SchNet - A deep learning architecture for molecules and materials:

The reach of the model

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Frontiers of Science Award

https://www.google.com/url?sa=i&url=https%3A%2F%2Fgeology.com%2Fworld%2Fmexico-satellite-image.shtml&psig=AOvVaw1TcCtd2UARtlKTt1tfzaS1&ust=1704791911199000&source=images&cd=vfe&ved=0CBEQjRxqFwoTCODToo-8zYMDFQAAAAAdAAAAABAE

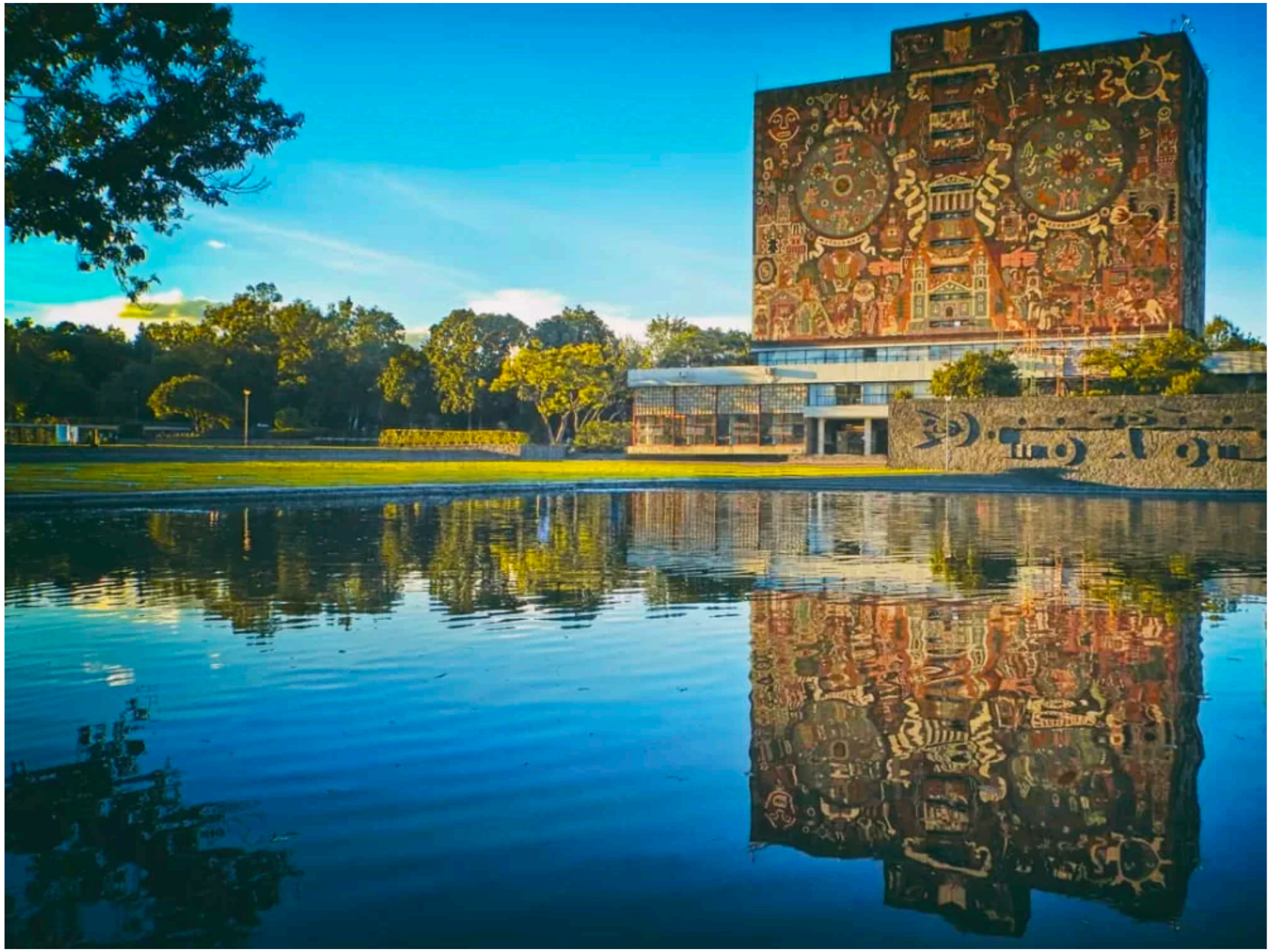
UNIVERSIDAD NACIONAL AUTONOMA DE MEXICO

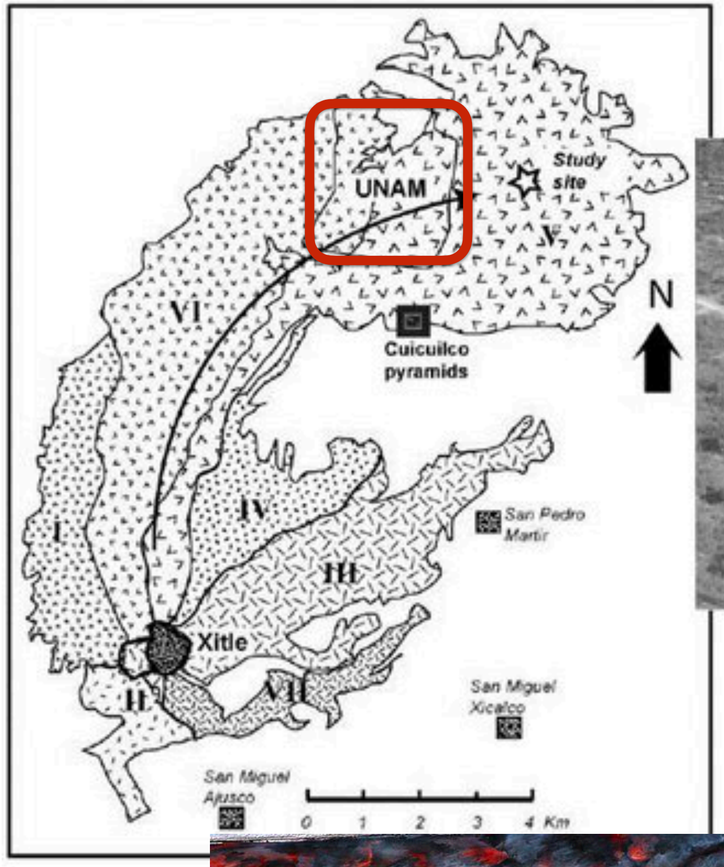
POR MI RAZA HABLARA EL ESPIRITU

VNIVERSIDAD NACIONAL AVTNOMA DE MEXICO

(founding goes back to 1551)

UNESCO World Heritage



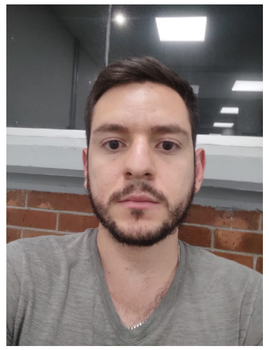

UNAM
Study site
N
VI
Cuicuilco pyramids
I
IV
San Pedro Martir
III
Xitle
II
VII
San Miguel Xicalco
San Miguel Ajusco
0 1 2 3 4 Km

~ 140 Researchers

The Team

Machine Learning for Simulations @ iF

Jessica Martínez-Marcelo (B)



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Roman Armenta (PhD)

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Carlos Cureño-Ayluardo (B)

Carlos Vital-José (PhD)

Diana-Sanchez-Barrios (M)

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Diego Peña-Angeles (M)

Research

Machine Learning for Simulations @

Atomistic simulations

Nuclear quantum effects

Force fields learning
(Development)

Metal clusters'
Physics

Battery physics

Propagator learning

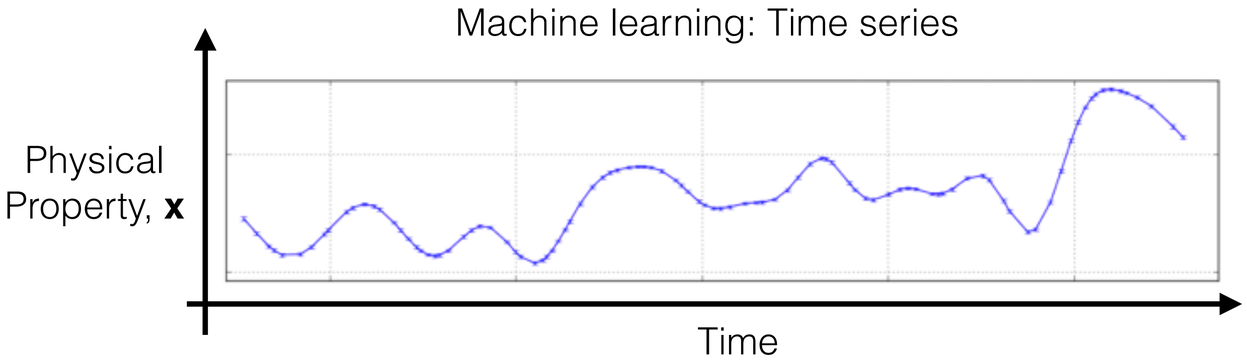
Dynamical processes
(Nuclear and electronic)

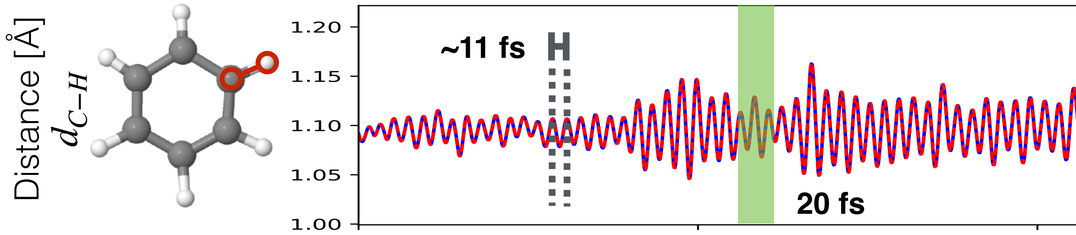
Electronic structure

ML and Quantum Monte Carlo
(First and second quantization)

Research

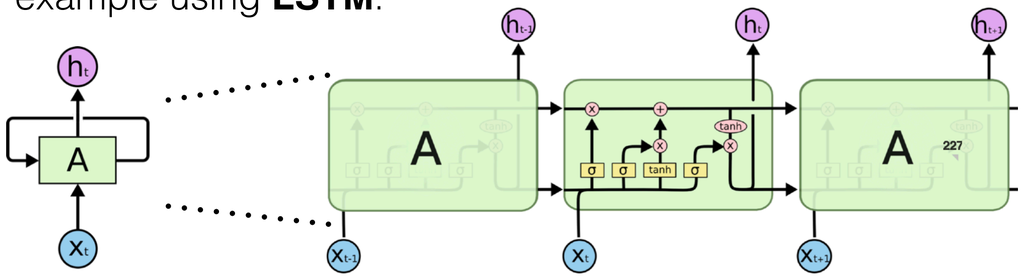
Machine Learning for Simulations @





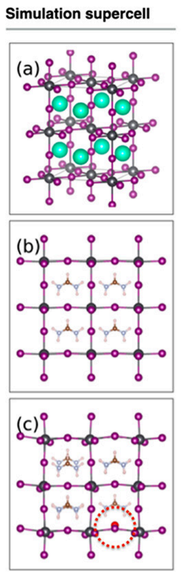
Mach. Learn.: Sci. Technol. 3, 025011 (**2022**)

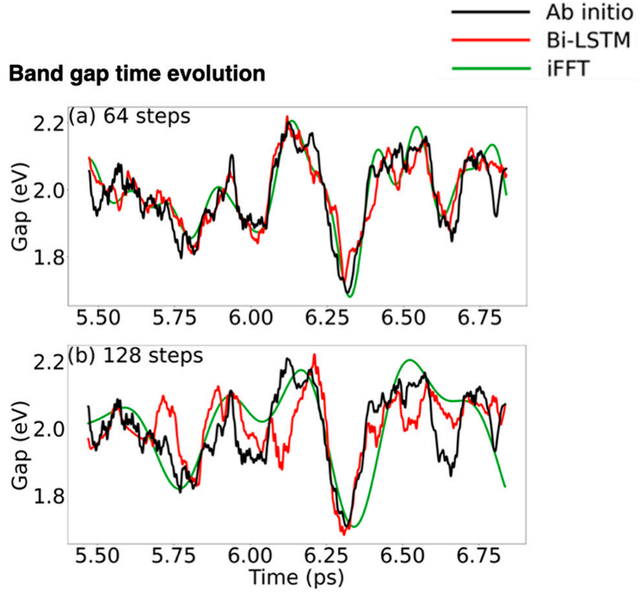
For example using **LSTM**:



Propagator learning

Dynamical processes (Nuclear and electronic)



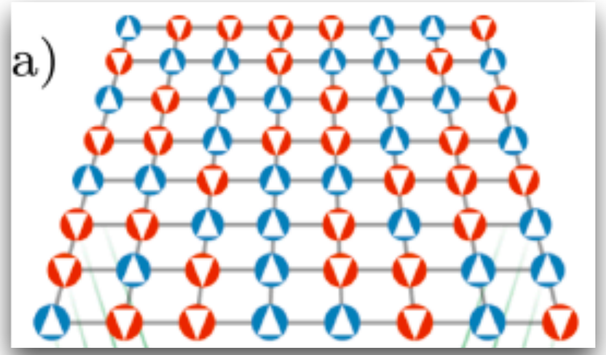


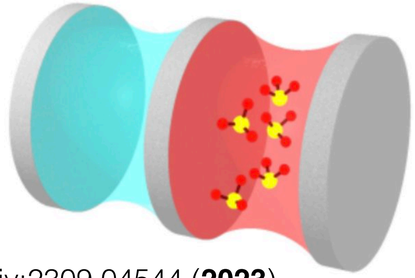
J. Phys. Chem. Lett. 14, 7092 (**2023**)

Research

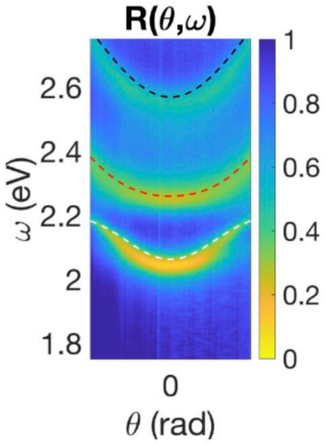
Machine Learning for Simulations @

Carlos
Cureño-Ayluardo



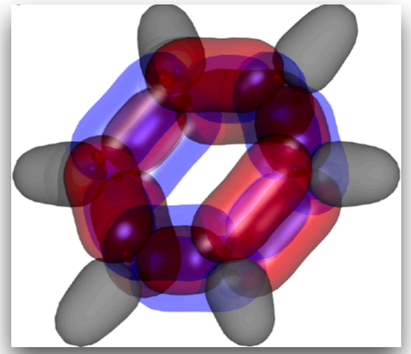


arXiv:2309.04544 (**2023**)
Under review



Roman Armenta

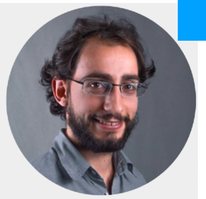
Diego
Gonzalez-Baños



PIIF2023

Dr Arturo Camacho Guardian

Dr Hugo Alberto Lara García



Dr Giuseppe Pirruccio

Electronic structure

ML and Quantum Monte Carlo
(First and second quantization)

THE JOURNAL OF CHEMICAL PHYSICS **148**, 241722 (2018)

SchNet – A deep learning architecture for molecules and materials

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Frontiers of Science Award
AI for Physical Sciences (Material, Physics and Chemistry)

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2018

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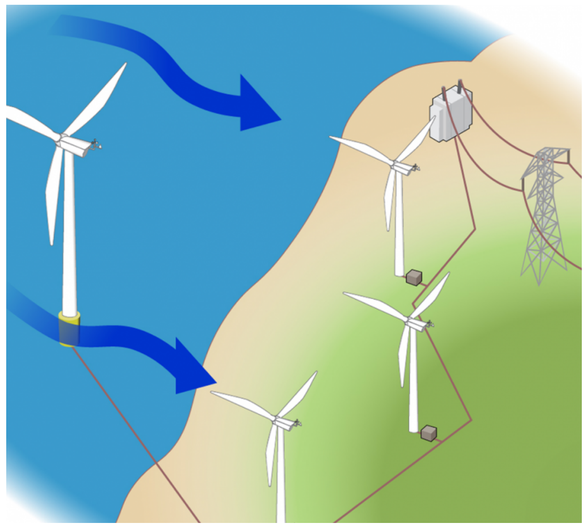
Google DeepMind

BIFOLD

Outline

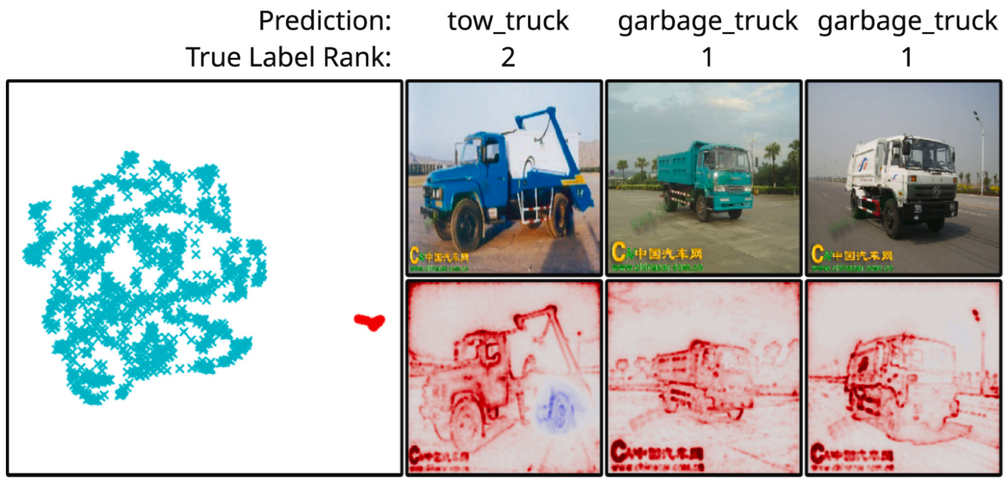
- SchNet
  - Evolution
  - Applications
- Kernel Methods
- Simulations

- Some uses of ML

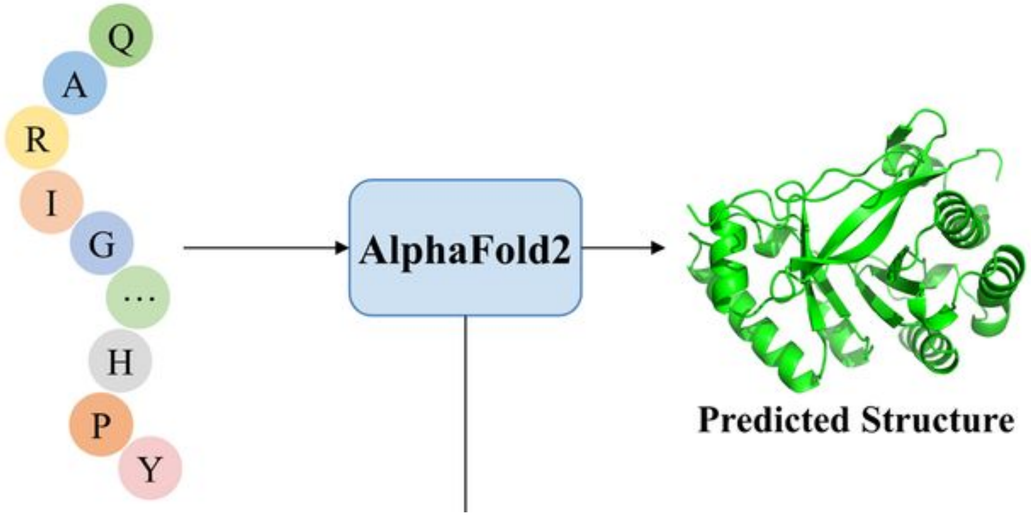


Resources management

Computation efficiency



Explainable AI



Machine Learning

Learning force fields

$$\mathcal{H}\Psi = V_{BO}\Psi$$

$$-\mathbf{F} = \langle \Psi^* | \partial\mathcal{H}/\partial\mathbf{x} | \Psi \rangle$$

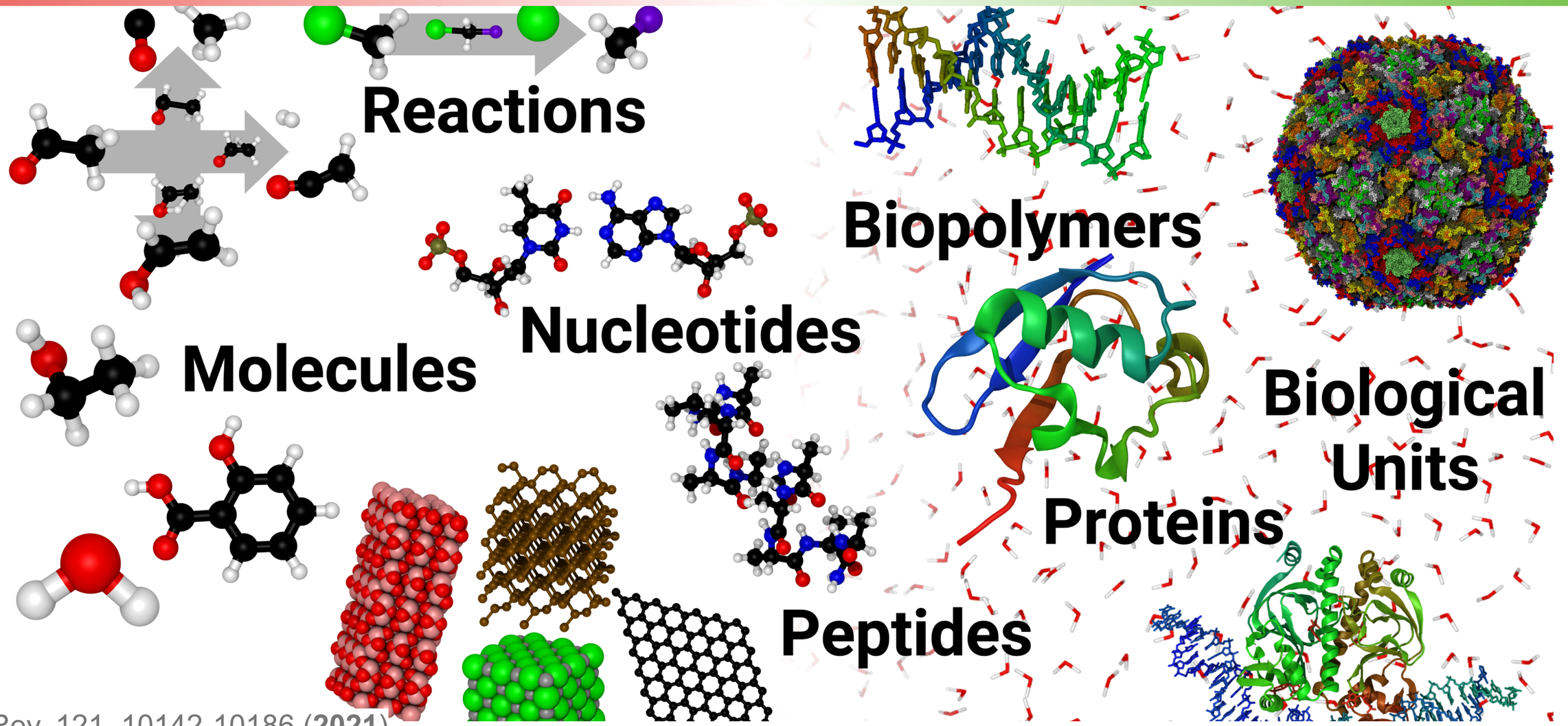
The problem…

Limitations of ab initio molecular dynamics

Predictive simulations: Energies and forces

Ab initio

Force Fields

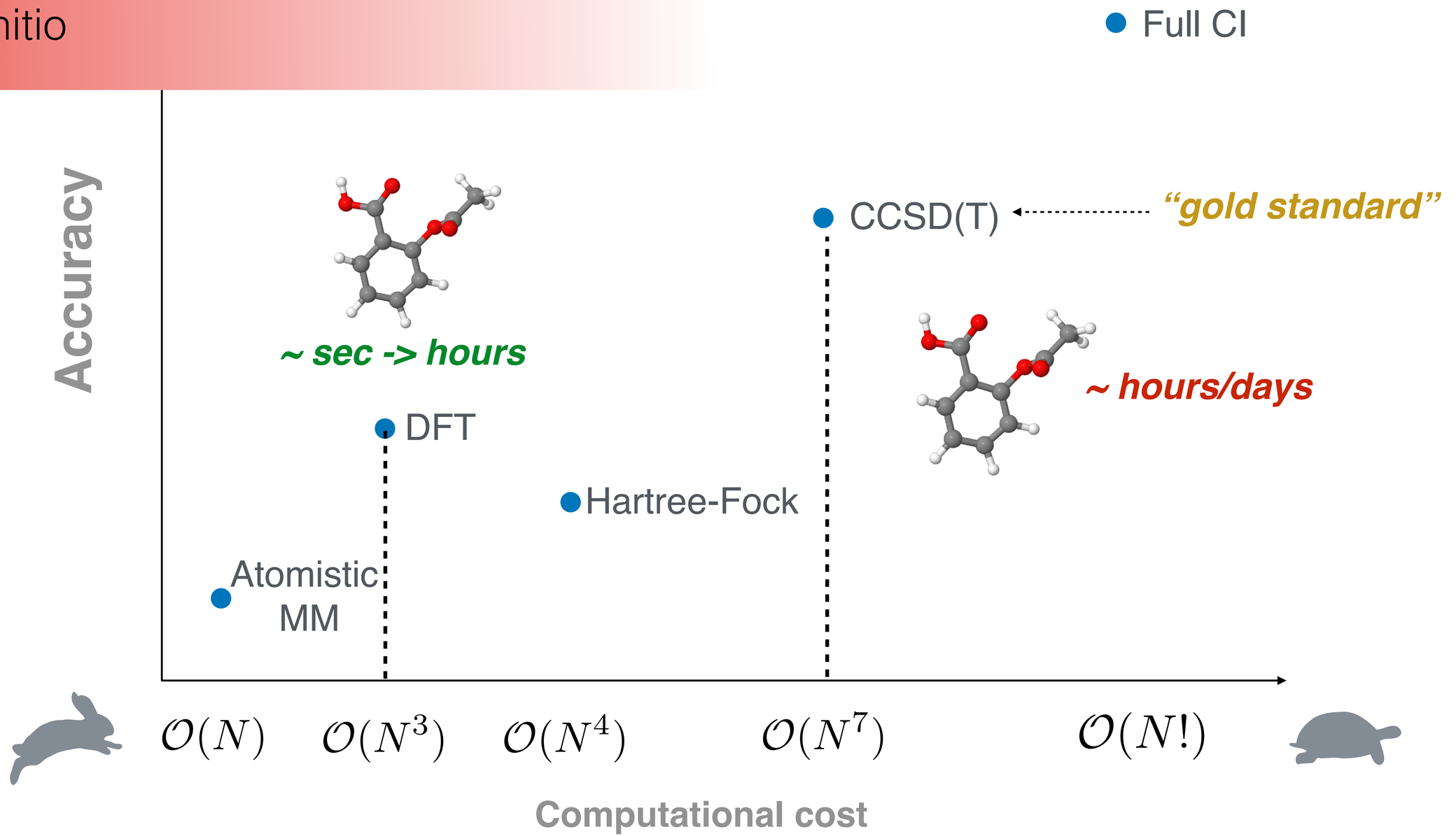


Chem. Rev. 121, 10142-10186 (**2021**)

Predictive simulations: Energies and forces

$$\mathcal{H}\Psi = E\Psi$$

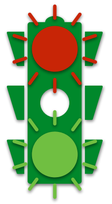
Ab initio



Predictive simulations:

$$\mathcal{H}\Psi = E\Psi$$

Ab initio + Molecular dynamics

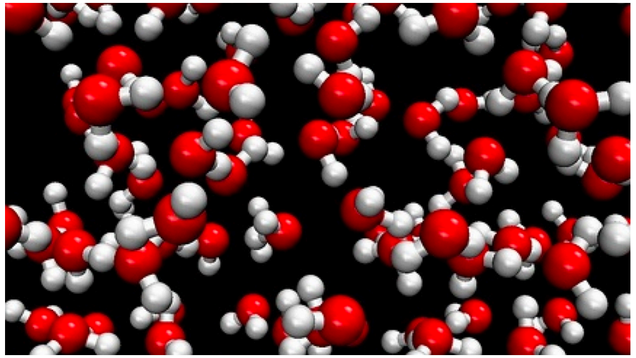


ML

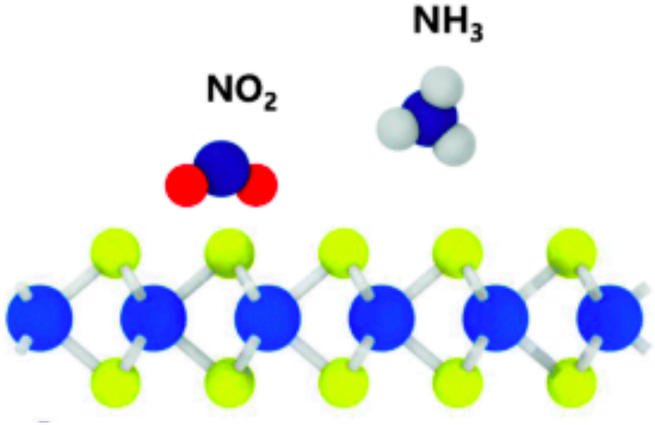
Converged thermodynamics: $\sim 10^6 * \mathcal{O}(N^3)$

?

~10 s/s.p.c. ▶ ~100 days



Water



Molecule + 2D material

ML in physics and chemistry…

CHEMICAL REVIEWS

Machine Learning Force Fields

Oliver T. Unke, Stefan Chmiela, Huziel E. Sauceda, Michael Gastegger, Igor Poltavsky, Kristof T. Schütt, Alexandre Tkatchenko*, and Klaus-Robert Müller*

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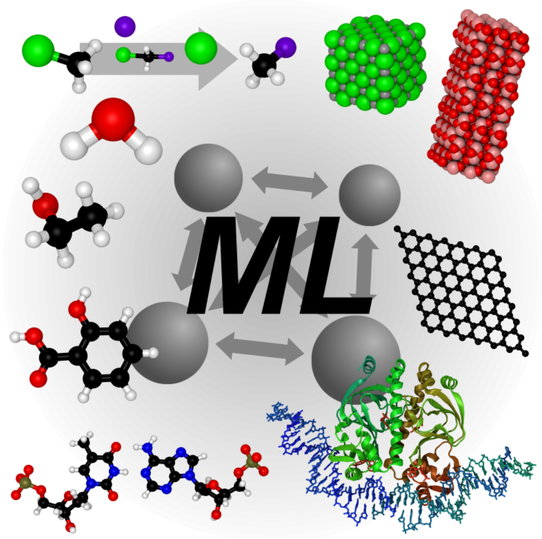
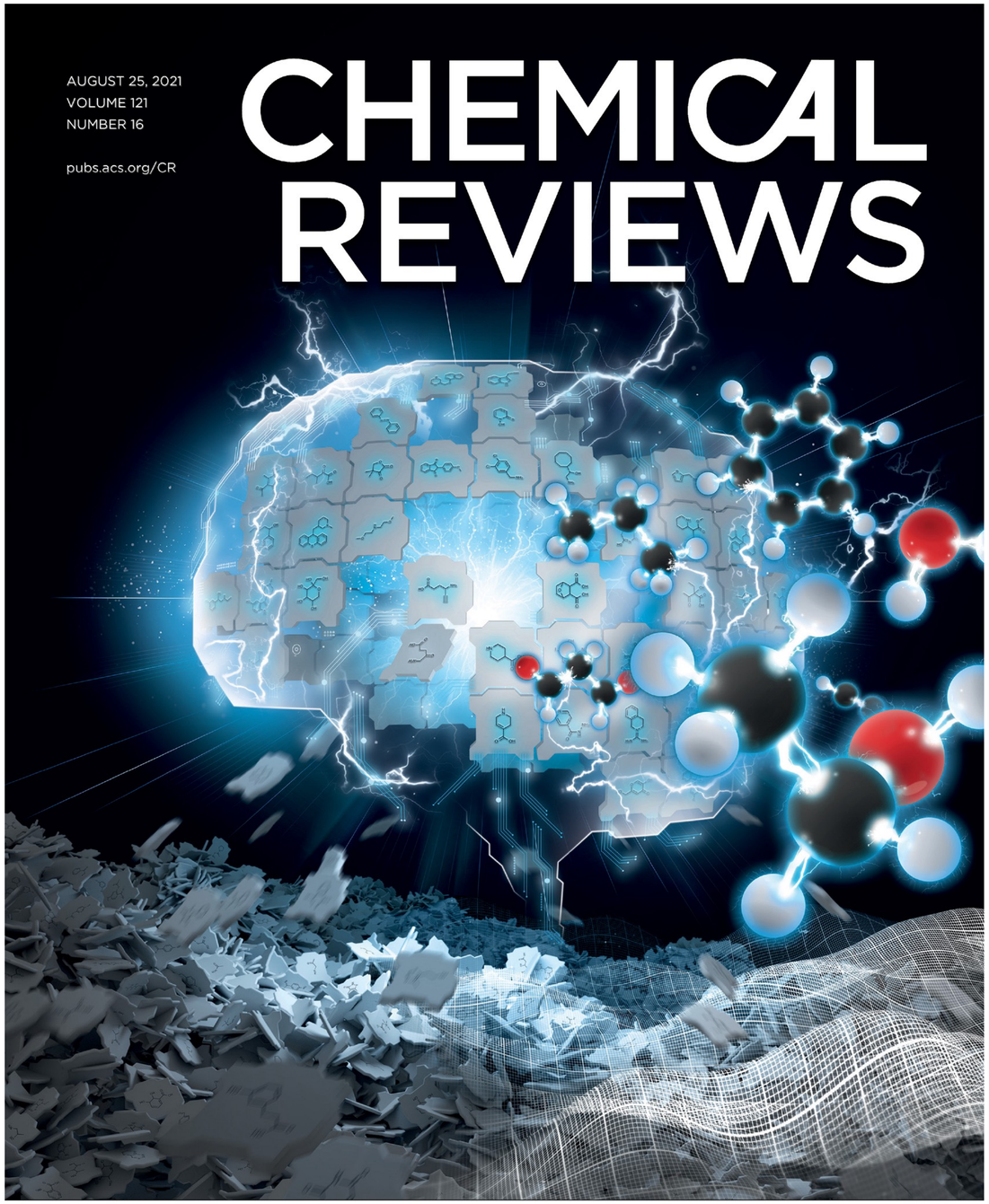


Chem. Rev. 121, 10142-10186 (**2021**)



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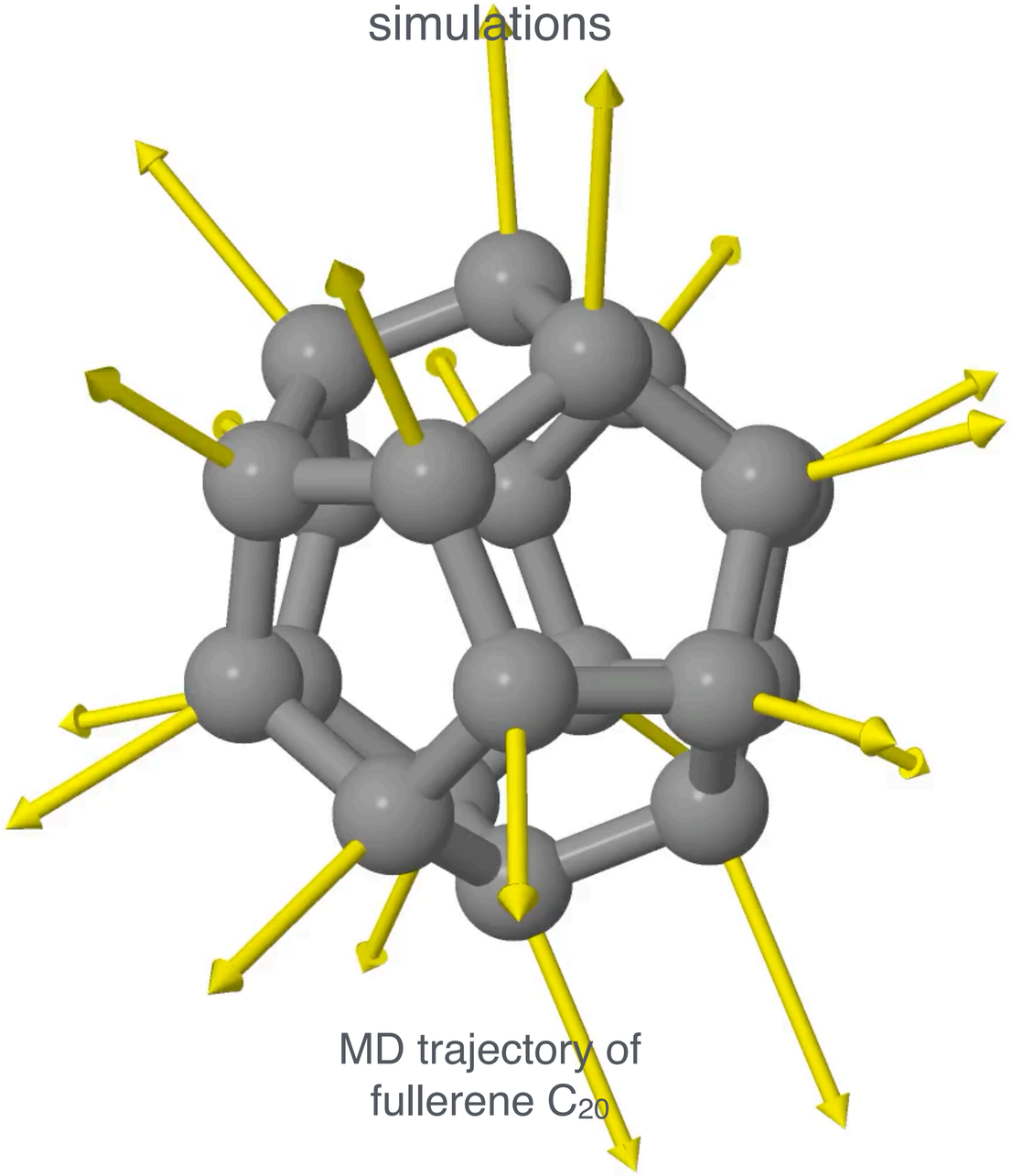
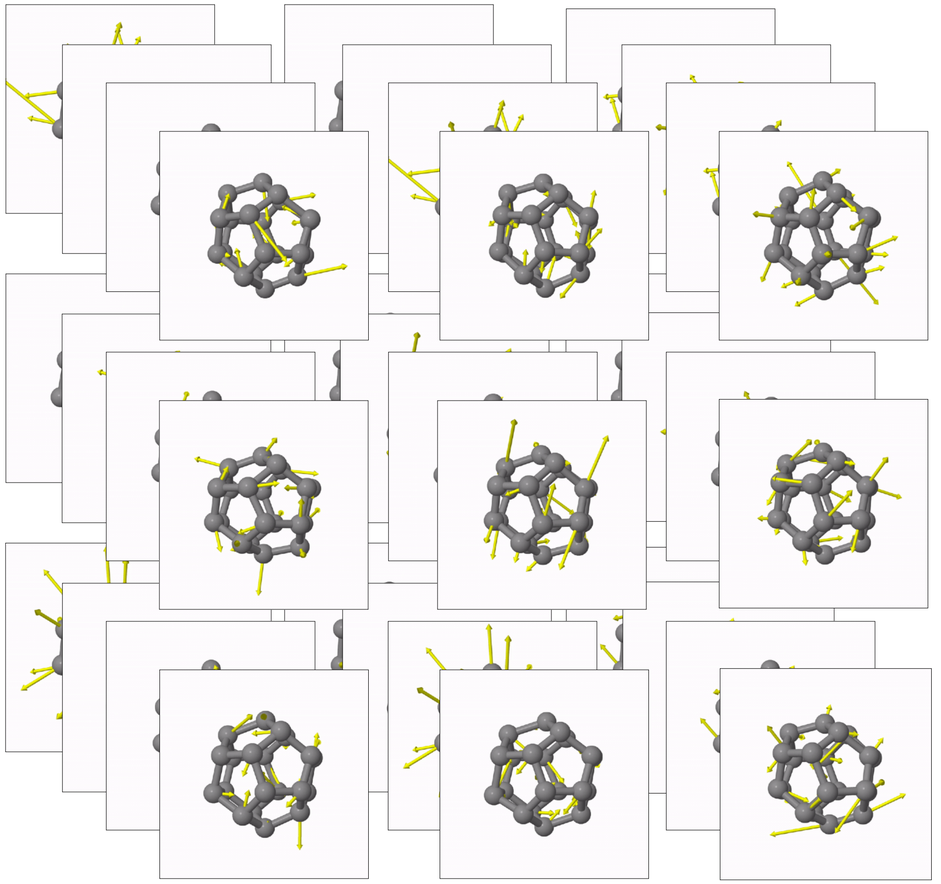
Molecular dynamics (MD) simulations



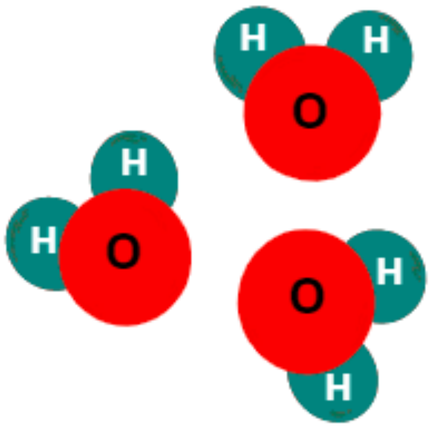
MD trajectory of fullerene C_{20}

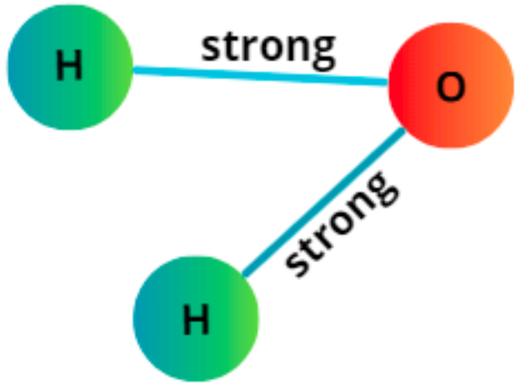


Nat. Commun., 9, 3887 (**2018**).

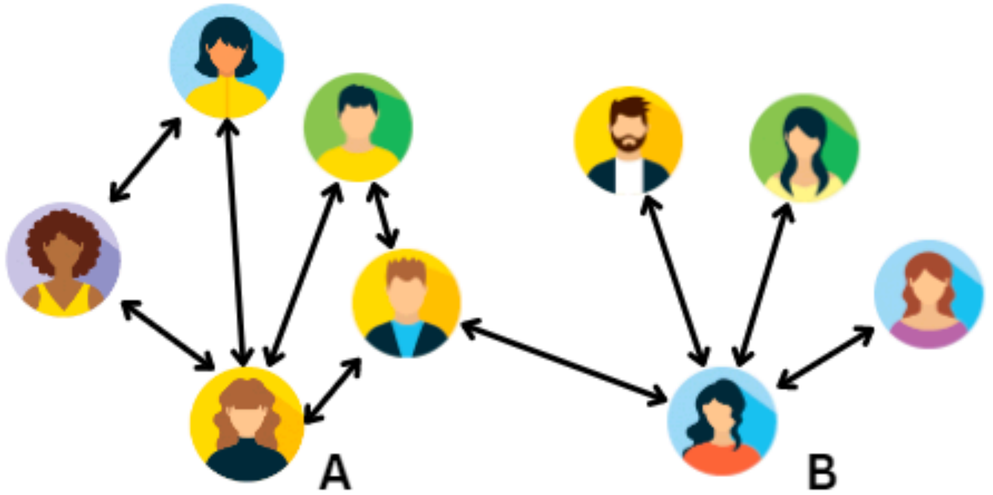
Graphs

Brain networks





Chemical compounds

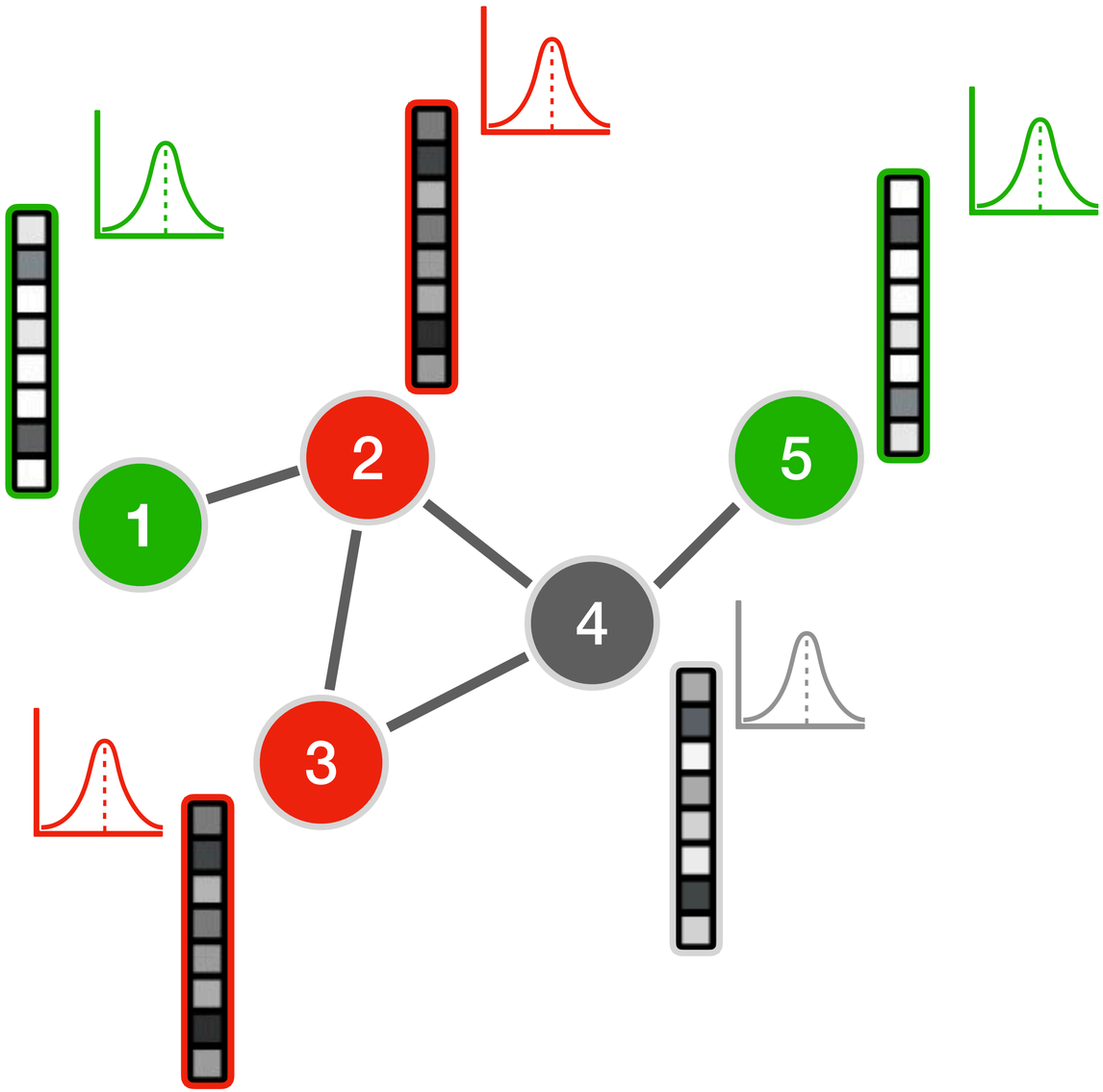


Social networks

https://miro.medium.com/v2/resize:fit:1029/1*txzoFgR0XvAy4PpIgbUyvQ.png

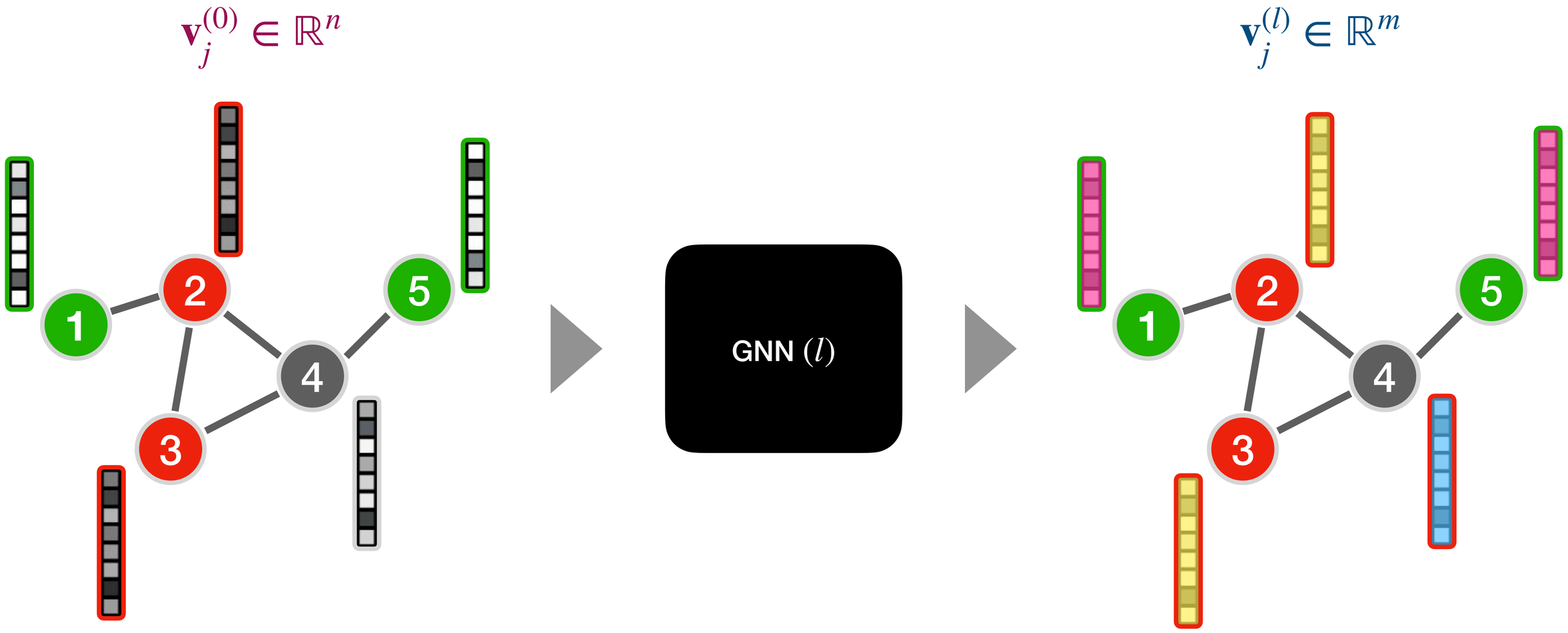
Graph Neural Networks

$$G = (V, E)$$

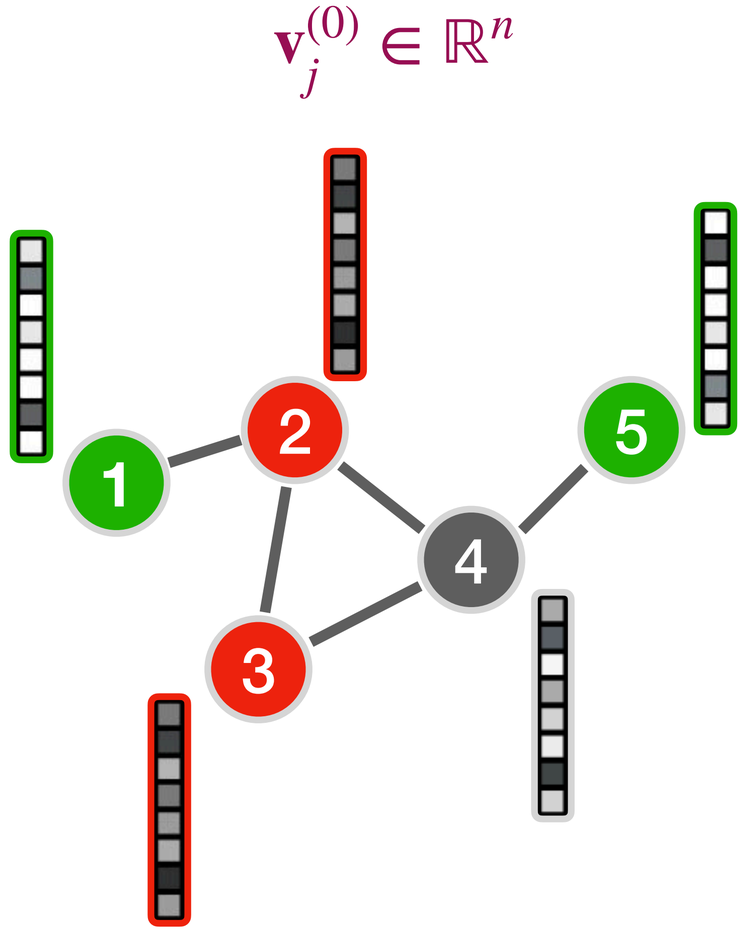


$$\mathbf{v}_j = \begin{bmatrix} \\ \\ \\ \\ \\ \\ \end{bmatrix} \in \mathbb{R}^n$$

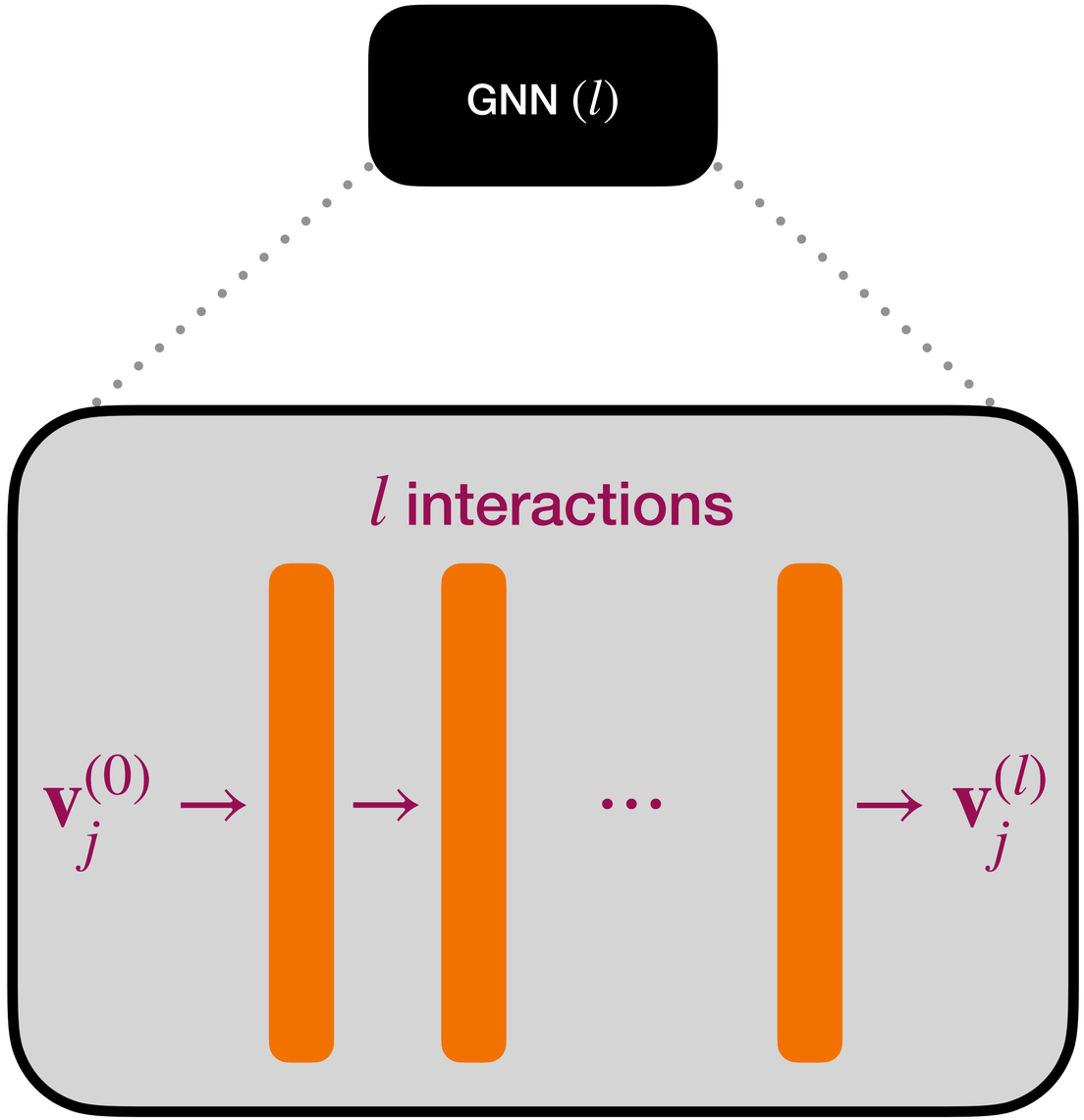
Graph Neural Networks



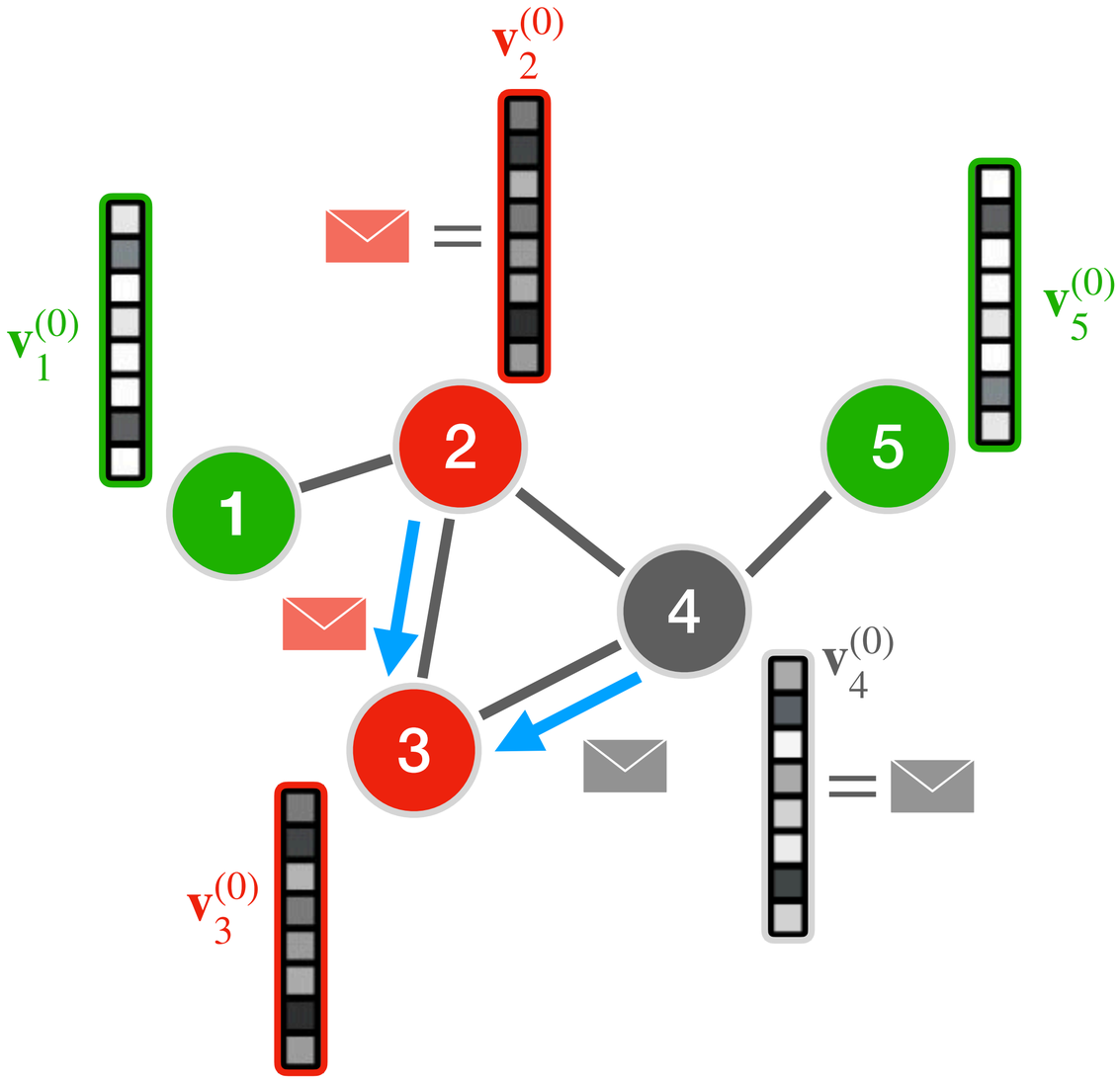
Graph Neural Networks



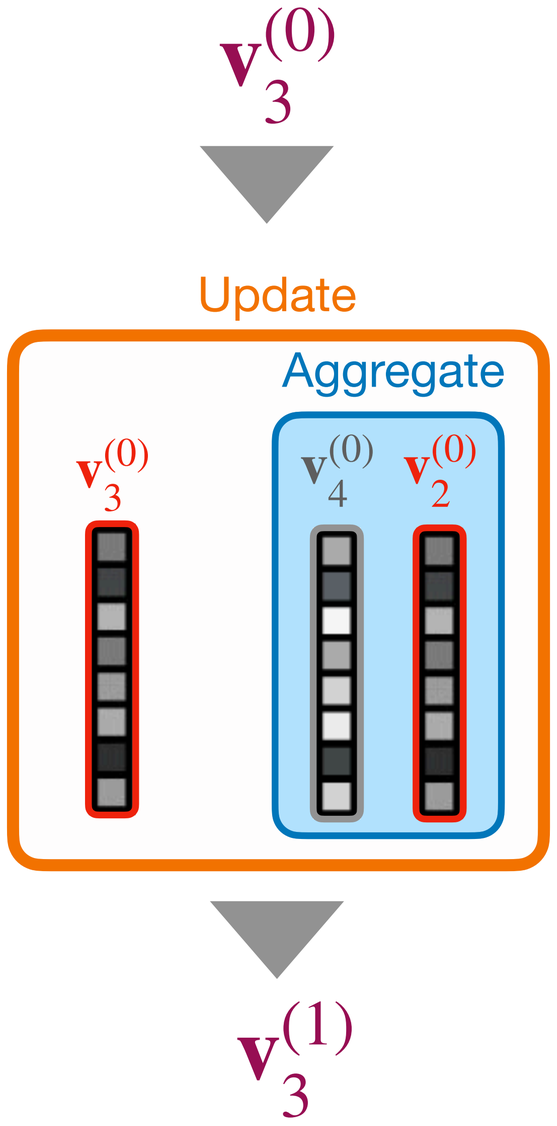
Message exchange



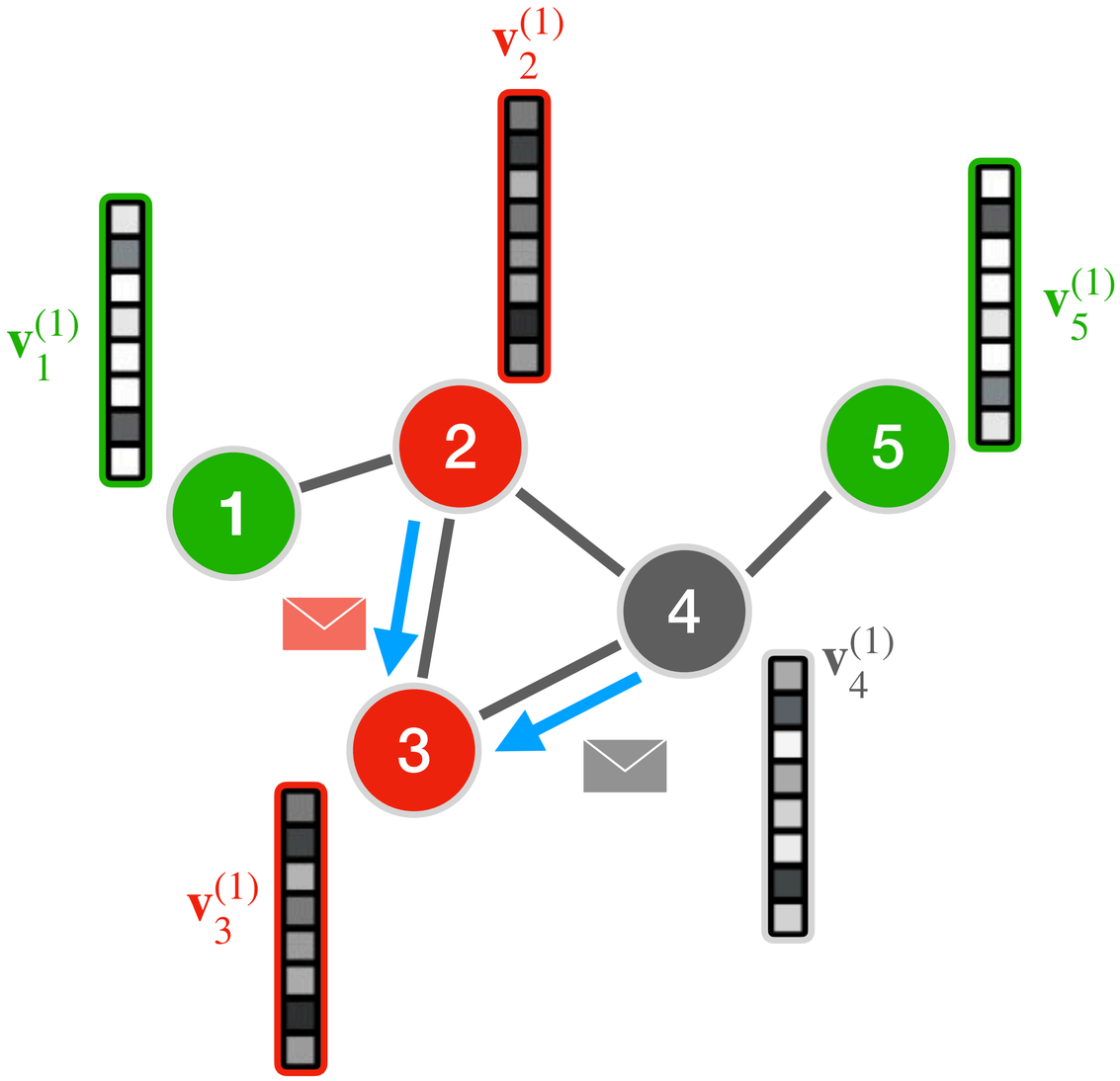
Graph Neural Networks



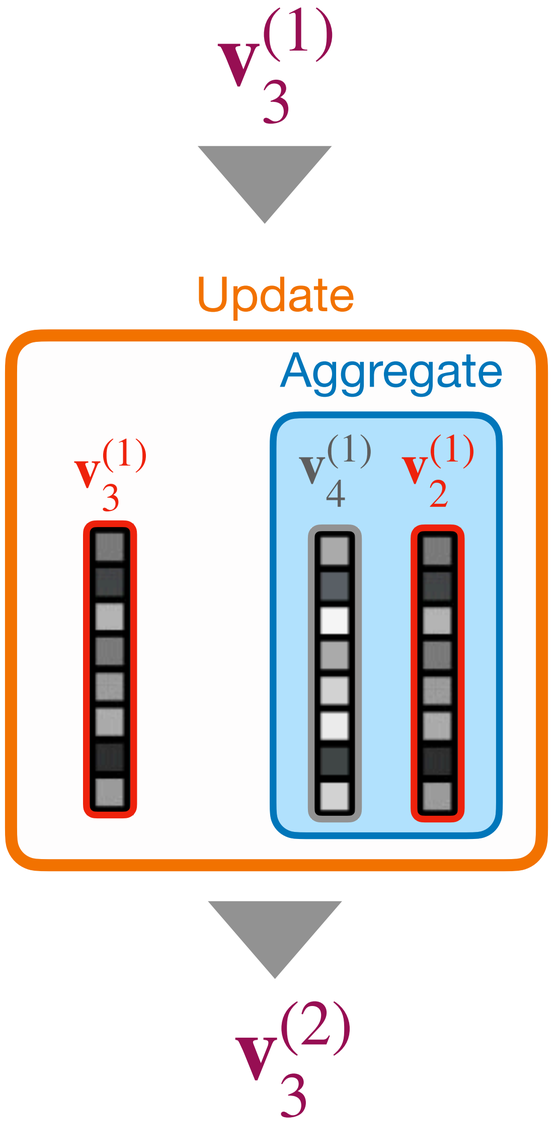
Message exchange



Graph Neural Networks



Message exchange



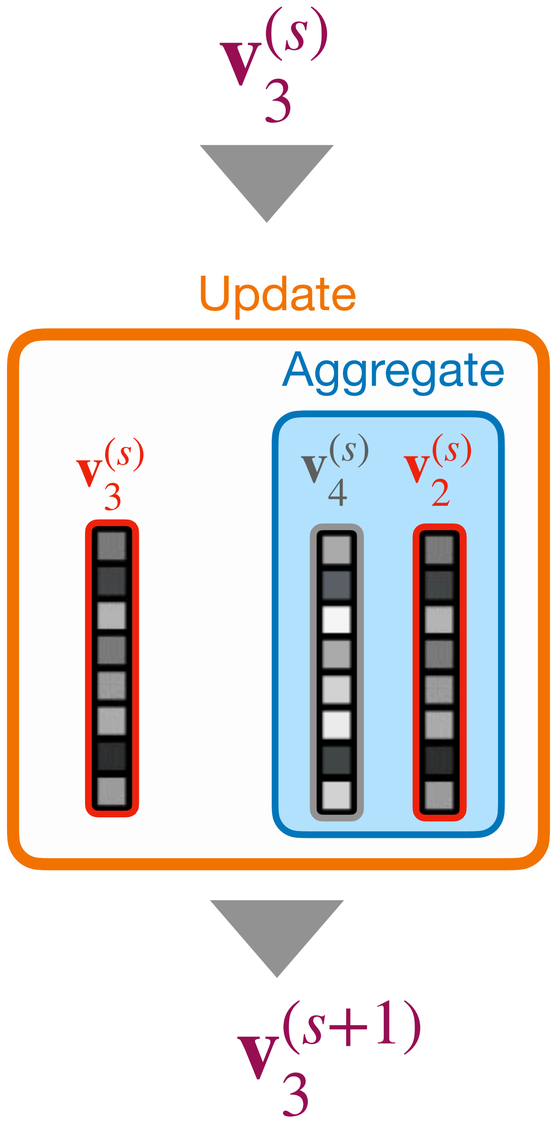
Graph Neural Networks

Message exchange

$$\mathbf{v}_j^{(s+1)} = \text{update}^{(s)}(\mathbf{v}_j^{(s)}, \text{aggregate}^{(s)}(\{\mathbf{v}_i^{(s)}; i \in \mathcal{N}_j\}))$$

- Min
- Max
- MLP
- RNN

- Min
- Max
- MLP
- Norm



Graph Neural Networks

$$\mathbf{v}_j^{(s+1)} = \text{update}^{(s)}(\mathbf{v}_j^{(s)}, \text{aggregate}^{(s)}(\{\mathbf{v}_i^{(s)}; i \in \mathcal{N}_j\}))$$

Graph Convolutional Networks, Kipf and Welling [2016]

$$\mathbf{h}_v^{(k)} = \sigma\left(\mathbf{W}^{(k)} \sum_{v \in \mathcal{N}(u) \cup \{u\}} \frac{\mathbf{h}_v}{\sqrt{|\mathcal{N}(u)||\mathcal{N}(v)|}}\right)$$

Self-loop

Sum of normalized neighbor embeddings

Multi-Layer-Perceptron as Aggregator, Zaheer et al. [2017]

$$\mathbf{m}_{\mathcal{N}(u)} = \boxed{\text{MLP}_\theta}\left(\sum_{v \in N(u)} \text{MLP}_\phi(\mathbf{h}_v)\right)$$

Aggregated message

trainable!

Send states through a MLP

Graph Attention Networks, Veličković et al. [2017]

$$\mathbf{m}_{\mathcal{N}(u)} = \sum_{v \in \mathcal{N}(u)} \alpha_{u,v} \mathbf{h}_v \qquad \alpha_{u,v} = \frac{\exp\left(\mathbf{a}^\top [\mathbf{W}\mathbf{h}_u \oplus \mathbf{W}\mathbf{h}_v]\right)}{\sum_{v' \in \mathcal{N}(u)} \exp\left(\mathbf{a}^\top [\mathbf{W}\mathbf{h}_u \oplus \mathbf{W}\mathbf{h}_{v'}]\right)}$$

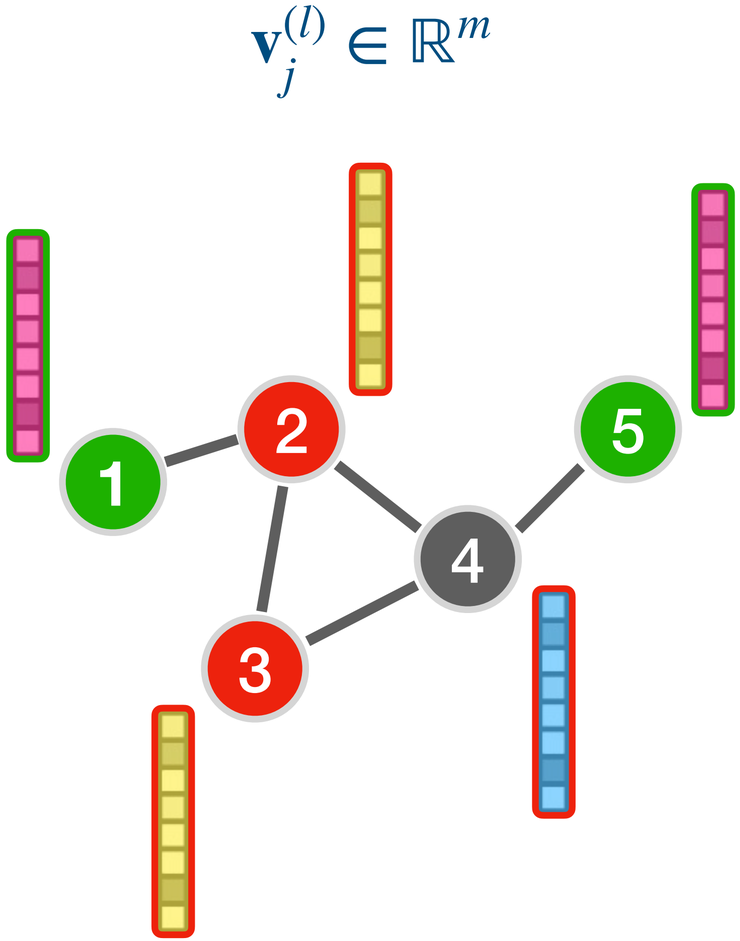
Attention weights

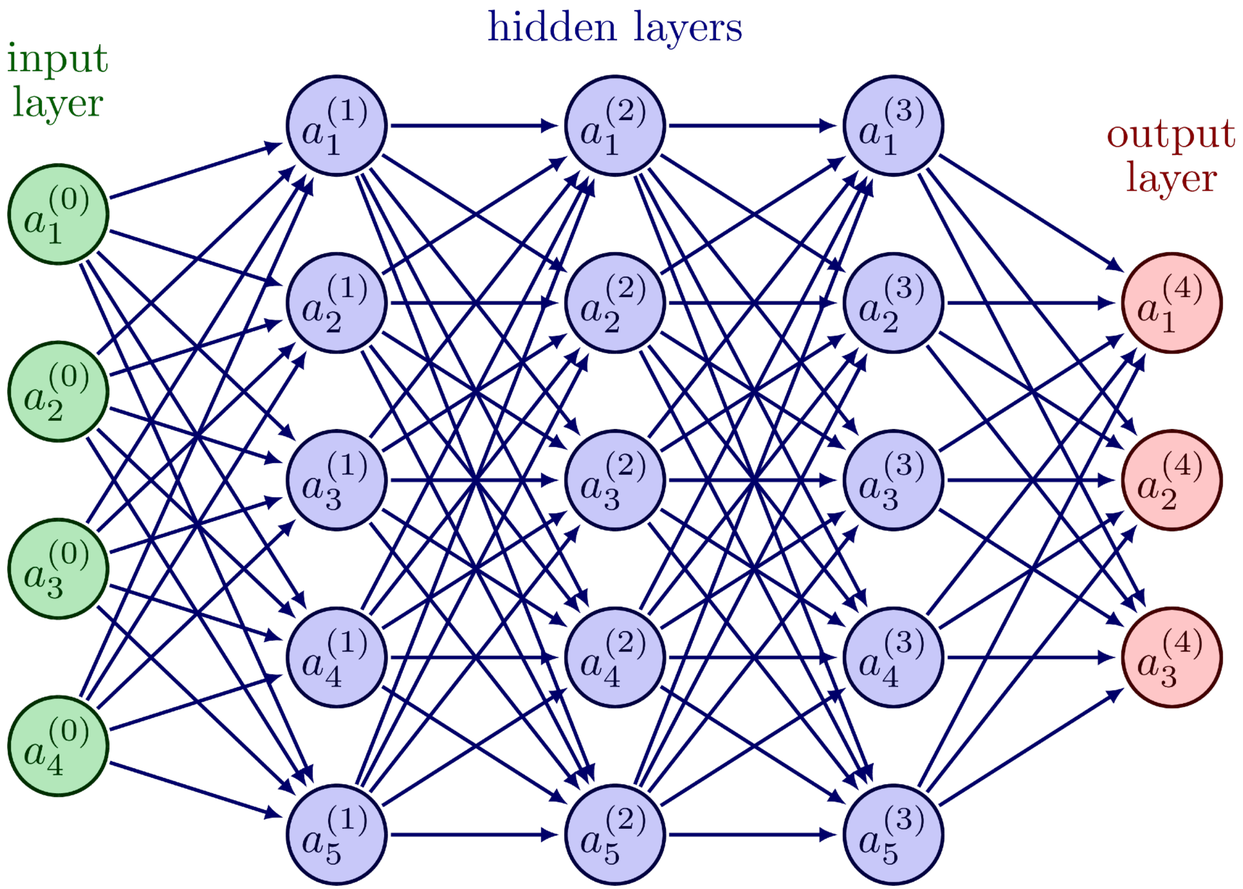
Gated Graph Neural Networks, Li et al. [2015]

$$\mathbf{h}_u^{(k)} = \text{GRU}(\mathbf{h}_u^{(k-1)}, \mathbf{m}_{\mathcal{N}(u)}^{(k)})$$

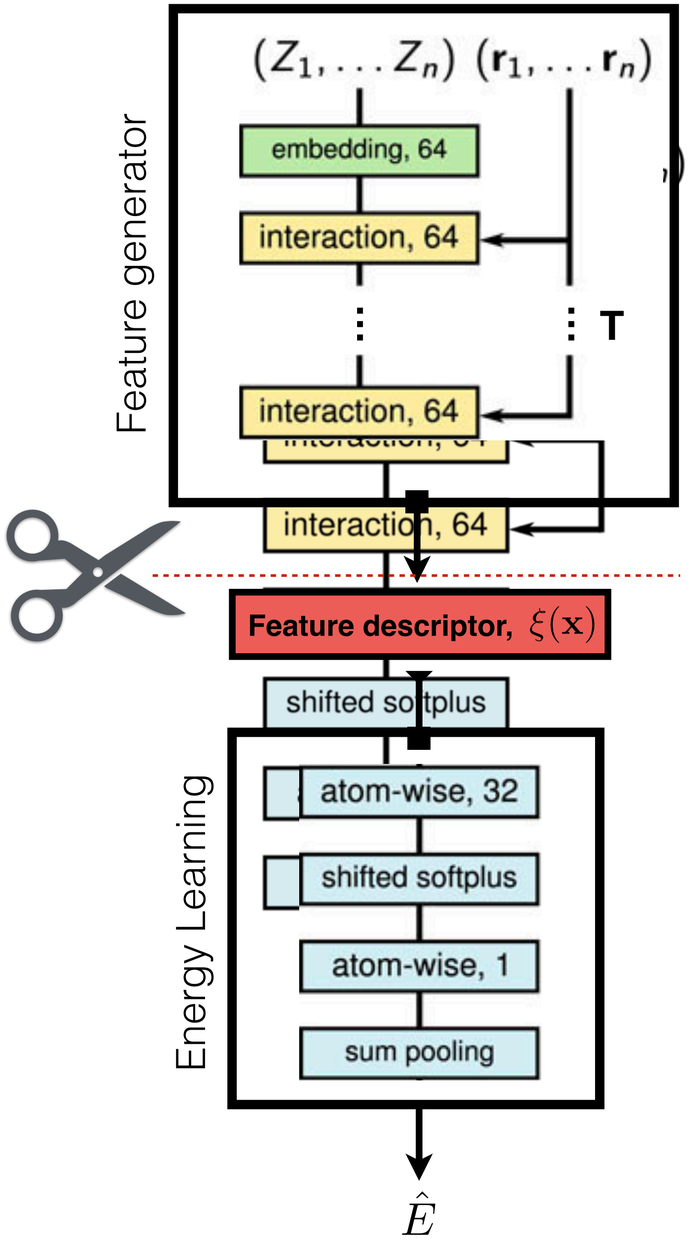
Recurrent update of the state

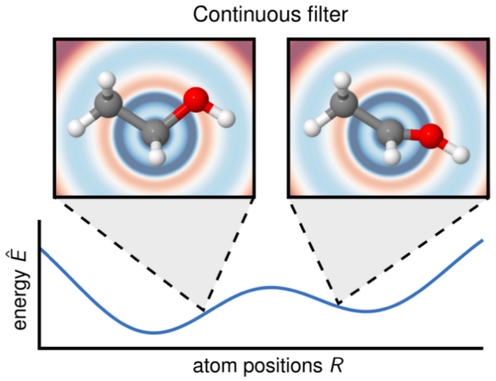
Graph Neural Networks



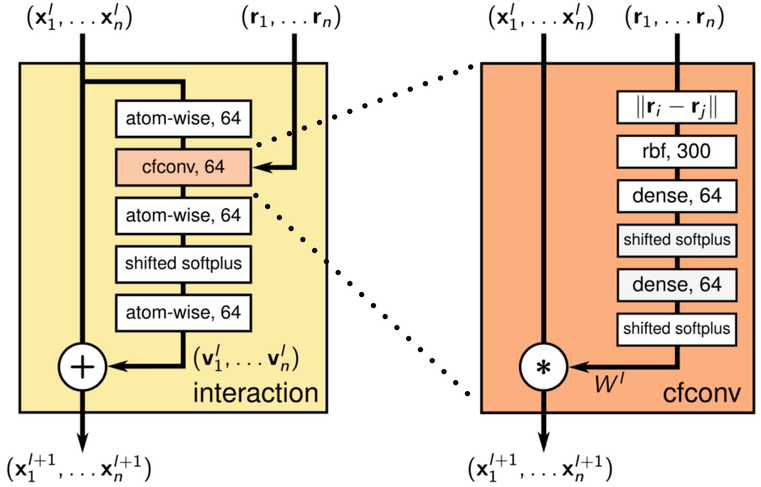


SchNet: A continuous-filter convolutional neural network for modeling quantum interactions





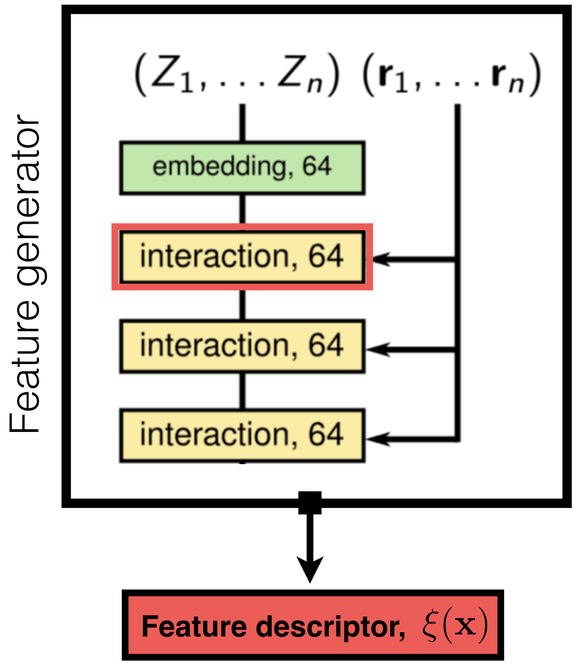
$$(\mathbf{x} * W)(\mathbf{r}_i) = \sum_{j=1}^{N_{\text{atom}}} \mathbf{x}_j^{(t)} \circ \underbrace{W^{(t)}(\mathbf{r}_i - \mathbf{r}_j)}_{\text{neural network}}$$



NeurIPS 30, pp. 992 (**2017**)

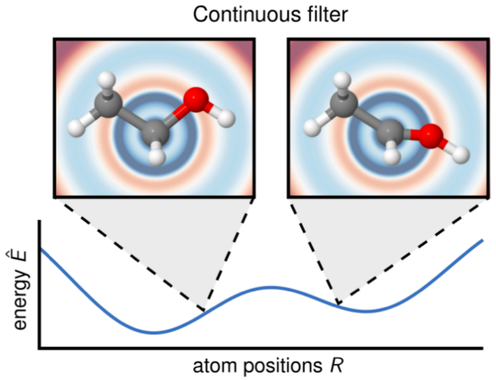
J. Chem. Phys. 148, 241722 (**2018**)

SchNet: A continuous-filter convolutional neural network for modeling quantum interactions



$$\xi = [\mathbf{x}_{H_1}, \mathbf{x}_{O_1}, \mathbf{x}_{H_2}]$$

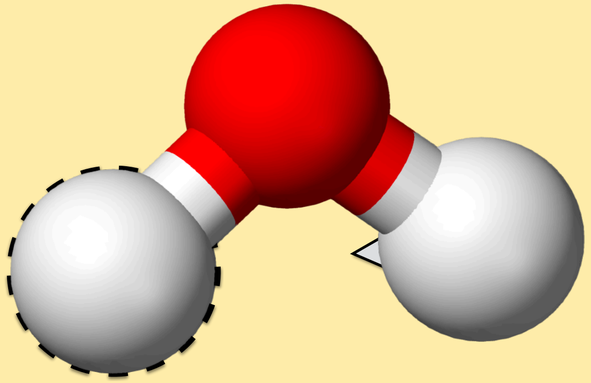
$$\mathbf{x}_{H_1} \in \mathbb{R}^{64}$$



$$(\mathbf{x} * W)(\mathbf{r}_i) = \sum_{j=1}^{N_{\text{atom}}} \mathbf{x}_j^{(t)} \circ \underbrace{W^{(t)}(\mathbf{r}_i - \mathbf{r}_j)}_{\text{neural network}}$$

Interaction 1

$\mathbf{x}_{H_1}^{(1)}$



NeurIPS 30, pp. 992 (**2017**)

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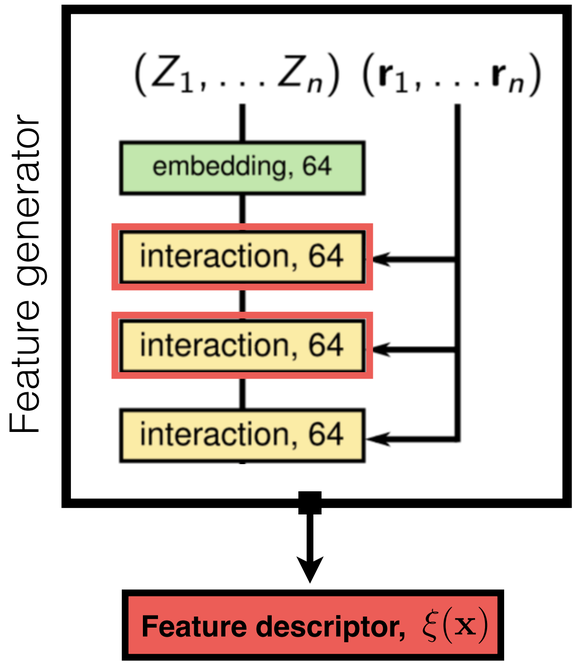
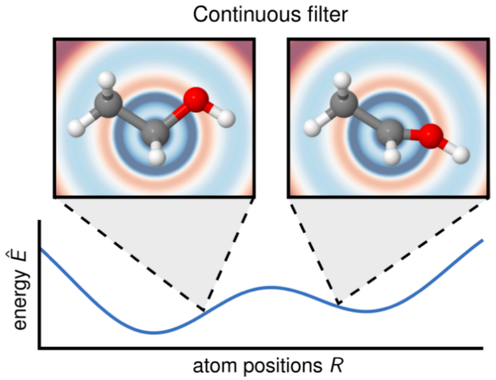
SchNet: A continuous-filter convolutional neural network for modeling quantum interactions



$$\xi = [\mathbf{x}_{H_1}, \mathbf{x}_{O_1}, \mathbf{x}_{H_2}]$$

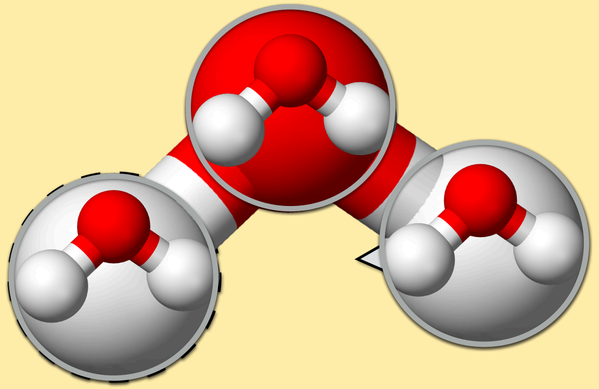
$$\mathbf{x}_{H_1} \in \mathbb{R}^{64}$$



$$(\mathbf{x} * W)(\mathbf{r}_i) = \sum_{j=1}^{N_{\text{atom}}} \mathbf{x}_j^{(t)} \circ \underbrace{W^{(t)}(\mathbf{r}_i - \mathbf{r}_j)}_{\text{neural network}}$$

Interaction 1

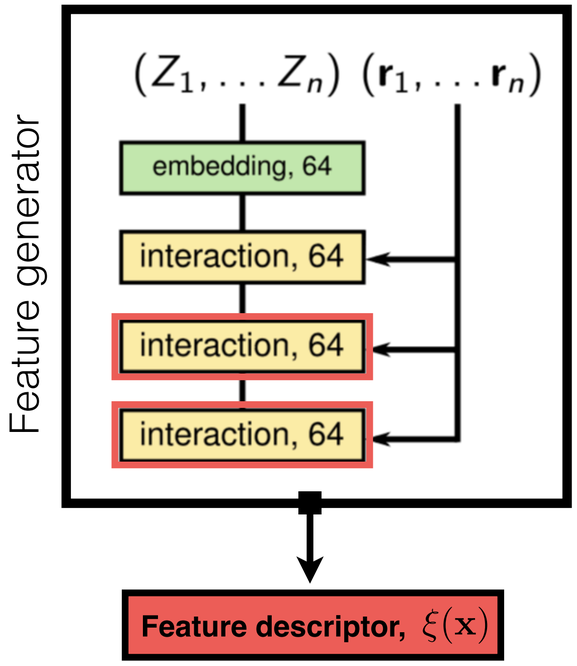
$\mathbf{x}_{H_1}^{(1)}$



NeurIPS 30, pp. 992 (**2017**)

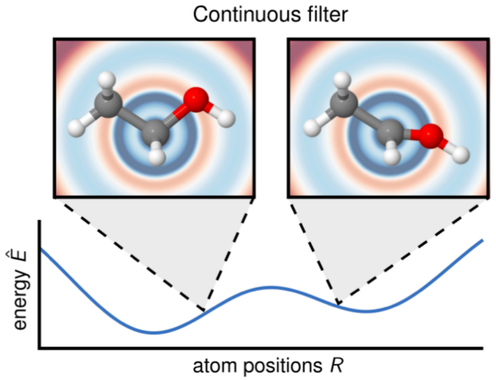
J. Chem. Phys. 148, 241722 (**2018**)

SchNet: A continuous-filter convolutional neural network for modeling quantum interactions



$$\xi = [\mathbf{x}_{H_1}, \mathbf{x}_{O_1}, \mathbf{x}_{H_2}]$$

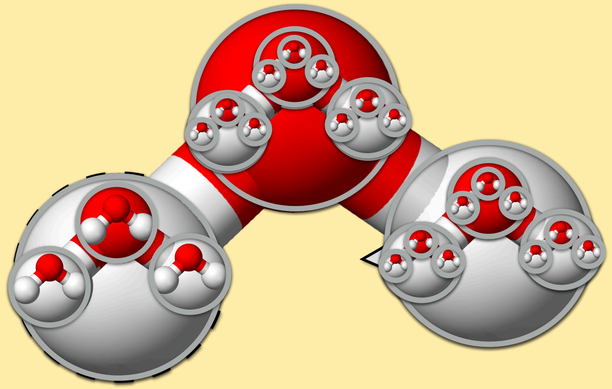
$$\mathbf{x}_{H_1} \in \mathbb{R}^{64}$$



$$(\mathbf{x} * W)(\mathbf{r}_i) = \sum_{j=1}^{N_{\text{atom}}} \mathbf{x}_j^{(t)} \circ \underbrace{W^{(t)}(\mathbf{r}_i - \mathbf{r}_j)}_{\text{neural network}}$$

Interaction 3

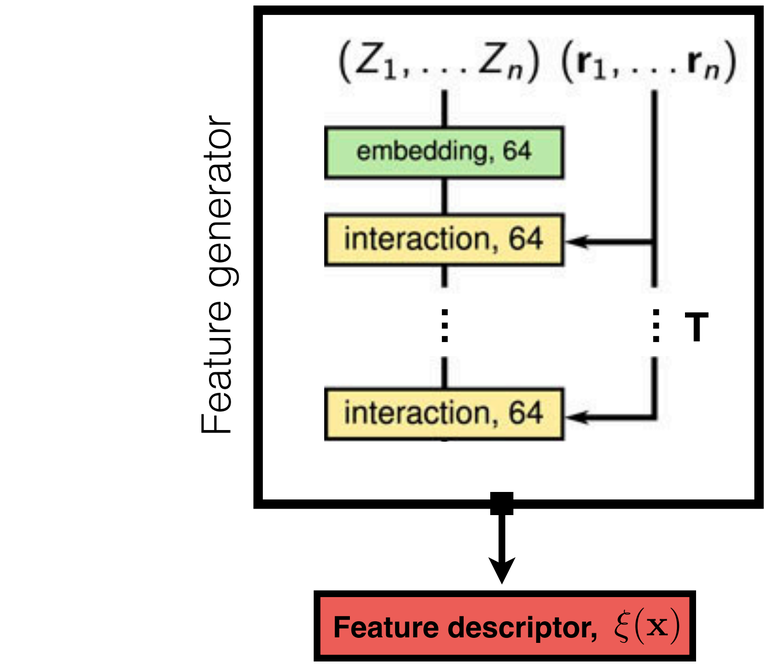
$\mathbf{x}_{H_1}^{(3)}$

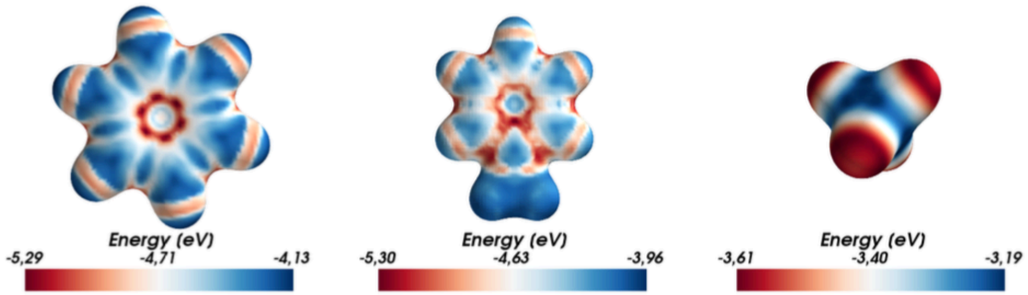


NeurIPS 30, pp. 992 (**2017**)

J. Chem. Phys. 148, 241722 (**2018**)

SchNet: A continuous-filter convolutional neural network for modeling quantum interactions



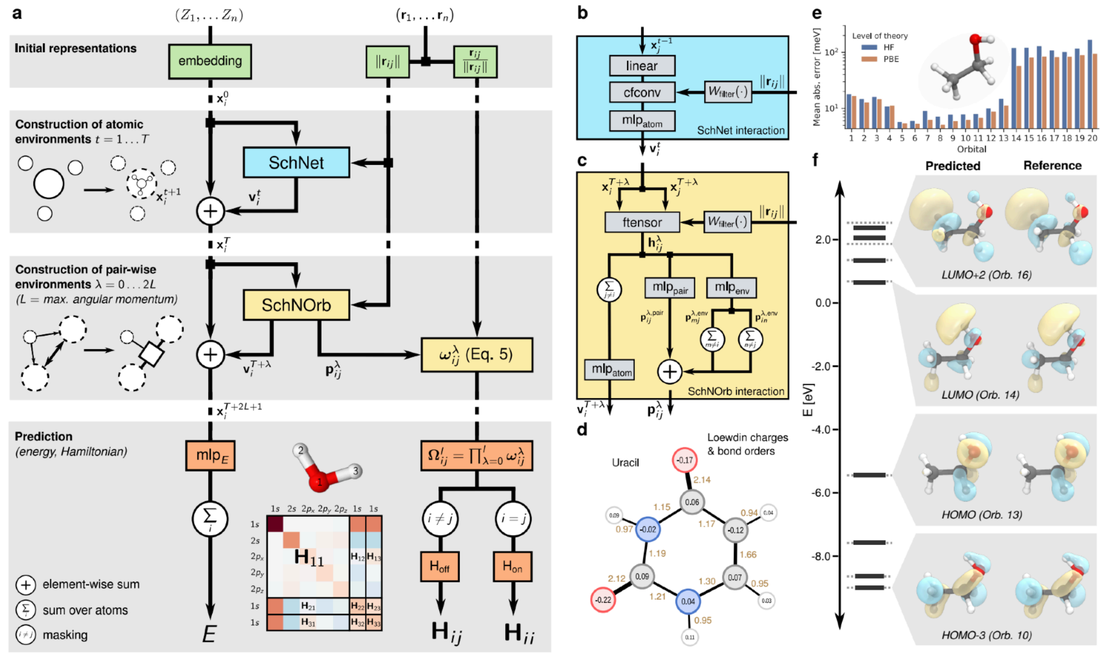


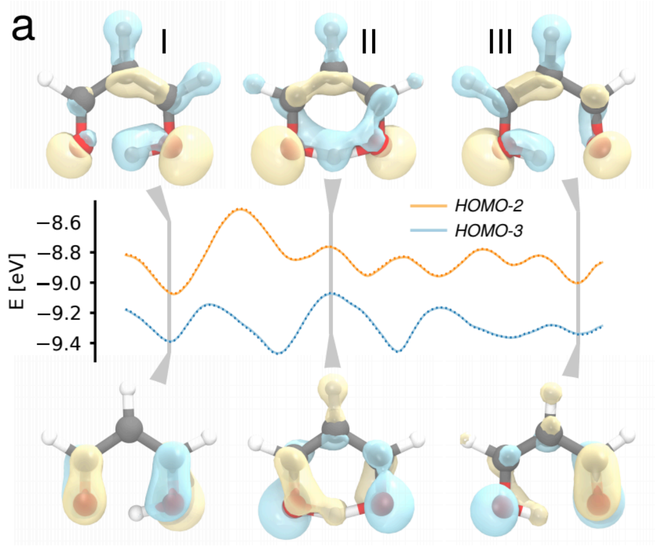
NeurIPS 30, pp. 992 (**2017**)

J. Chem. Phys. 148, 241722 (**2018**)

SchNOrb

$$\mathbf{H} = \begin{bmatrix} \mathbf{H}_{11} & \cdots & \mathbf{H}_{1j} & \cdots & \mathbf{H}_{1n} \\ \vdots & \ddots & \vdots & & \vdots \\ \mathbf{H}_{i1} & \cdots & \mathbf{H}_{ij} & \cdots & \mathbf{H}_{in} \\ \vdots & & \vdots & \ddots & \vdots \\ \mathbf{H}_{n1} & \cdots & \mathbf{H}_{nj} & \cdots & \mathbf{H}_{nn} \end{bmatrix}$$





ARTICLE

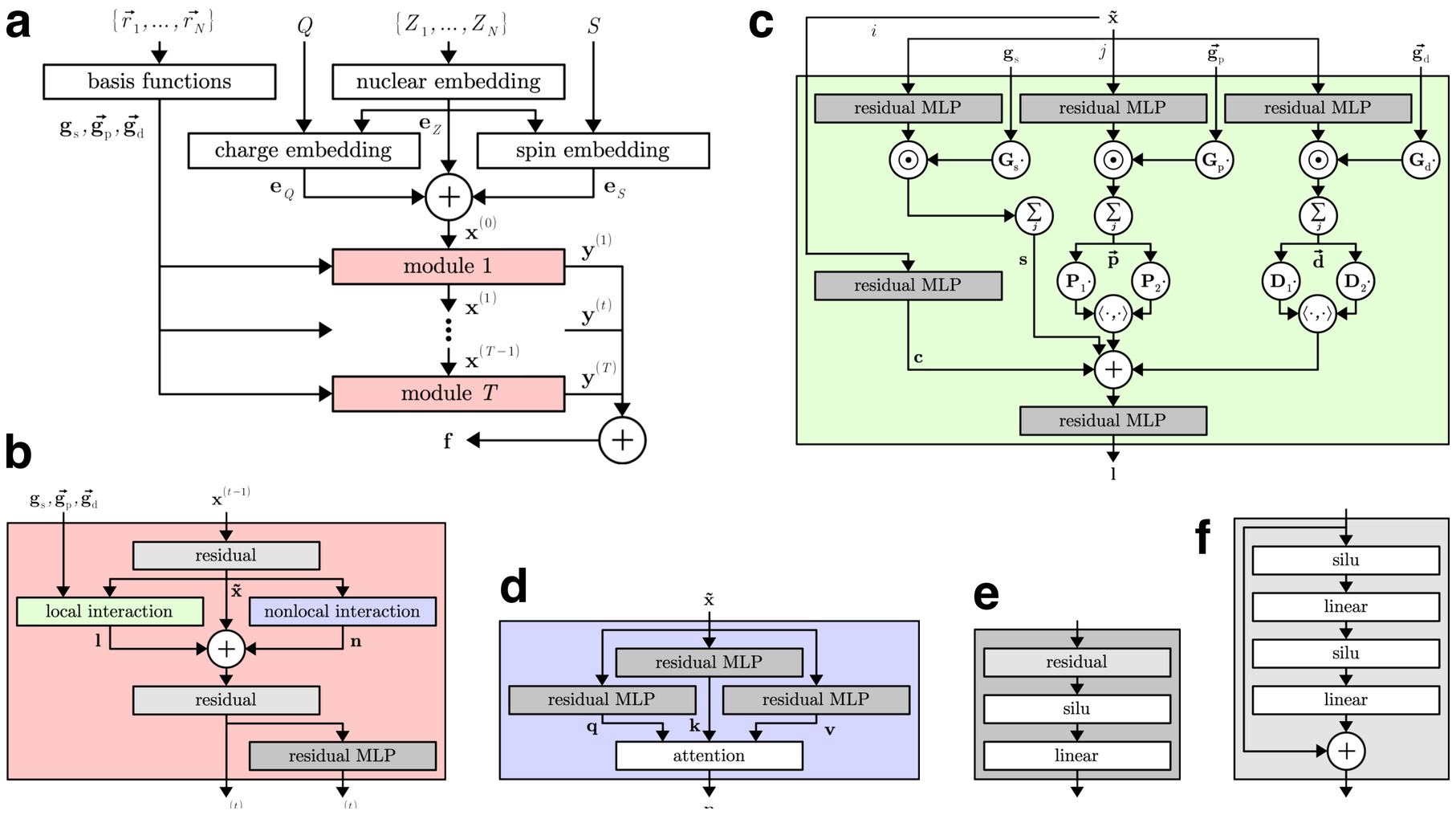
https://doi.org/10.1038/s41467-021-27504-0 OPEN

SpookyNet: Learning force fields with electronic degrees of freedom and nonlocal effects

Oliver T. Unke[1,2✉], Stefan Chmiela[1], Michael Gastegger[1,2], Kristof T. Schütt[1], Huziel E. Sauceda[1,3] & Klaus-Robert Müller[1,4,5,6,7✉]

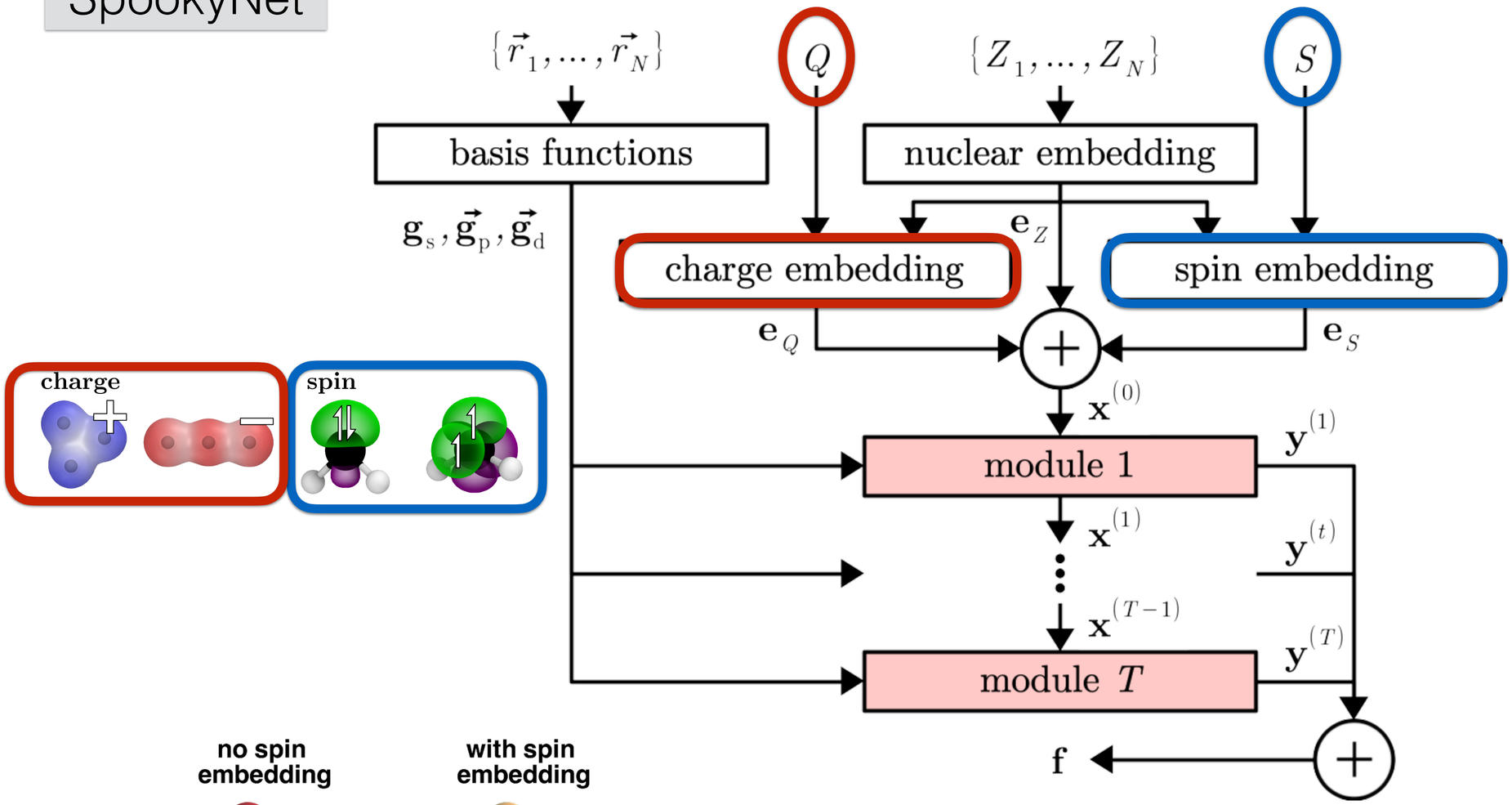
Unke *et al.*
Nature Communications (**2021**) 12, 7273.

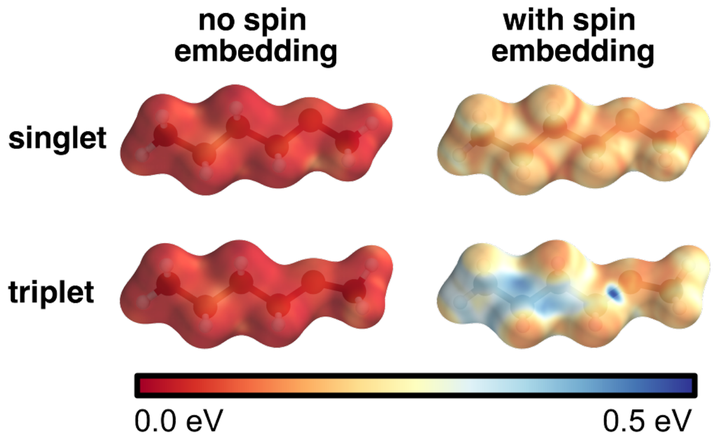
SpookyNet



Unke *et al.*
Nature Communications (**2021**) 12, 7273.

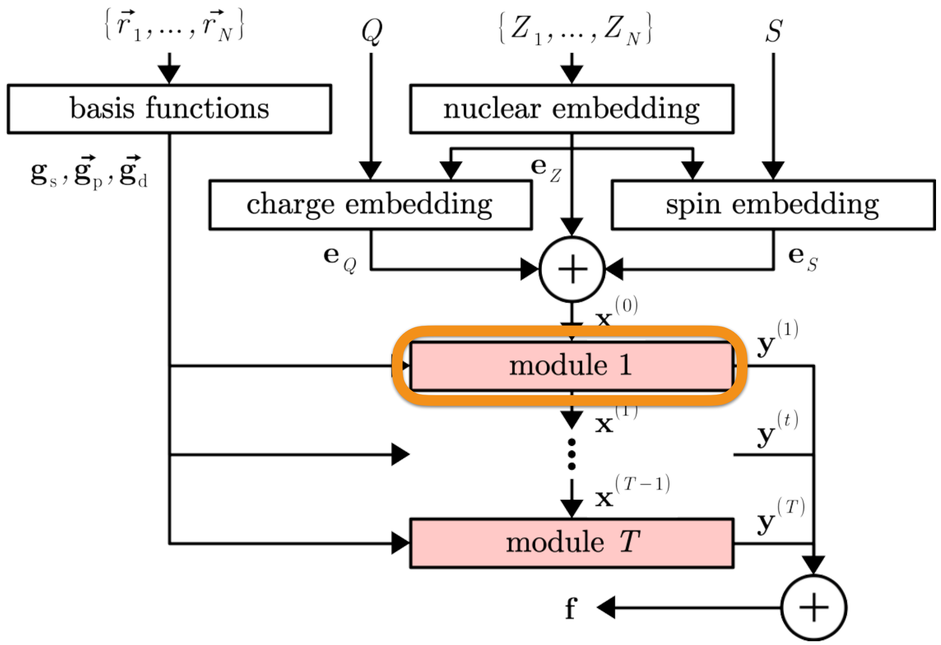
SpookyNet

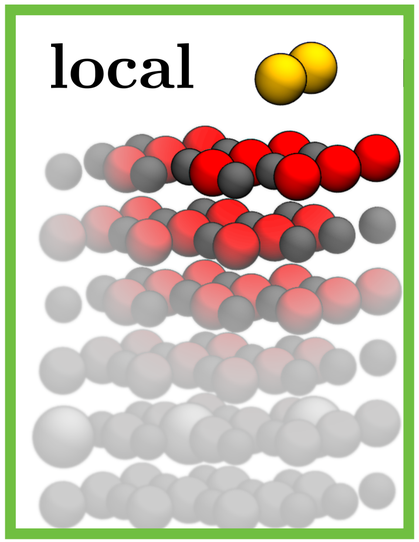


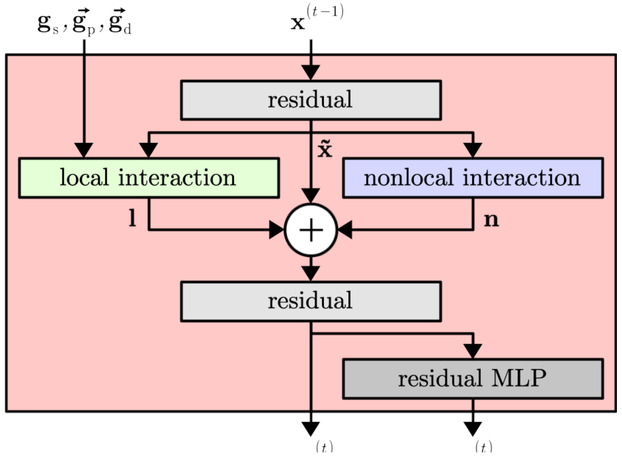


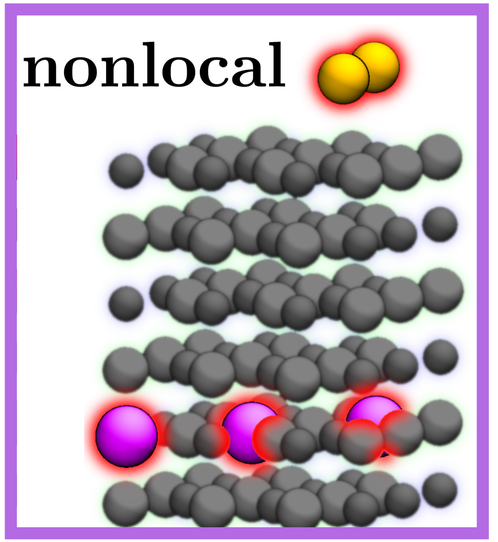
Unke *et al.*
Nature Communications **(2021)** 12, 7273.

SpookyNet



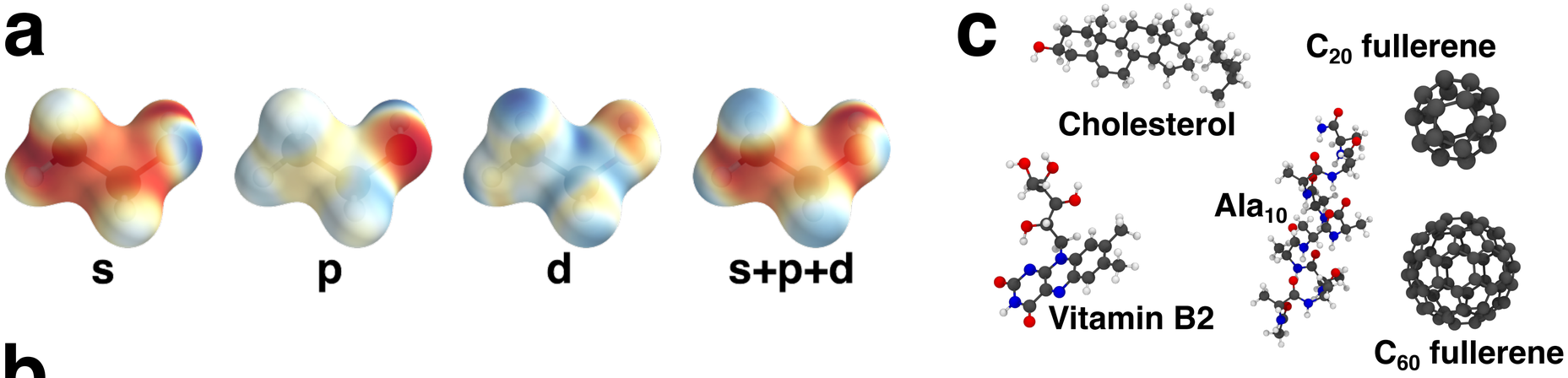






Unke *et al.*
Nature Communications **(2021)** 12, 7273.

SpookyNet



Unke *et al.*
Nature Communications **(2021)** 12, 7273.

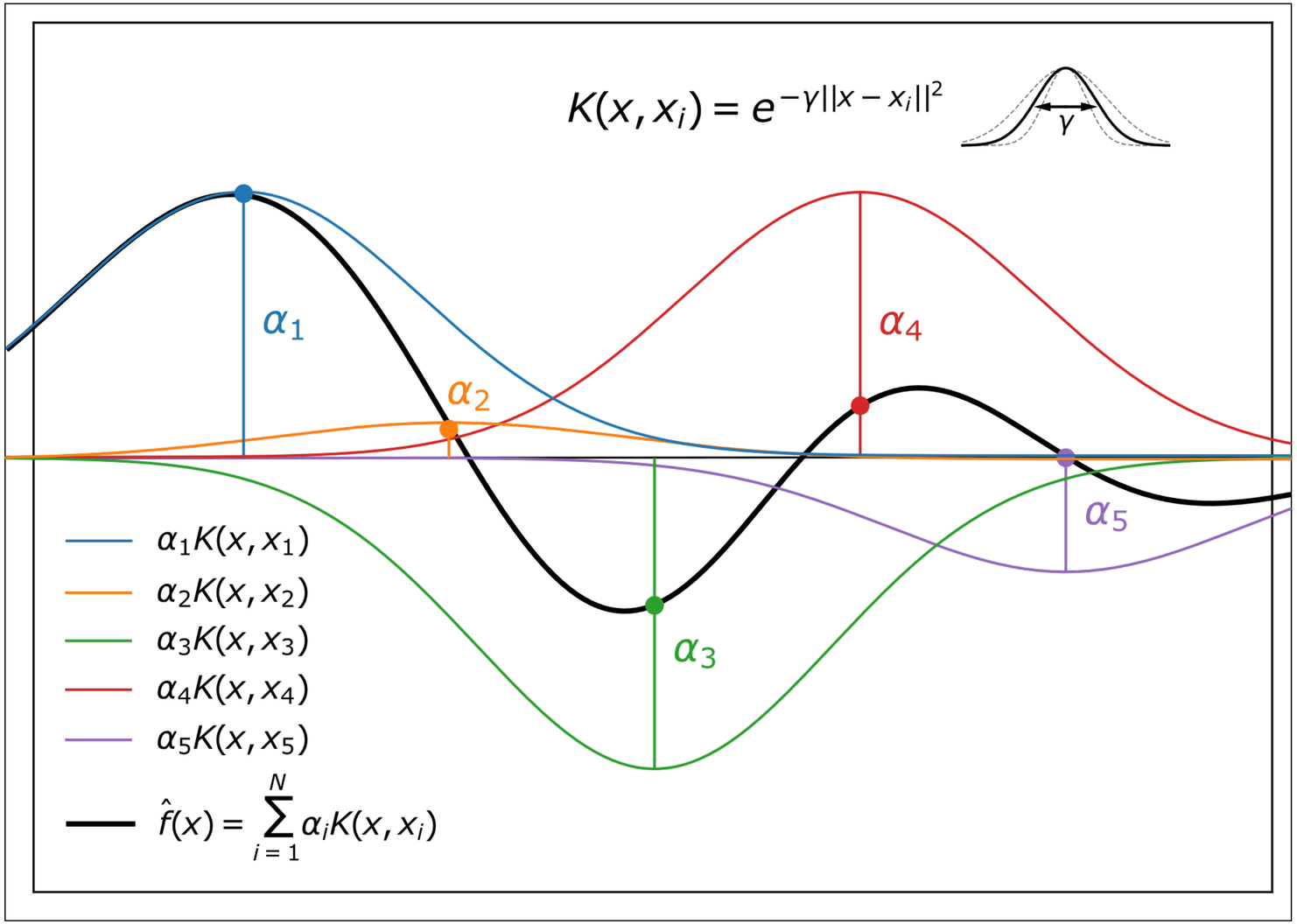
Machine Learning

Learning force fields

$$\mathcal{H}\Psi = V_{BO}\Psi$$

$$-\mathbf{F} = \langle \Psi^* | \partial\mathcal{H}/\partial\mathbf{x} | \Psi \rangle$$

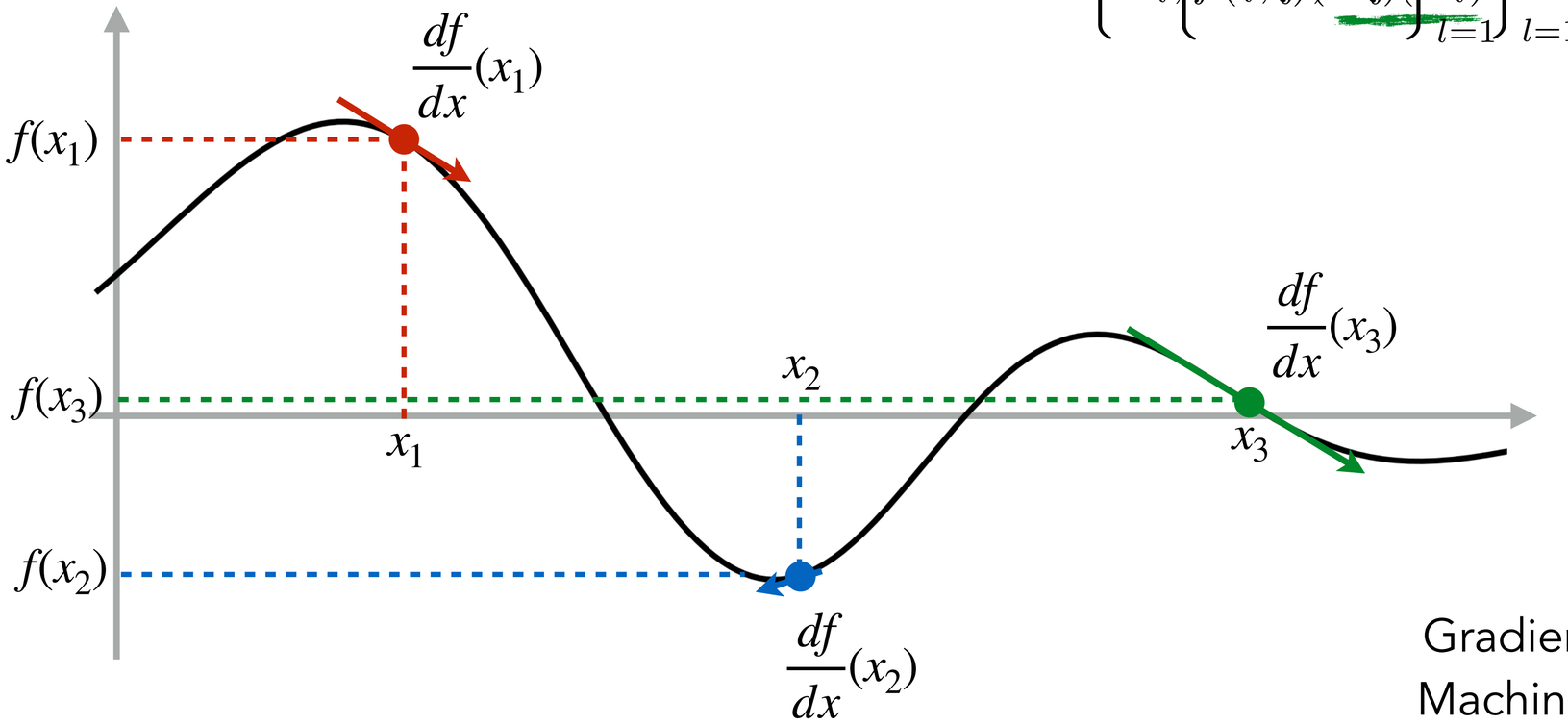
Kernel ridge regression



$$f(\mathbf{R}) = \sum_{l=1}^{M} \kappa(\mathbf{D}(\mathbf{R}), \mathbf{D}(\mathbf{R}_l))\alpha_l$$

Chem. Rev. 121 (16), 10142 (**2021**)

Kernel ridge regression



$$(\mathbf{K} + \lambda \mathbf{I})\vec{\alpha} = \vec{f}$$

$$\vec{f} = \left[\frac{df}{dx}(x_1), \frac{df}{dx}(x_2), \ldots, \frac{df}{dx}(x_M)\right]^{\mathrm{T}}$$

$$\mathrm{k}(x_i, x_j) = \frac{\partial^2}{\partial x \partial x'} e^{-||x-x'||^2/2\sigma}\Big|_{(x,x')=(x_i,x_j)}$$

Gradient Domain Machine Learning (**GDML**)

$$\frac{df}{dx}(x) = \sum_{l=1}^{M} \alpha_l \frac{d^2}{dx^2}\kappa(x, x_l)$$

$$f(x) = \sum_{l=1}^{M} \alpha_l \frac{d}{dx}\kappa(x, x_l)$$

Sci. Adv. **3**, e1603015 (**2017**)

The GDML framework

GDML

$$\hat{\mathbf{f}}_{\mathbf{F}}(\vec{x}) = \sum_{i=1}^{M} (\vec{\alpha}_i \cdot \nabla) \nabla \kappa(D(\vec{x}), D(\vec{x}_i))$$

Sci. Adv. **3**, e1603015 (**2017**)

sGDML

$$\hat{\mathbf{f}}_{\mathbf{F}}(\vec{x}) = \sum_{i=1}^{M} \sum_{\mathbf{P} \in \mathcal{F}} (\mathbf{P}\vec{\alpha}_i \cdot \nabla) \nabla \kappa(D(\vec{x}), D(\mathbf{P}\vec{x}_i))$$

Nat. Commun., 9, 3887 (**2018**)

BIGDML

$$\hat{\mathbf{f}}_{\mathbf{F}}(\vec{x}) = \sum_{i=1}^{M} \sum_{\mathbf{T} \in \mathcal{T}} \sum_{\mathbf{P} \in \mathcal{F}} (\mathbf{TP}\vec{\alpha}_i \cdot \nabla) \nabla \kappa(D(\vec{x}), D(\mathbf{TP}\vec{x}_i))$$

Nat. Commun. 13 (1), 3733 (**2022**)

Numerical Optimizer

$$\alpha_t = \alpha_{t-1} - \gamma \left[(\mathbf{K} + \lambda \mathbb{I}) \alpha_{t-1} - \mathbf{y} \right]$$

$$\mathbf{P}^{-1} = \lambda^{-1} [\mathbb{I} - \mathbf{K}_{mk} (\lambda \mathbf{K}_{kk} + \mathbf{K}_{mk}^{\top} \mathbf{K}_{mk})^{-1} \mathbf{K}_{mk}^{\top}]$$

Sci. Adv. 9, eadf0873 (**2023**)

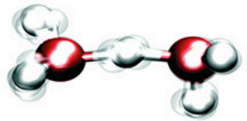
Path integral molecular dynamics

Formulation

Nuclear Quantum Effects

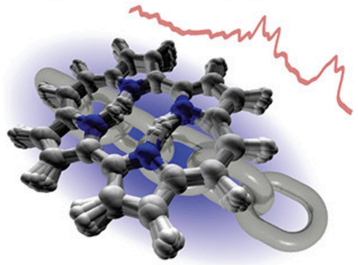
Protons/hydrogen atoms NQE

1: Magnetic shielding



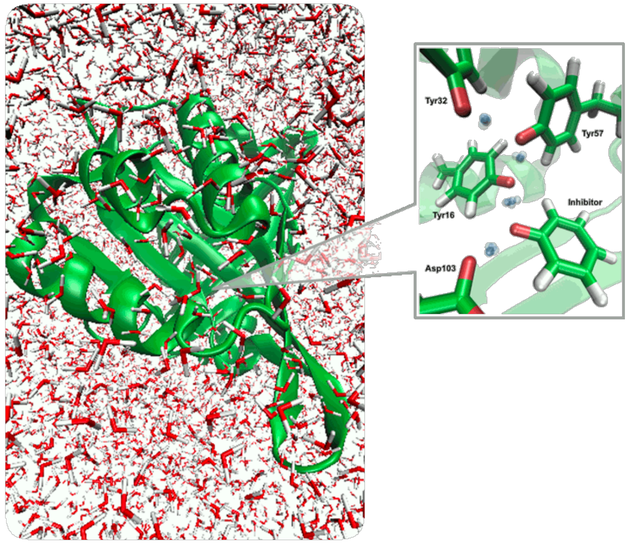
Phys. Chem. Chem. Phys. **2015**, 17, 14355–14359.

3: Spectroscopy



J. Am. Chem. Soc. **2019**, 141, 2526– 2534

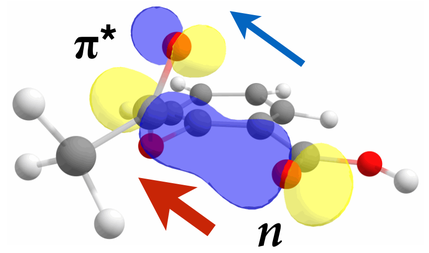
2: Enzyme proton networks

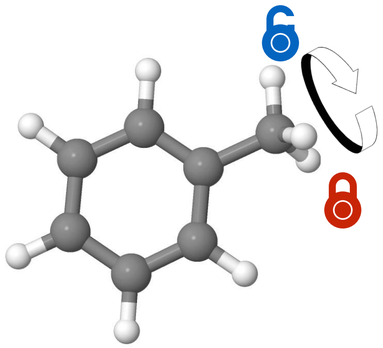


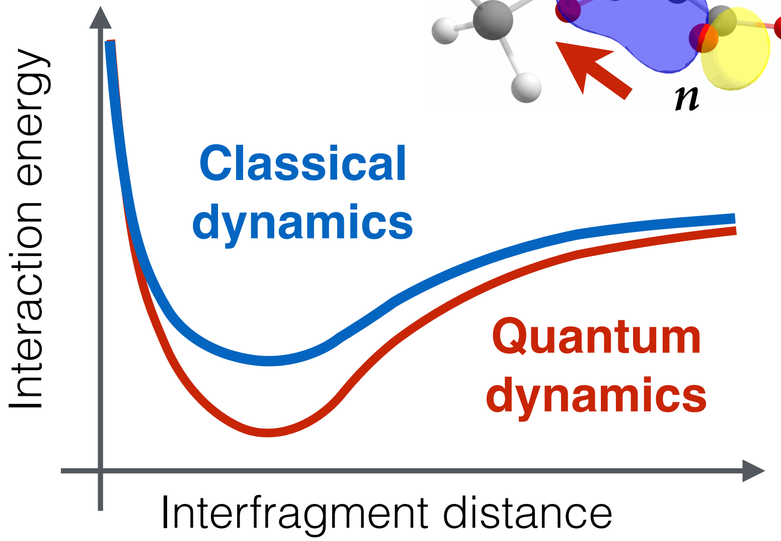
Markland et al. ***J. Phys. Chem. B.***, 121 (42), 9807-9815 (**2017**)
Proc. Natl. Acad. Sci., 111 (52), 18454-18459 (**2014**)

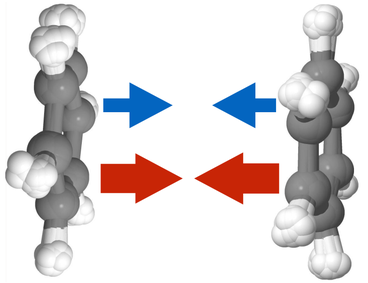
NQE beyond hydrogen atoms

4: Interactions enhancement







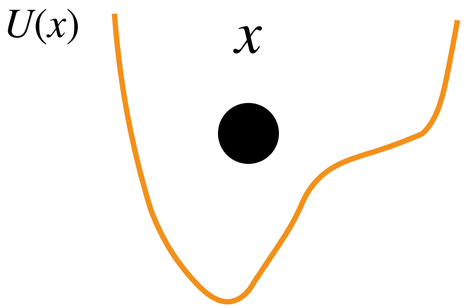


Sci. Adv. **3**, e1603015 (**2017**)
Nat. Commun., 9, 3887 (**2018**)
*J. Chem. Phys. 150 (11), 114102 (**2019**)*
*J. Chem. Phys. 153 (12), 124109 (**2020**)*
Nat. Commun., 12, 442 (***2021***)

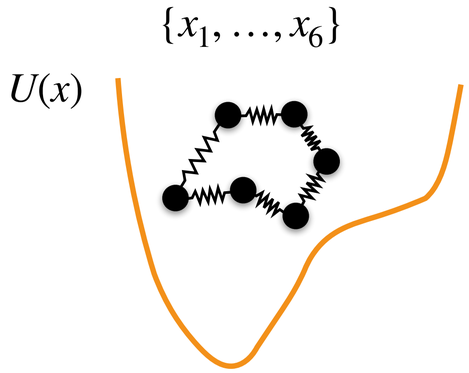
Ring Polymer Molecular Dynamics: Summary

$$H = \frac{p^2}{2m} + U(x)$$

$$H = \sum_{l=1}^{P} \left[\frac{p_l^2}{2m'} + \frac{1}{2} m\omega_P^2 (x_{l+1} - x_l)^2 + \frac{1}{P} U(x_l) \right]_{x_{P+1}=x_1}$$



Classical particle



Ring polymer

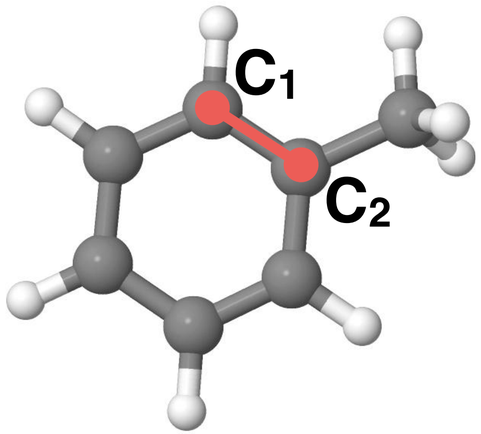
$$\omega_P = \frac{\sqrt{P}}{\beta\hbar}$$

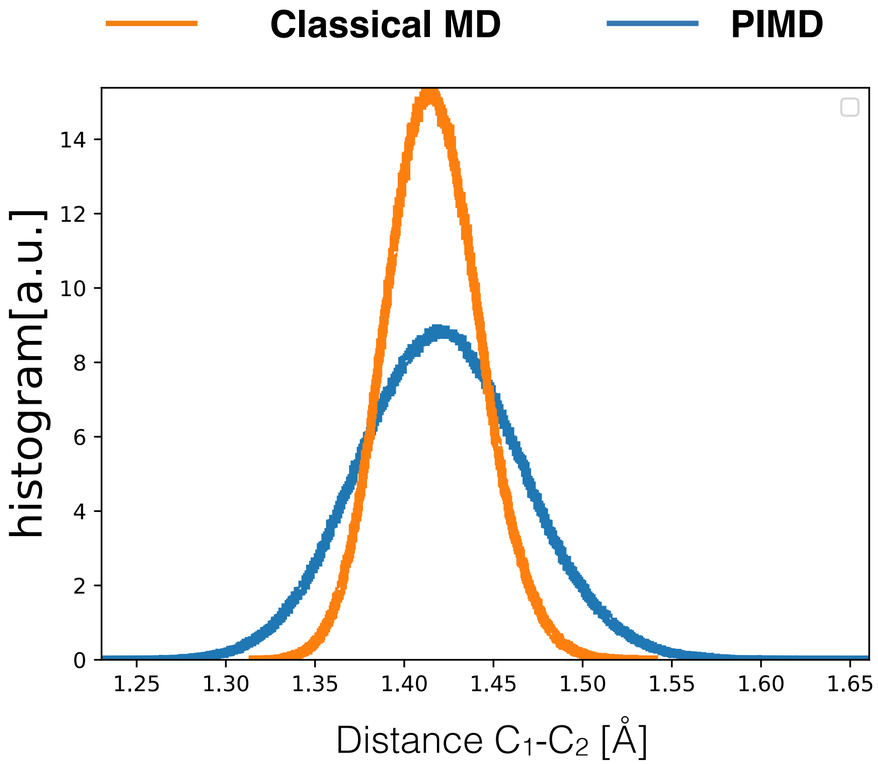
Classical simulation provides quantum results

Chem. Rev. 121 (16), 10142 (**2021**)

Nuclear Quantum Effects

Molecular bond delocalization during MD simulations

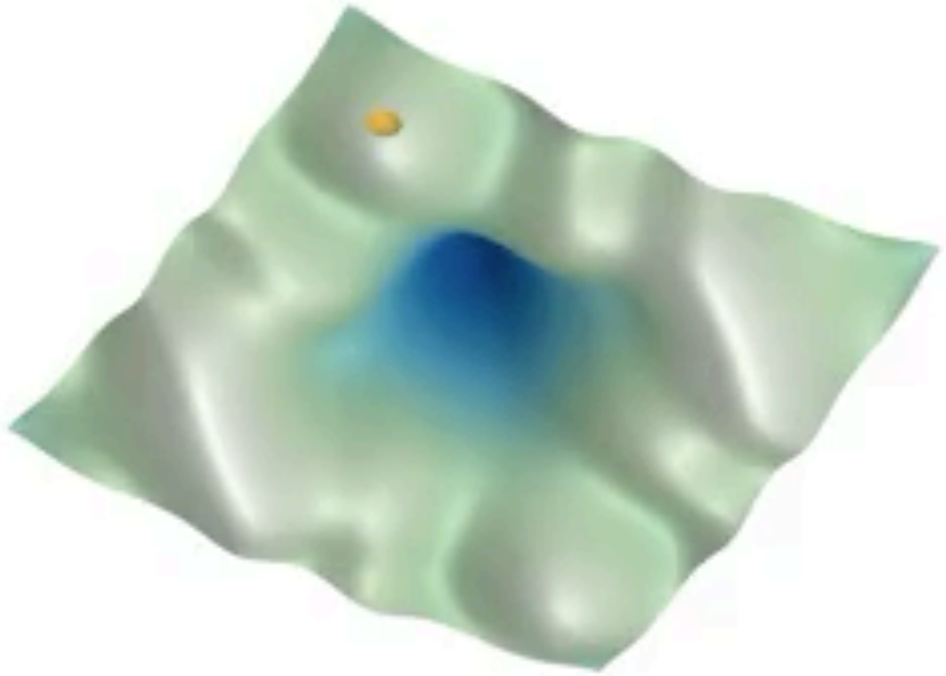


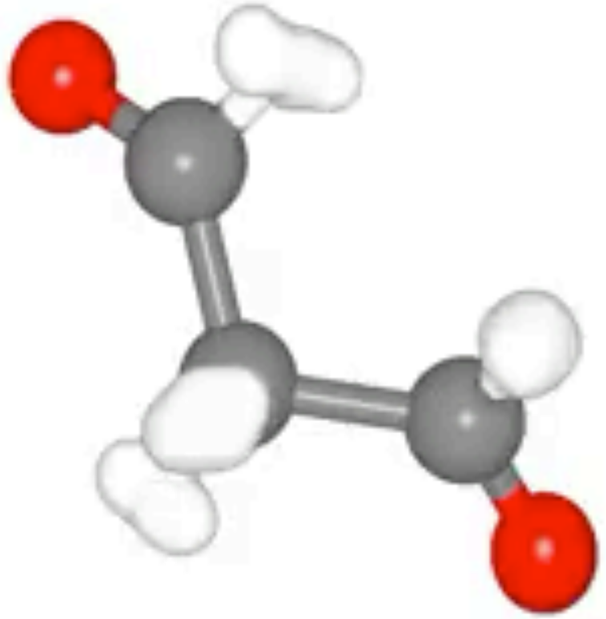


Quantum interatomic *dilation*

HES *et al. Nat. Commun.*, 12, 442 ***(2021)***

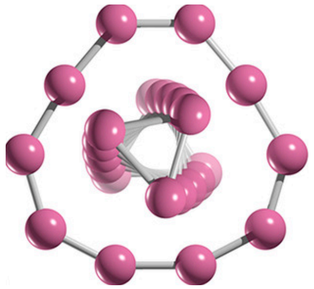
Research



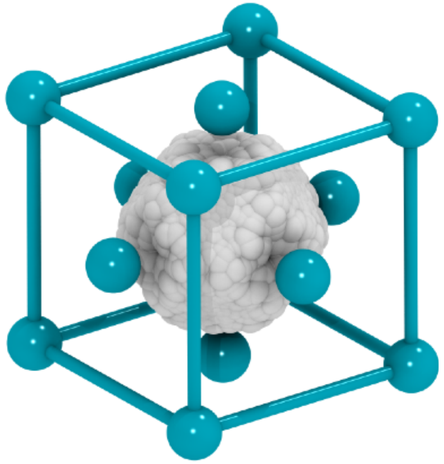


Applications

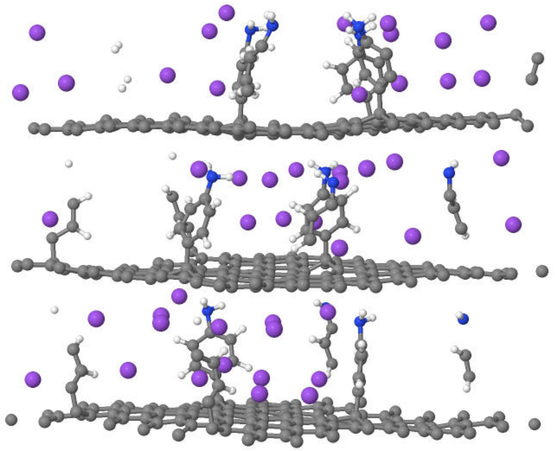
Spectroscopy



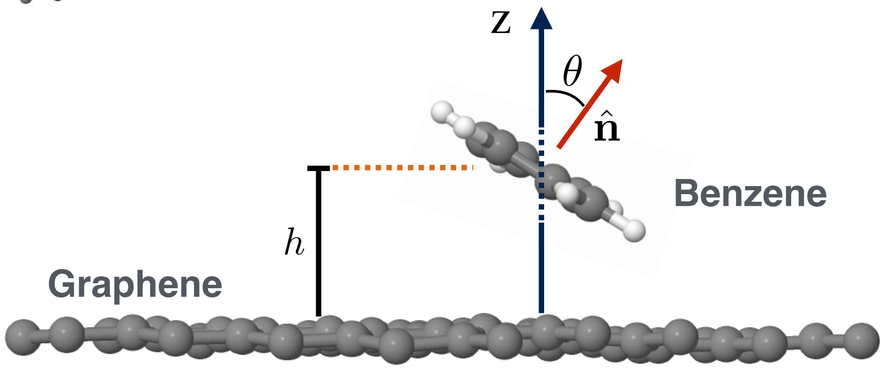
Diffusion



Batteries

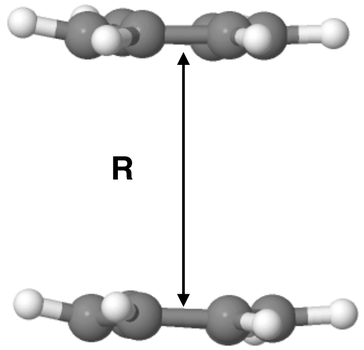


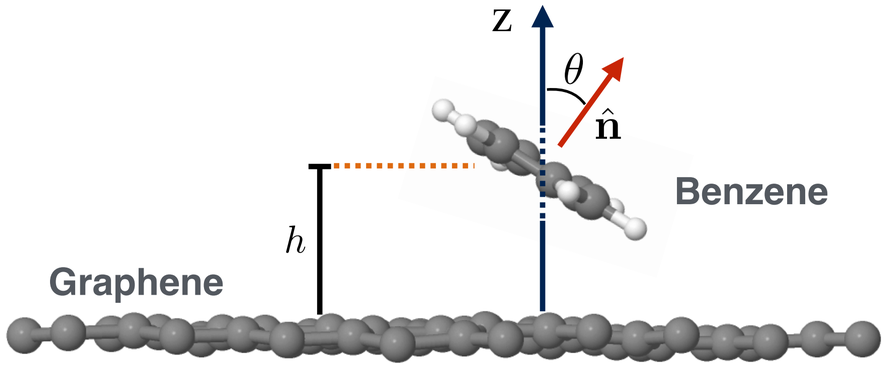
Dispersion Interactions

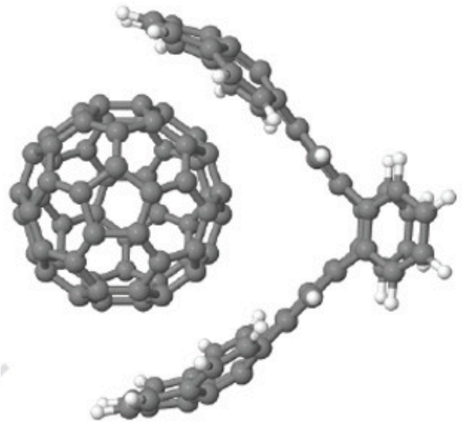


Applications

Dispersion Interactions

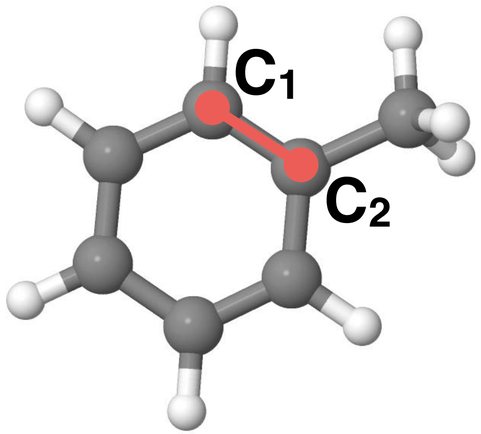


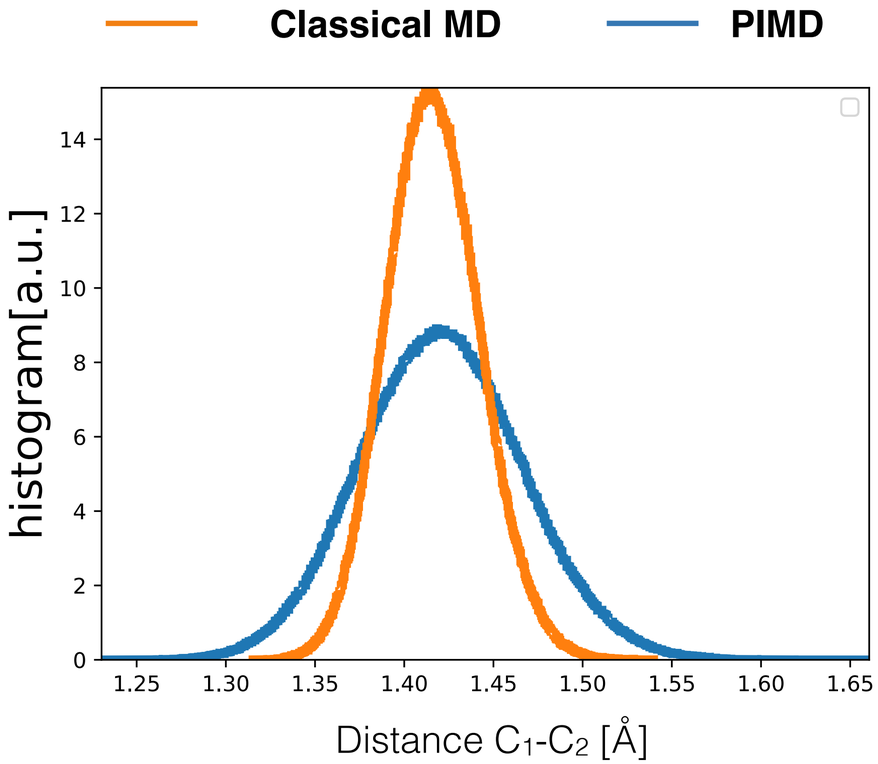




Nuclear Quantum Effects

Molecular bond delocalization during MD simulations





Quantum interatomic *dilation*

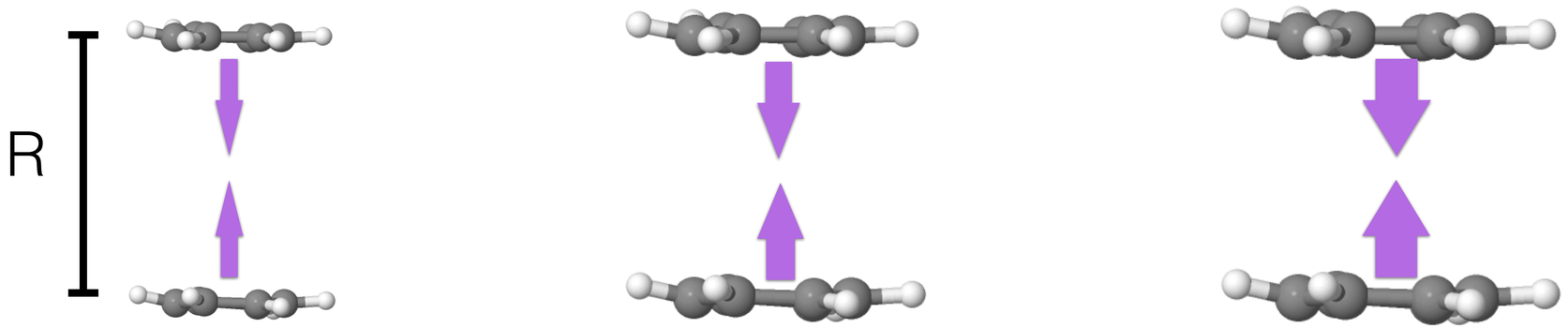
HES, V. Vassilev-Galindo, S. Chmiela, K.-R. Müller, A. Tkatchenko *Nat. Commun.*, 12, 442 ***(2021)***

Nuclear Quantum Effects: van der Waals interaction

$$E^{(2)}_{vdW} = -\frac{C_6^{AB}}{R_{AB}^6} \quad \Rightarrow \quad C_6^{AB} = \frac{3\hbar}{\pi}\int_0^\infty \alpha_A(i\omega)\alpha_B(i\omega)d\omega \quad \Rightarrow \quad \alpha \sim V^b$$

$b = 7/3$

Fedorov *et al.*
PRL **121**, 183401, (2018)



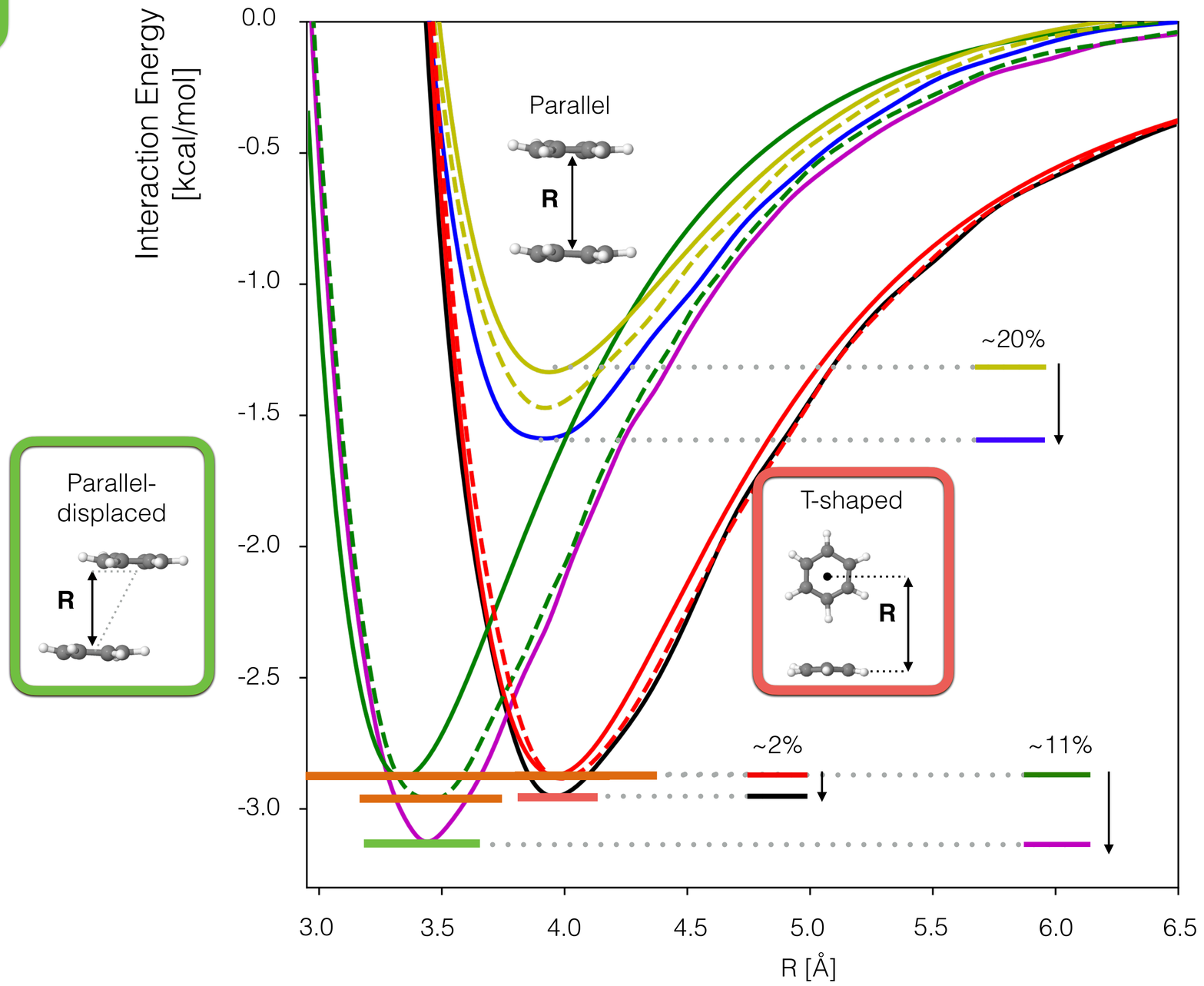
Quantum interatomic *dilation*

HES *et al. Nat. Commun.*, 12, 442 (**2021**)
HES *et al. Nat. Commun.*, 13, 3733 (**2022**)
Chmiela *et al. Sci. Adv. 9, eadf0873* (**2023**)

Nuclear Quantum Effects:
van der Waals interaction

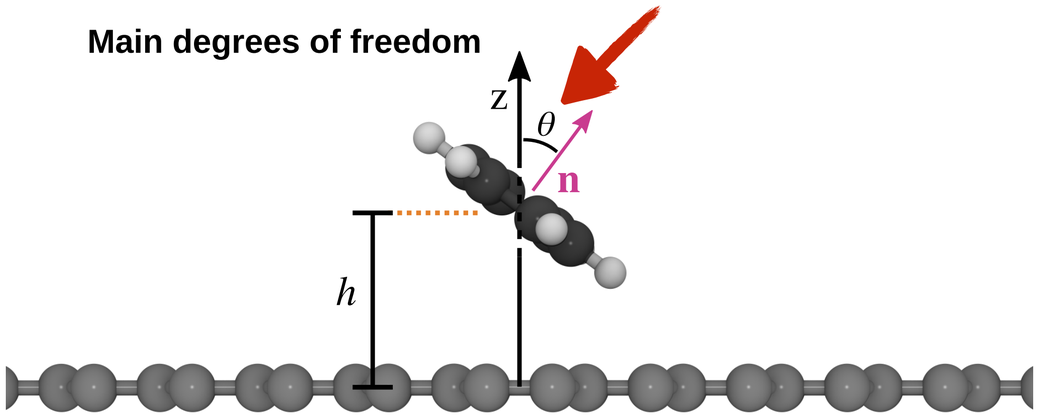
Benzene dimer
non-covalent interaction

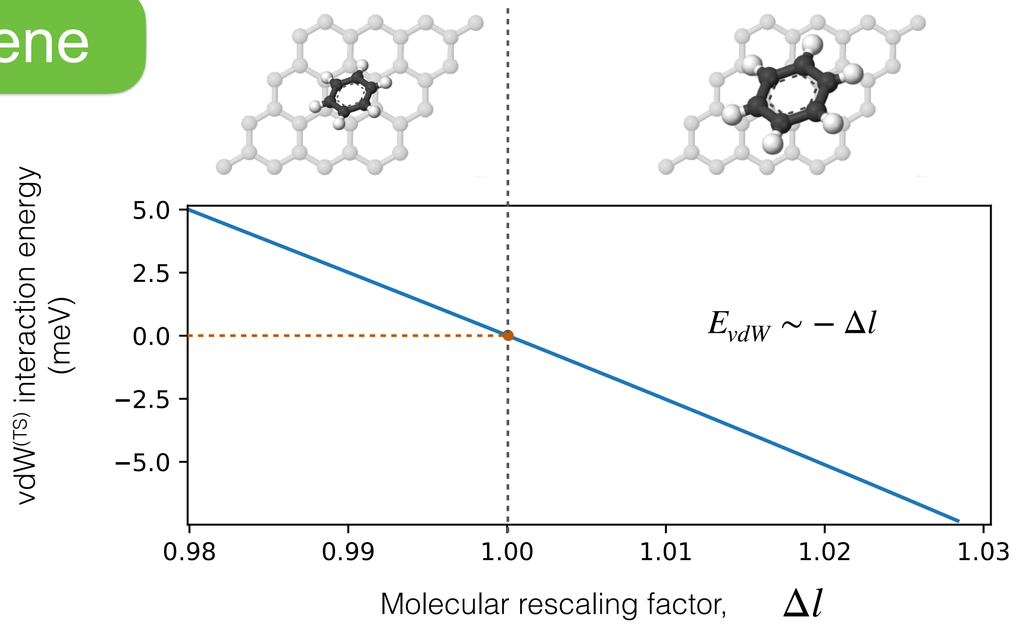
$$E_{vdW} \overset{!}{\sim} -\frac{V_A^b * V_B^b}{R_{AB}^6}$$



HES *et al. Nat. Commun.*, 12, 442 (***2021***)

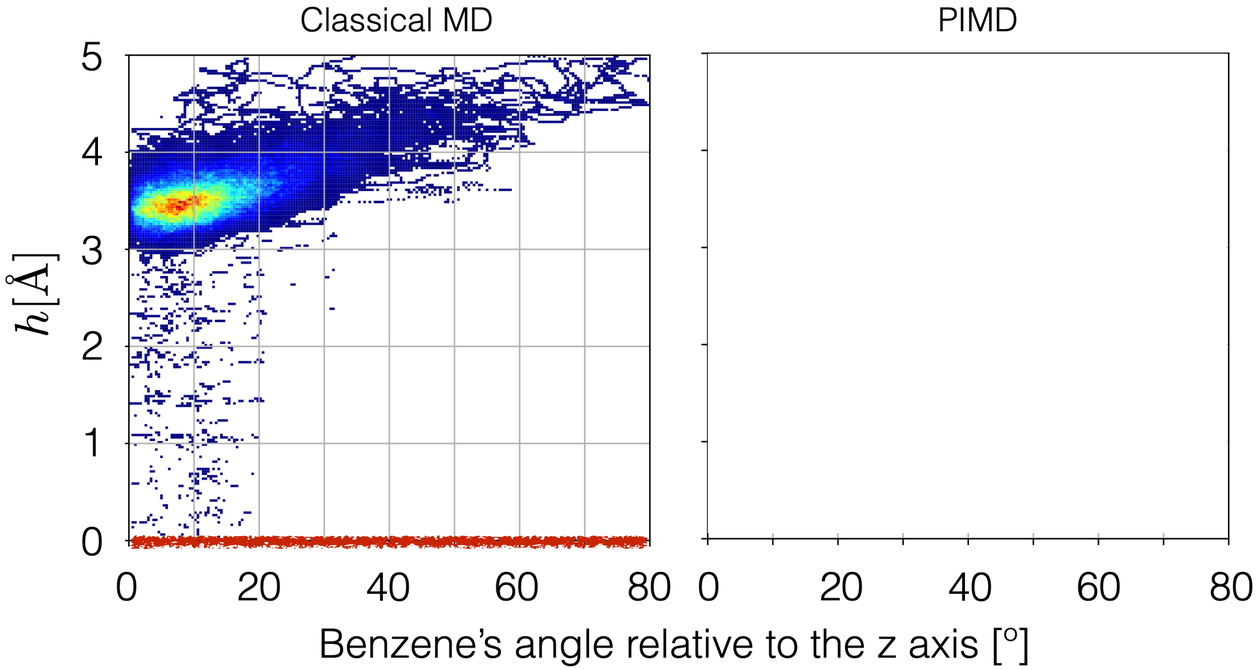
Nuclear Quantum Effects: vdW in benzene@graphene





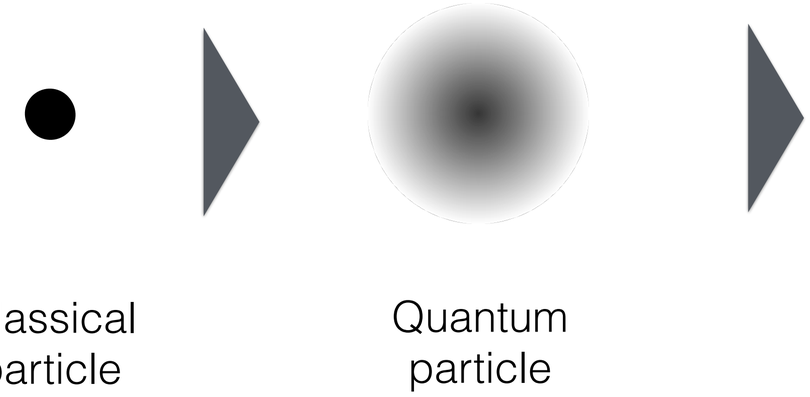
$$E_{vdW} \overset{!}{\sim} -\frac{V_A^b * V_B^b}{R_{AB}^6}$$

Dynamics of the system

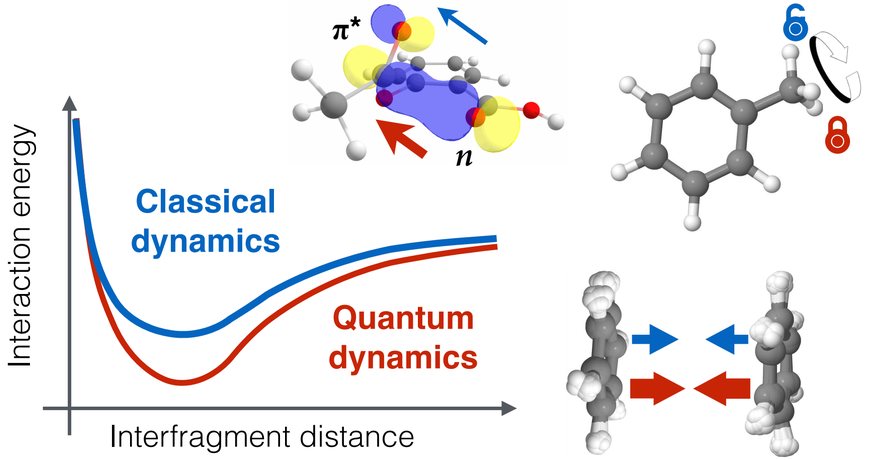


Nat. Commun., 13, 3733 (**2022**)

Dynamics

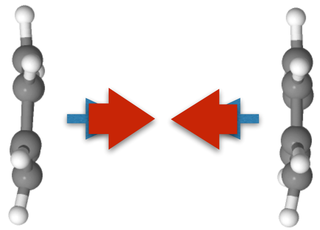


Interactions enhancement



Dynamical strengthening

Thermal fluctuations

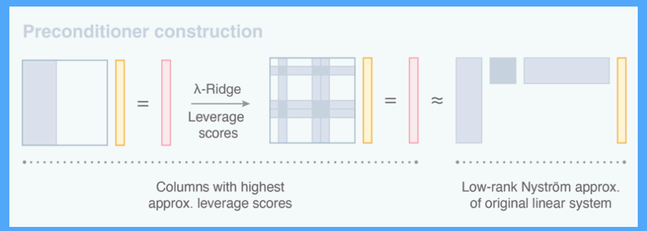


Nat. Commun., 12, 442 (**2021**)
Nat. Commun., 13, 3733 (**2022**)
Sci. Adv. 9, eadf0873 (**2023**)

Summary

Force fields learning

$$F = -\nabla E$$

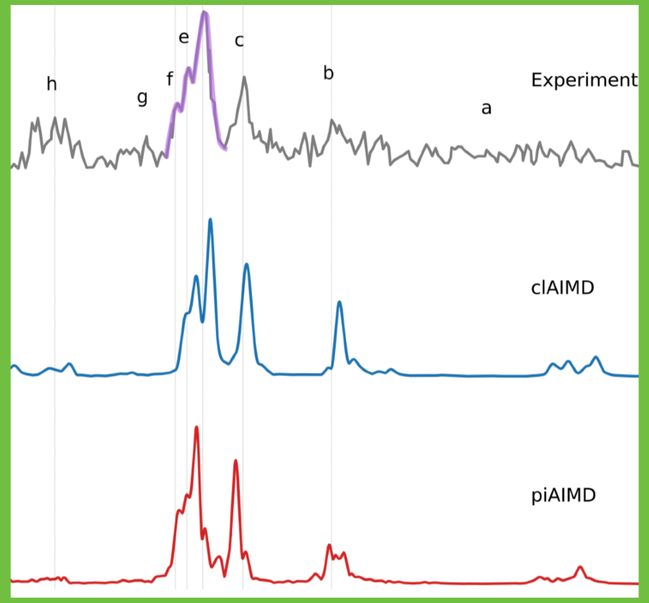


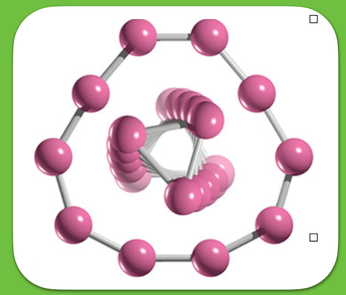
$$\alpha_t = \alpha_{t-1} - \gamma\left[(\mathbf{K} + \lambda\mathbb{I})\alpha_{t-1} - \mathbf{y}\right]$$

Nat. Commun., 13, 3733 (**2022**)

Sci. Adv. 9, eadf0873 (**2023**)

Nuclear quantum effects



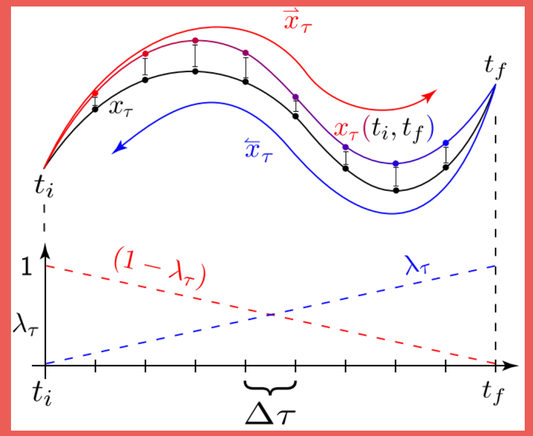


Nat. Commun., 12, 442 (**2021**)

Nat. Commun., 13, 3733 (**2022**)

Under Review (**2023**)

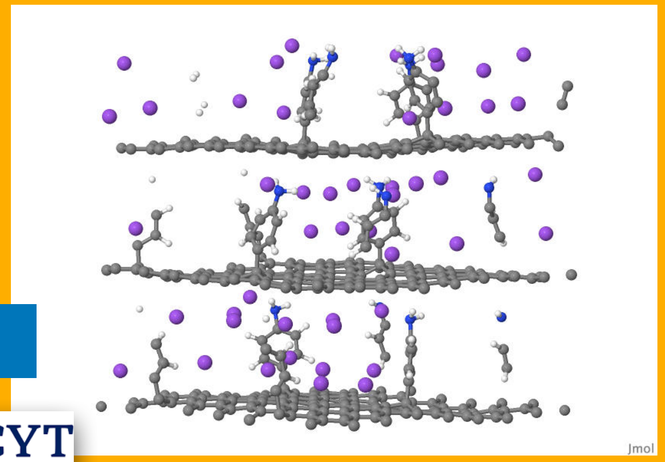
Dynamical processes



Mach. Learn.: Sci. Technol. 3, 025011 (**2022**)

J. Phys. Chem. Lett. 14, 7092 (**2023**)

Battery physics



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CIENCIAS Y TECNOLOGÍAS

Under Review at Google (**2023**)