Ethanol (9 atoms)			Malonaldehyde (9 atoms)			Uracil (12 atoms)		
		$H\downarrow$ $[\mu E_h]$	$\epsilon_{\mathrm{occ}}\downarrow$ $[\mu E_h]$	$\mathcal{S}_c\uparrow$ [%]	$H\downarrow$ $[\mu E_h]$	$\epsilon_{\mathrm{occ}}\downarrow$ $[\mu E_h]$	$\mathcal{S}_c\uparrow$ [%]	$H\downarrow$ $[\mu E_h]$	$\epsilon_{\mathrm{occ}}\downarrow$ $[\mu E_h]$	$\mathcal{S}_c\uparrow$ [%]	$H\downarrow$ $[\mu E_h]$	$\epsilon_{\mathrm{occ}}\downarrow$ $[\mu E_h]$	$\mathcal{S}_c\uparrow$ [%]
(2019)	SchNOrb	165.4	279.3	**100.00**	187.4	334.4	**100.00**	191.1	400.6	99.00	227.8	1760.	90.00
(NIPS'21)	PhiSNet	15.67	85.53	**100.00**	20.09	102.04	99.81	21.31	100.6	99.89	18.65	143.36	99.86
(ICML'23)	QHNet*	11.70	26.06	**100.00**	27.99	99.33	99.99	29.60	100.16	99.92	26.80	127.93	99.87
(ICML'25)	SPHNet	23.18	182.29	**100.00**	21.02	82.30	**100.00**	20.67	95.77	**99.99**	19.36	118.21	**99.99**
	Ours	**4.93**	**19.29**	**100.00**	**5.33**	**29.03**	**100.00**	**3.80**	**22.68**	**99.99**	**3.68**	**30.54**	**99.99**

- Our model shows **71% error reduction** on Hamiltonian
- Our model shows lower error on **occupied energy** ϵ_{occ} and higher **coefficient similarity score** $\mathcal{S}_c$
  - Higher physical fidelity

DFT Approximation – QH9

- The **general molecule dataset**, which consists of various chemical formulas

(ICML'23) QHNet
(ICLR'25) WANet
(ICML'25) SPHNet

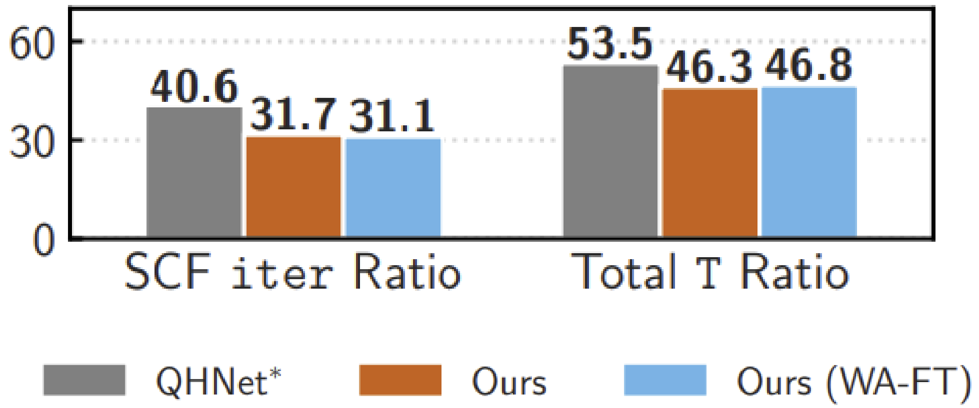
		H Error	*Energy related error*				
Dataset	**Model**	$H \downarrow [\mu E_h]$	$\epsilon_{occ} \downarrow [\mu E_h]$	$\mathcal{S}_c \uparrow [\%]$	$\epsilon_{LUMO} \downarrow [\mu E_h]$	$\epsilon_{HOMO} \downarrow [\mu E_h]$	$\epsilon_{\Delta} \downarrow [\mu E_h]$
QH9-stable (id)	QHNet*	77.72	963.45	94.80	18257.34	1546.27	17822.62
	WANet	80.00	833.62	96.86	-	-	-
	SPHNet	45.48	334.28	97.75	-	-	-
	Ours	**22.95**	119.67	99.51	437.96	179.48	553.87
w/ Finetuning	**Ours (WA-FT)**	23.85	**101.92**	**99.56**	**187.48**	**92.22**	**206.15**
QH9-stable (ood)	QHNet*	69.69	884.97	93.01	25848.83	1045.99	25370.10
	SPHNet	43.33	186.40	98.16	-	-	-
	Ours	**20.01**	84.54	99.04	321.20	130.74	395.83
	Ours (WA-FT)	20.55	**72.64**	**99.16**	**171.24**	**77.96**	**179.57**
QH9-dynamic (300k-geo)	QHNet*	88.36	1170.50	93.65	23269.41	2040.06	22407.96
	WANet	74.74	416.57	99.68	-	-	-
	SPHNet	52.18	100.88	99.12	-	-	-
	Ours	**25.94**	103.11	99.59	425.18	175.18	547.33
	Ours (WA-FT)	27.12	**89.03**	**99.65**	**136.63**	**84.17**	**154.68**
QH9-dynamic (300k-mol)	QHNet*	121.39	5554.36	86.02	53505.09	4352.76	50424.86
	SPHNet	108.19	1724.10	91.49	-	-	-
	Ours	**45.91**	442.56	98.65	1344.68	479.71	1605.03
	Ours (WA-FT)	46.60	**424.75**	**98.74**	**912.10**	**403.51**	**1047.88**

H: Hamiltonian MAE
ϵ_{occ}: occupied energy MAE
$\mathcal{S}_c$: Similarity score of the coefficients
ϵ_{LUMO}: LUMO energy MAE
ϵ_{HOMO}: HOMO energy MAE
ϵ_{Δ}: LUMO-HOMO energy diff. MAE

- Our model show a **53% error reduction** on average
- With the **finetuning (WA-FT),** additional **improvement in Energy** with a trade-off in **Hamiltonian error**

DFT Acceleration – QH9

Initialization of the SCF process



- Reduces the **SCF steps** calculations by **about 69% (= 1-0.31)**
- Reduces the **total time** of SCF convergence by **about 54% (= 1-0.46)** (Inference time included)

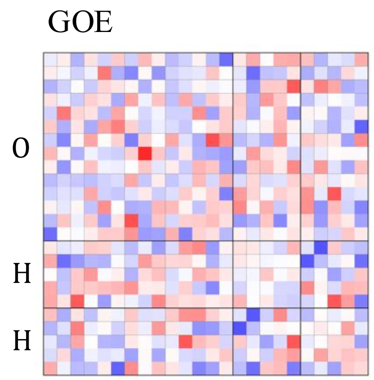
Here, 100% is the conventional initialization (*MinAO*), and a lower value implies more efficiency

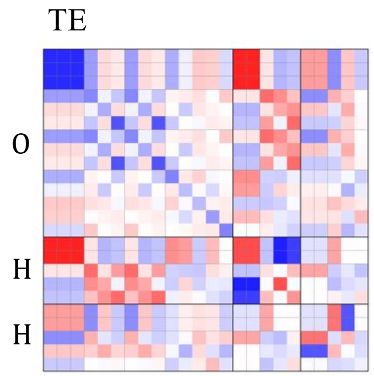
We tested on the first 300 samples from each test split

Ablation – Prior distribution

- Influence of the prior distribution on QH9

Data	Prior	$H \downarrow [\mu E_h]$	$\epsilon_{\text{occ}} \downarrow [\mu E_h]$	$\mathcal{S}_c \uparrow [\%]$
`id`	GOE	25.93	154.65	99.39
	TE	**22.95**	**119.61**	**99.51**
`ood`	GOE	20.41	87.32	98.95
	TE	**20.01**	**84.54**	**99.04**
`geo`	GOE	29.39	122.14	99.49
	TE	**25.94**	**103.11**	**99.59**
`mol`	GOE	46.78	**419.68**	98.65
	TE	**45.91**	442.56	**98.65**





- ***TE*** prior consistently yields lower errors than ***GOE***
- Highlights importance of designing appropriate priors for Hamiltonian prediction

ML-DFT vs. MLFF (not in paper)

Energy and Force evaluation / compared with MLFF

Molecule	Metric (MAE)	Hamiltonian (meV)	(Pred − Targ) Energy (meV)	E. Reduc. (%)	Force (meV/Å)	F. Reduc. (%)
Water	DFT-variance	-	0.000 08	-	0.0491	-
	UMA-omol (MLFF)	-	4326	-	362	-
	Equiformer (MLFF)	-	-	-	-	-
	QHNet (DFT)	0.323	0.048	-	0.803	-
	QHFlow (DFT)	**0.105**	**0.015**	-	**0.270**	-
Ethanol	DFT-variance	-	0.0002	-	0.088	-
	UMA-omol (MLFF)	-	8194	-	334	-
	Equiformer (MLFF)	-	2.2	0.0	2.9	0.0
	QHNet (DFT)	0.633	0.323	−85.3	2.513	−13.3
	QHFlow (DFT)	**0.152**	**0.019**	**−99.1**	**0.775**	**−73.3**
Malondialdehyde	DFT-variance	-	0.0004	-	0.1469	-
	UMA-omol (MLFF)	-	13 166	-	487	-
	Equiformer (MLFF)	-	3.2	0.0	5.4	0.0
	QHNet (DFT)	0.653	0.916	−71.4	4.949	−8.4
	QHFlow (DFT)	**0.116**	**0.035**	**−98.9**	**1.187**	**−78.0**
Uracil	DFT-variance	-	0.0004	-	0.2955	-
	UMA-omol (MLFF)	-	21 212	-	367	-
	Equiformer (MLFF)	-	4.3	0.0	3.3	0.0
	QHNet (DFT)	0.546	2.351	−45.3	6.798	106.0
	QHFlow (DFT)	**0.109**	**0.106**	**−97.5**	**1.869**	**−43.4**

- Vs. Equiformer on MD17
  - -98.5% error reduction on Energy
  - -64.9% error reduction on Forces

ML-DFT vs. MLFF (not in paper)

Energy and Force evaluation / compared with MLFF

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- Vs. Equiformer on MD17
  - -98.5% error reduction on Energy
  - -64.9% error reduction on Forces

Question & Answer

Thank you!

Open to talk!

Interested in *AI for science, computational biology, and material design!*

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