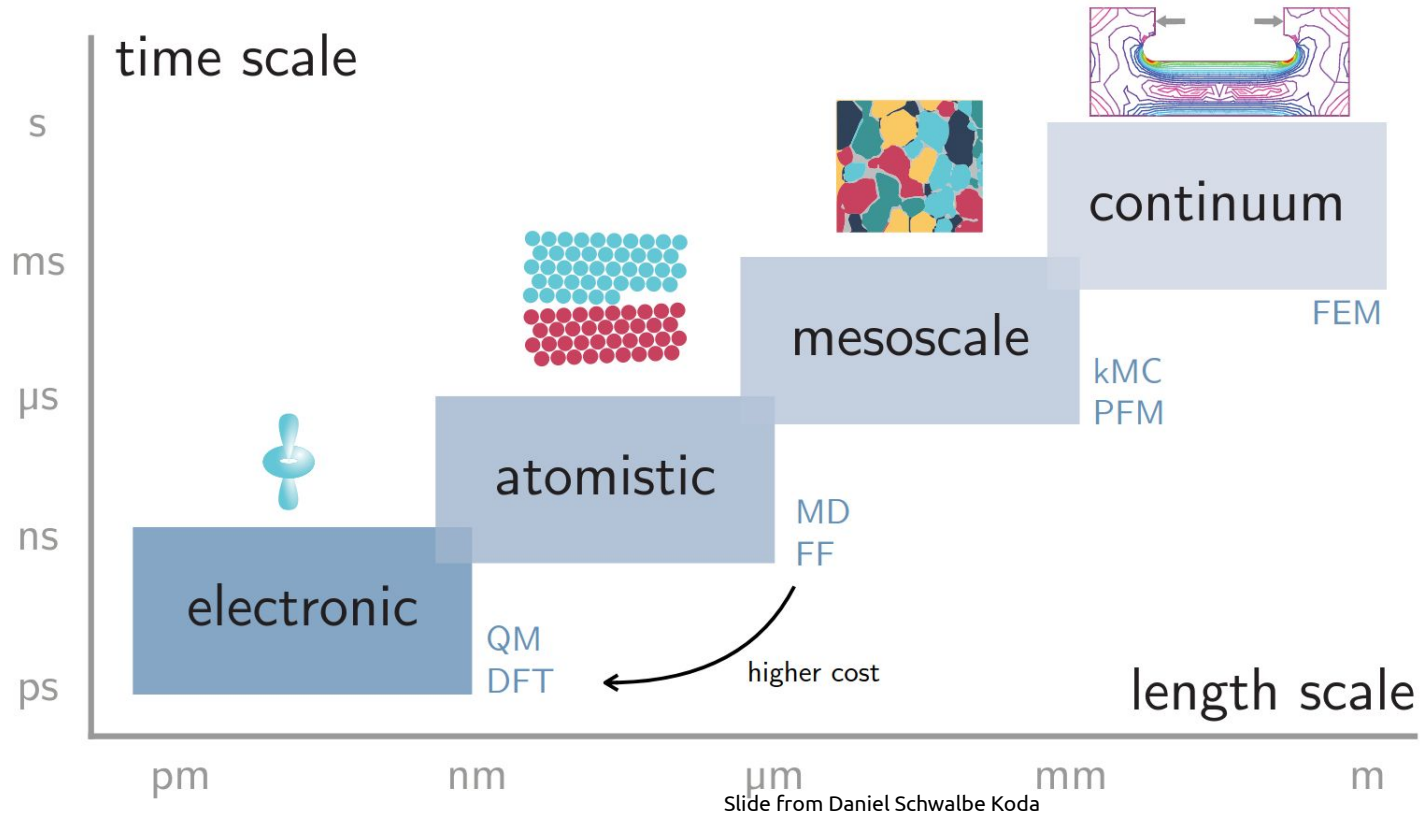
Machine learning for interatomic potentials

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COST NanoSpace – AI in Astrochemistry Training School 2025,
Espoo, Finland

Length and time scales of materials simulations



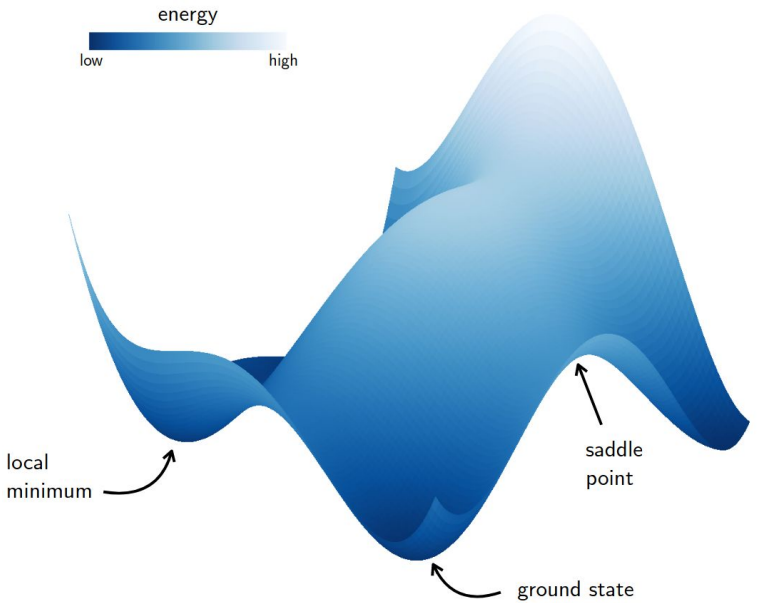
Slide from Daniel Schwalbe Koda

Potential Energy Surface (PES)

Properties of interest can be obtained from a potential energy surface (PES):

- geometries,
- reaction energies,
- mechanical properties
- etc.

The energy from atomistic configurations can be computed from the atomic numbers and coordinates



Slide adapted Daniel Schwalbe Koda

The cost of electronic structure calculations

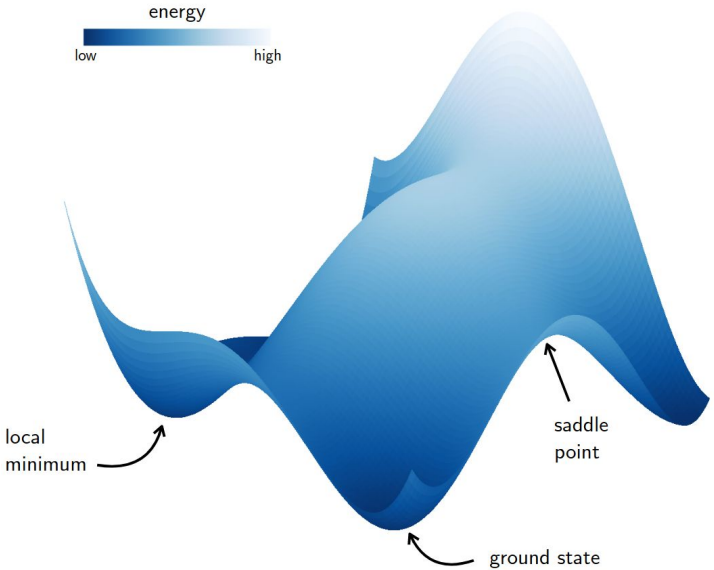
Low level DFT: 100 atoms, 1 node, ~1 hour

- Cubic scaling, N: number of atoms
- High level DFT: 20x
- Coupled-cluster theory

N^3

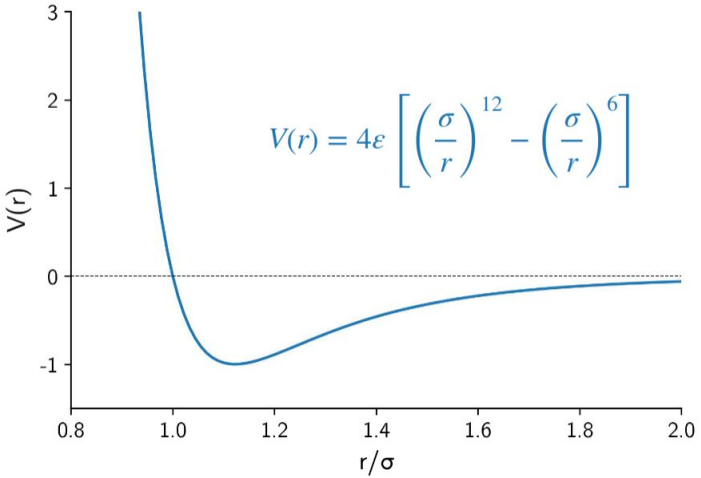
N^4

N^7



Classical potentials

- Use simpler models to describe interatomic interactions
- The computational cost is reduced

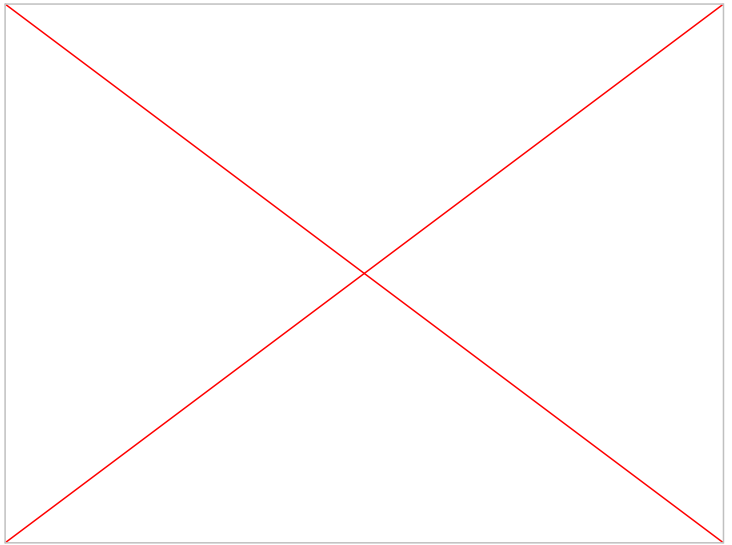


Lennard-Jones potential: a simple example of pair potential

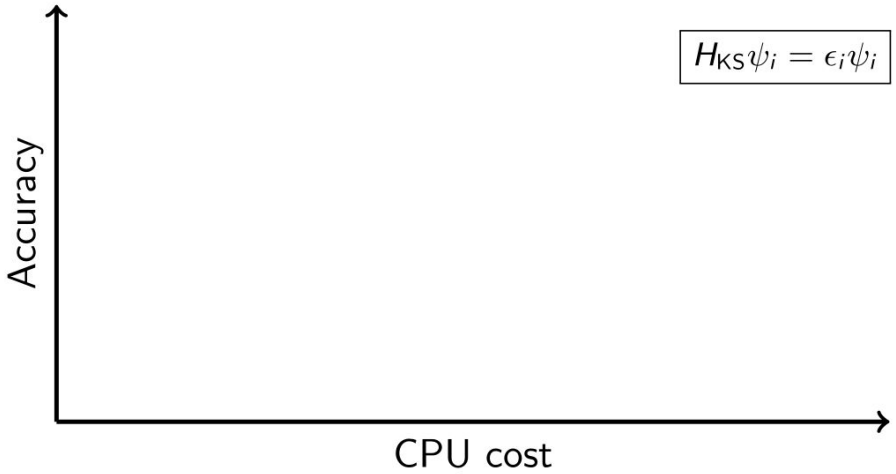
Classical potentials

Longstanding issues:

- Fixed functional form
- Fit to a certain problem
- Many parameters to consider
- Non reactive: no bond breaking and formation



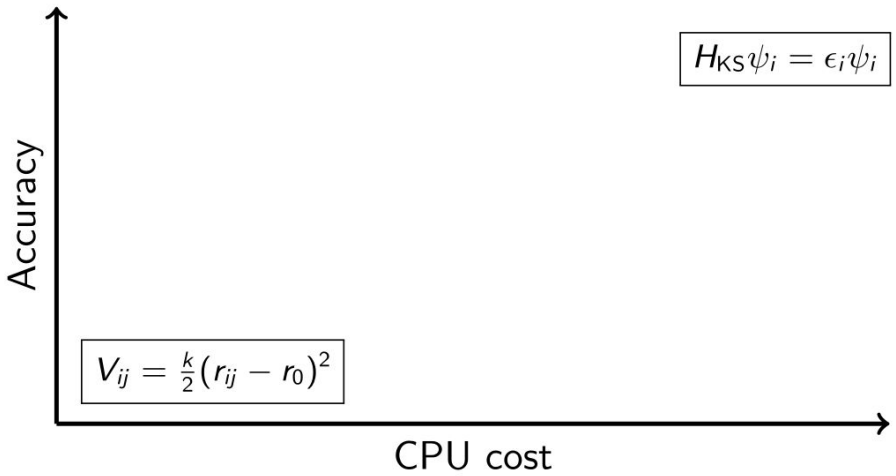
Atomistic simulations



$$H_{KS}\psi_i = \epsilon_i\psi_i$$

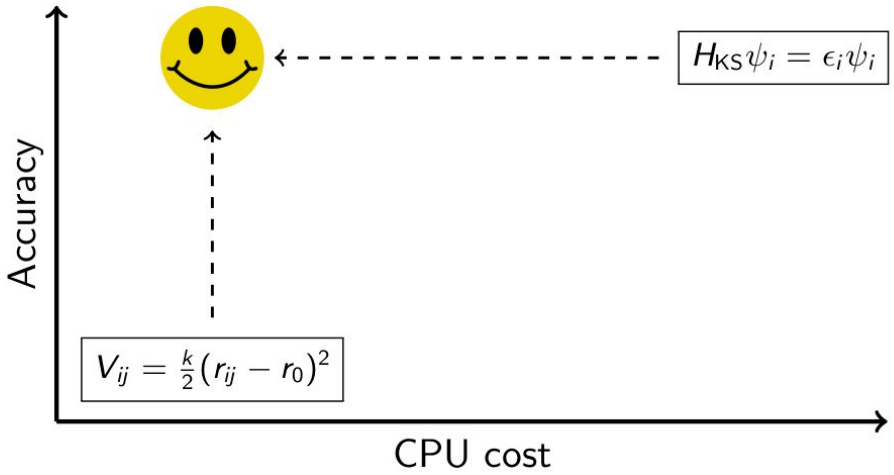
- Quantum mechanical description of atomic interactions is very expensive

Atomistic simulations



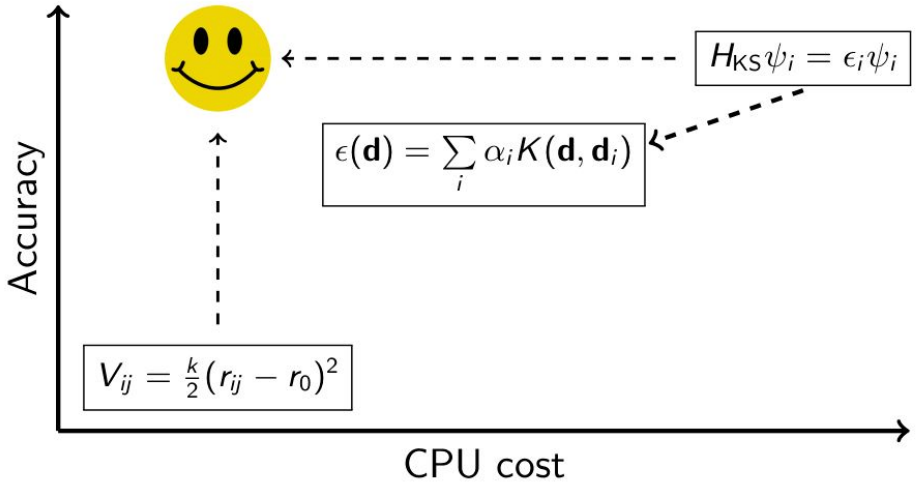
- Quantum mechanical description of atomic interactions is very expensive
- Classical interatomic potentials are not accurate enough

Atomistic simulations: The Dreamscape



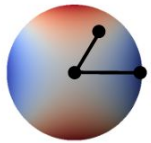
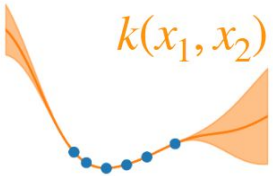
- Quantum mechanical description of atomic interactions is very expensive
- Classical interatomic potentials are not accurate enough

Atomistic simulations: The Dreamscape



- Quantum mechanical description of atomic interactions is very expensive
- Classical interatomic potentials are not accurate enough
- Machine learning interatomic potentials (MLIPs) bring us one step closer to the dreamscape!

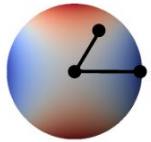
ML methods for interatomic potentials

	Linear Methods	**Kernel/Gaussian Process Regression**	**Neural Networks (NNs)**
			
ℹ️	Polynomial on many-body terms	Computes an explicit similarity between points	"Universal approximator" with non-linear mappings
😄	Simple and fast	Fewer data points (+uncertainty for GPR)	High accuracy
😞	Relies crafting a representation for the inputs	$O(N^3)$ complexity for training for GPR	Large number of trainable parameters

Slide from Daniel Schwalbe Koda

ML methods for interatomic potentials

Linear Methods

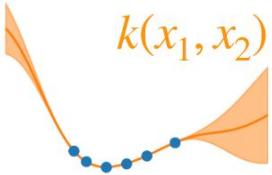


Spectral Neighbor Analysis Potential (SNAP) (Thompson et al.)

Moment Tensor Potentials (MTP) (Shapeev)

Atomic Cluster Expansion (ACE) (Drautz, Kovacs et al.)

Kernel/Gaussian Process Regression



Gaussian Approximation Potentials (GAP) (Bartok, Csanyi et al.)

MLOTF (Li et al.)

FLARE (Vandermause et al.)

sGDML (Chmiela et al.)

Coulomb matrices (Rupp et al.)

Neural Networks (NNs)



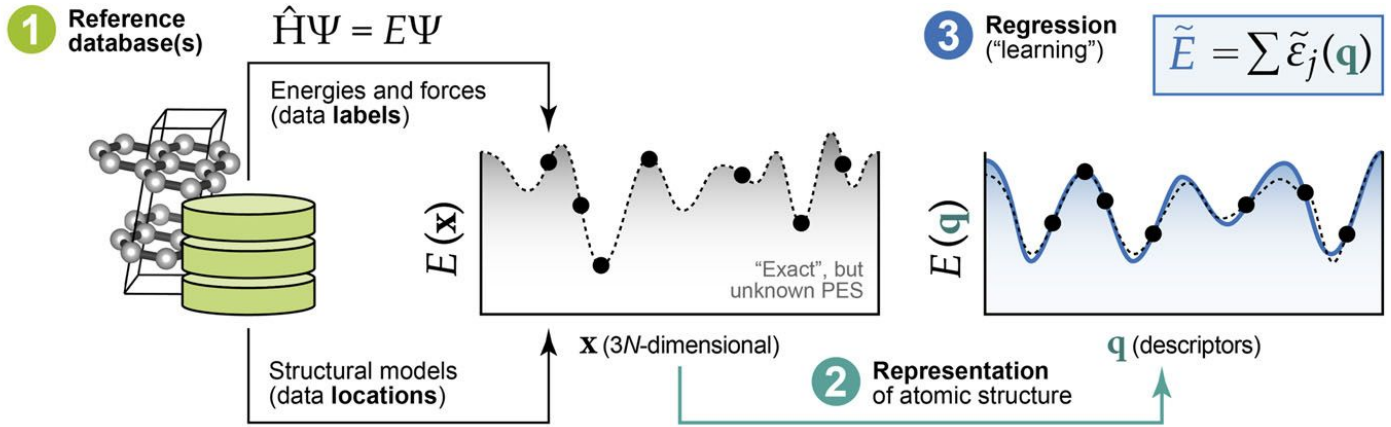
Behler–Parrinello Neural Network (BPNN)

SchNet

NequIP (Neural Equivariant Interatomic Potential)

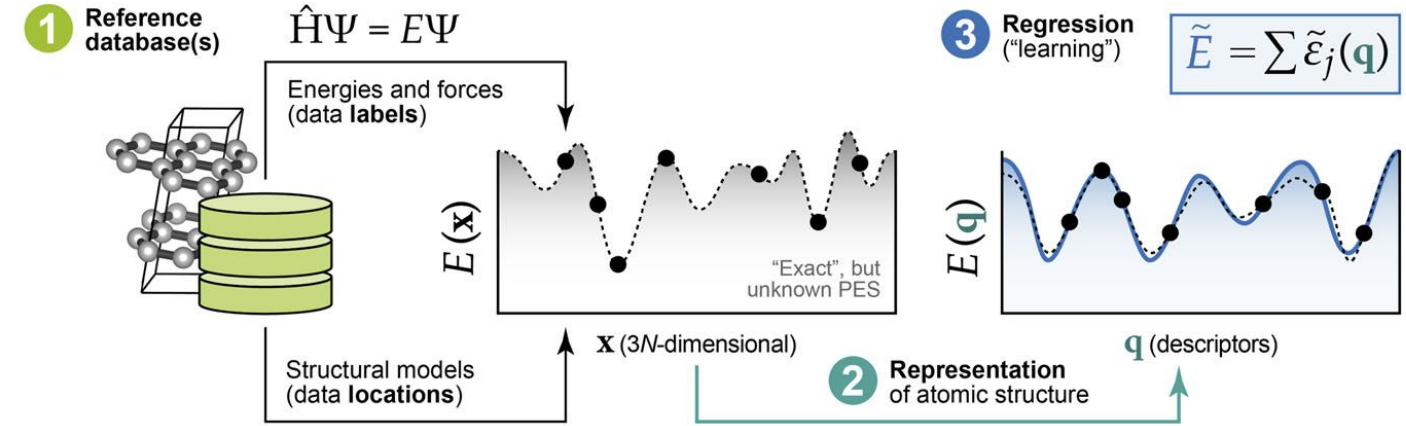
MACE (Message Passing ACE)

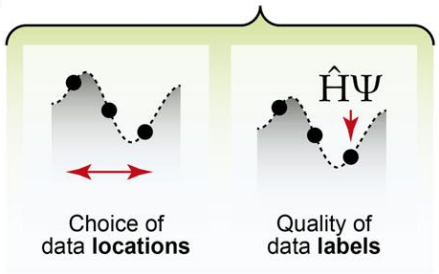
ML for interatomic potentials



Deringer, V. L., Caro, M. A., Csányi, G., Machine Learning Interatomic Potentials as Emerging Tools for Materials Science. *Adv. Mater.* 2019, 31

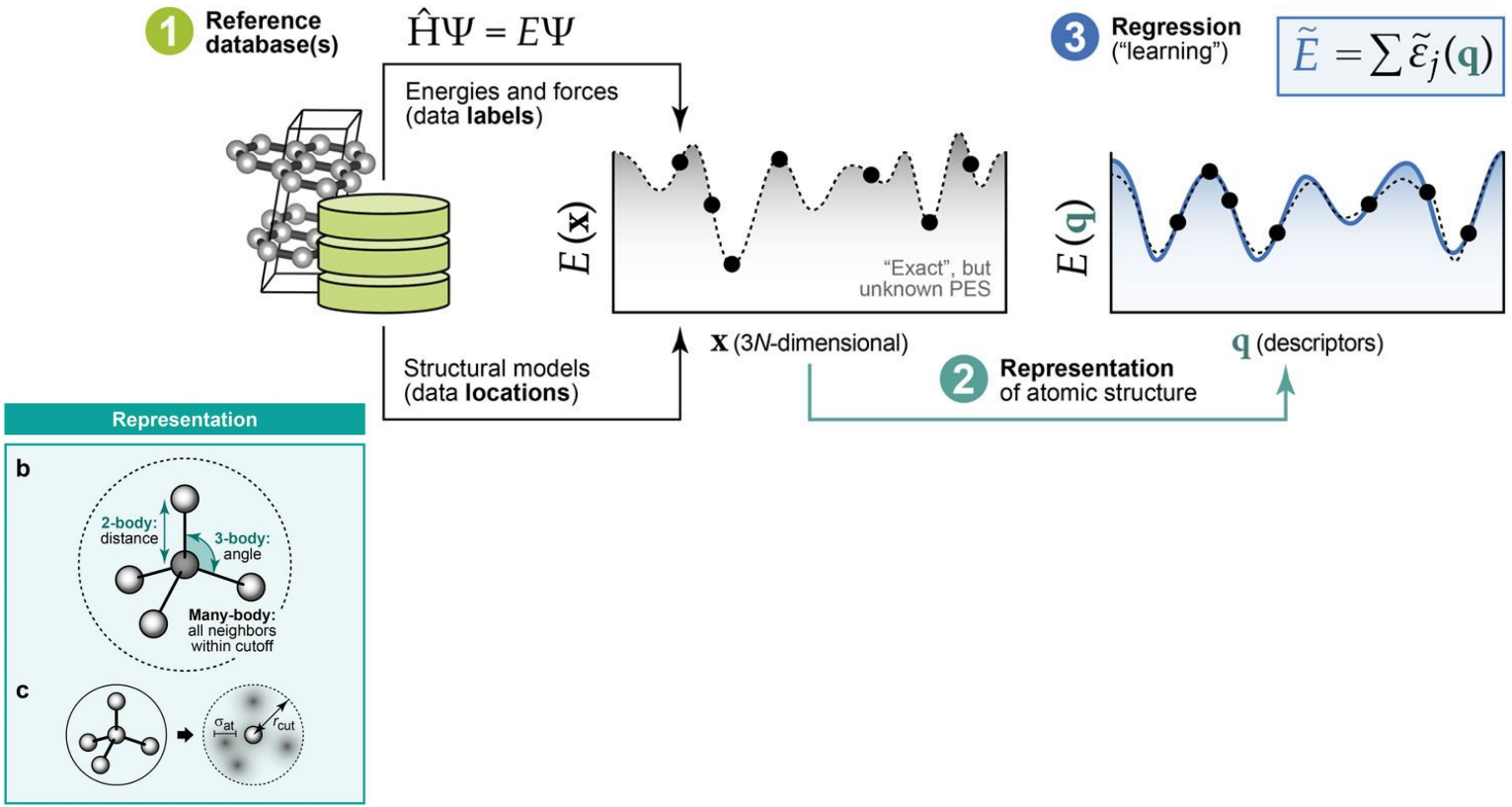
ML for interatomic potentials





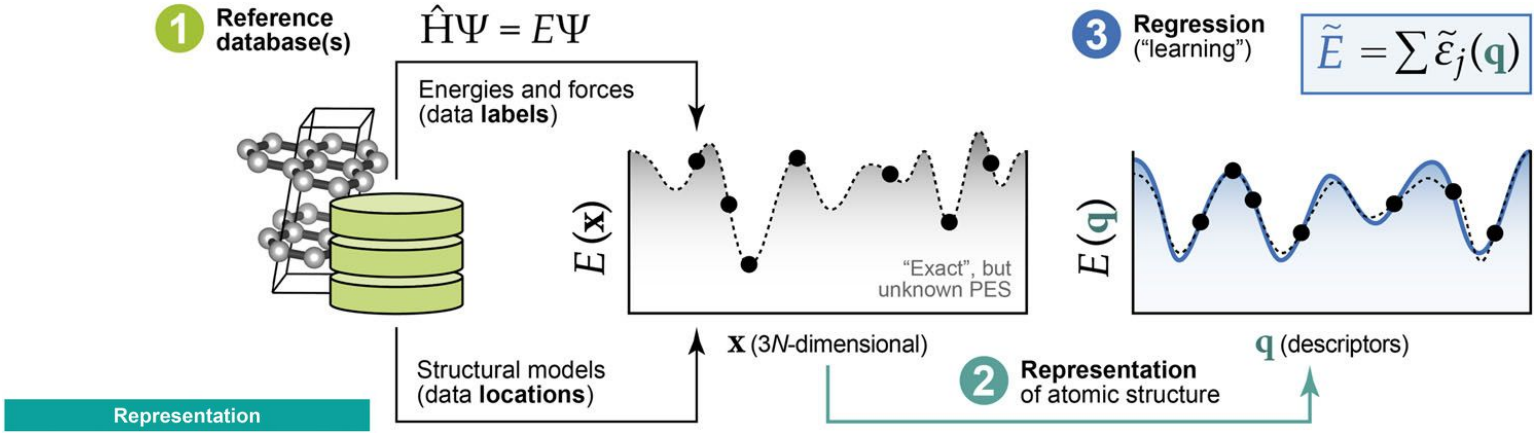
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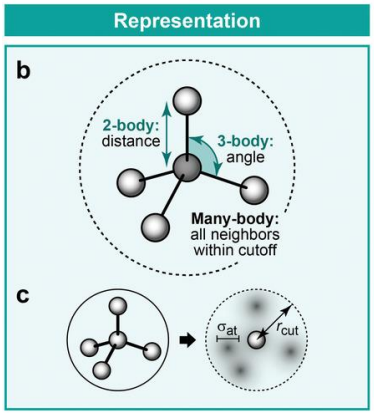
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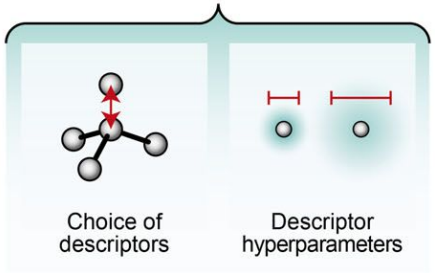


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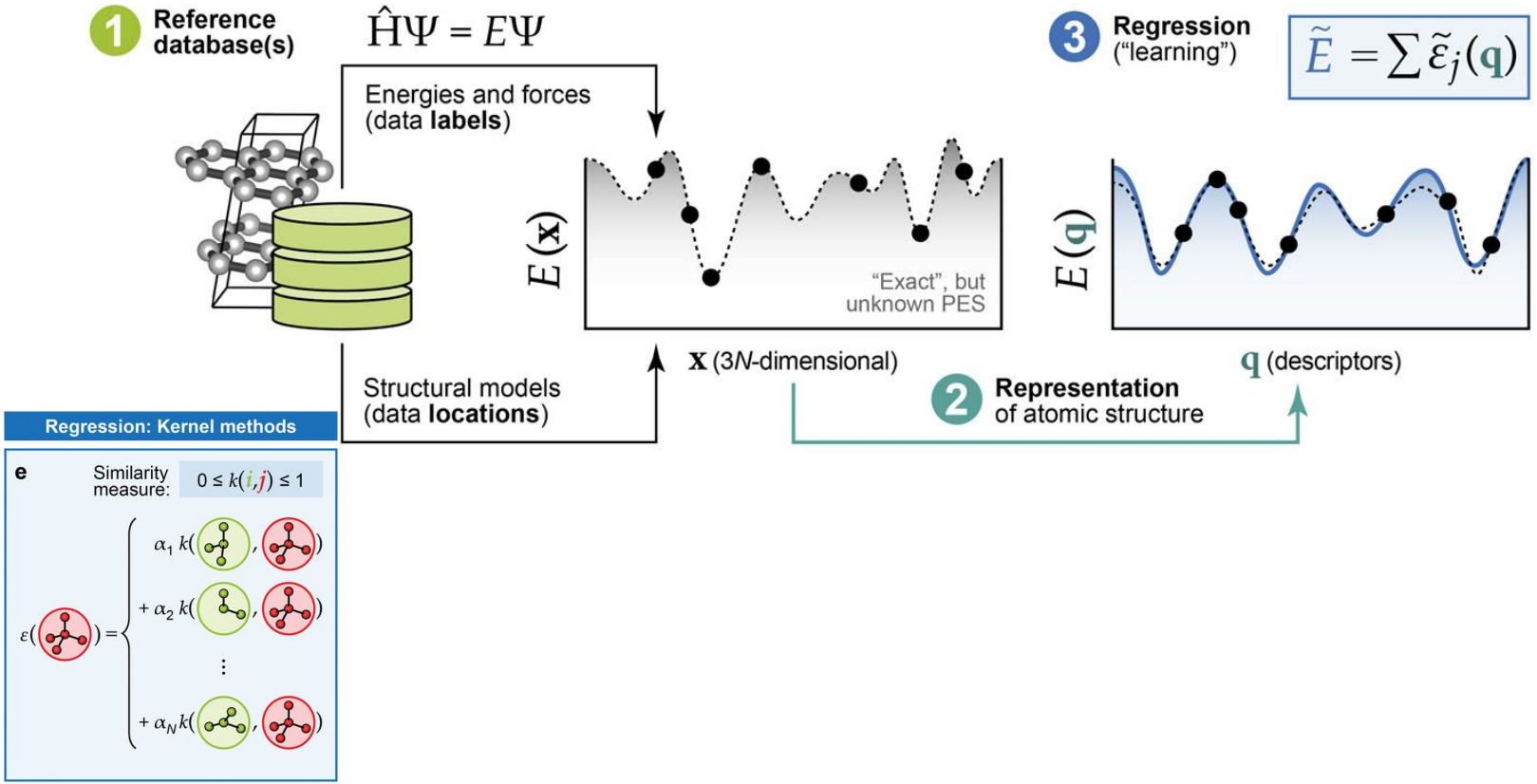






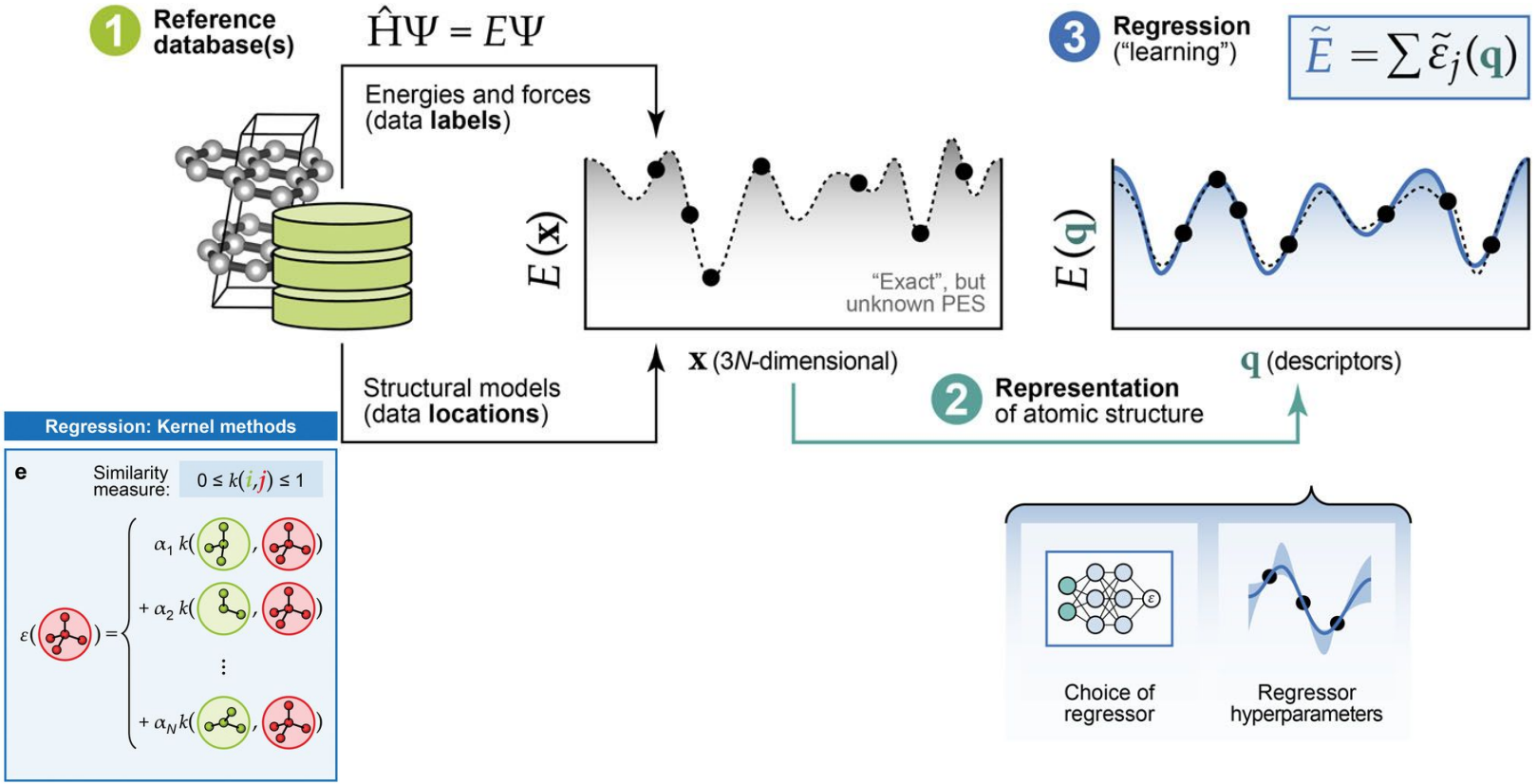
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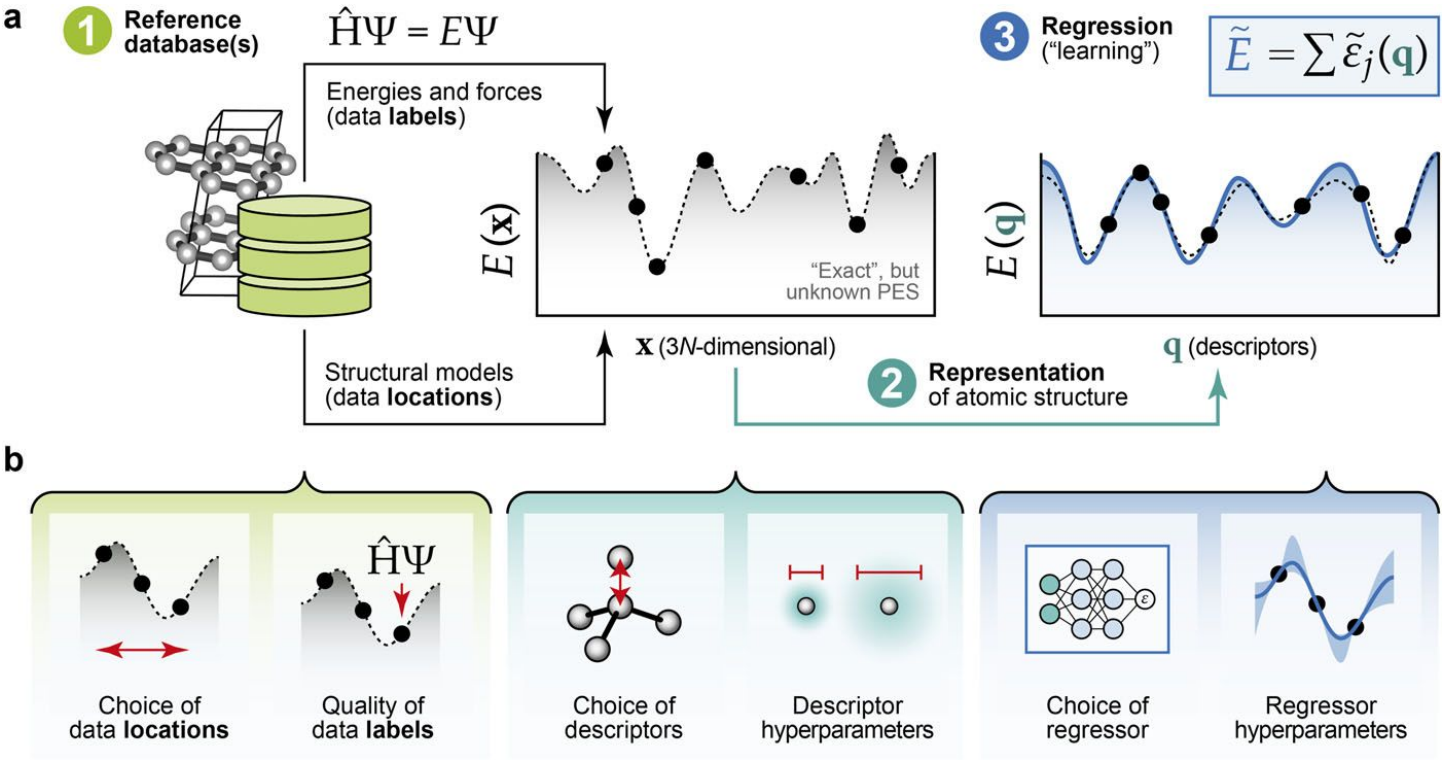
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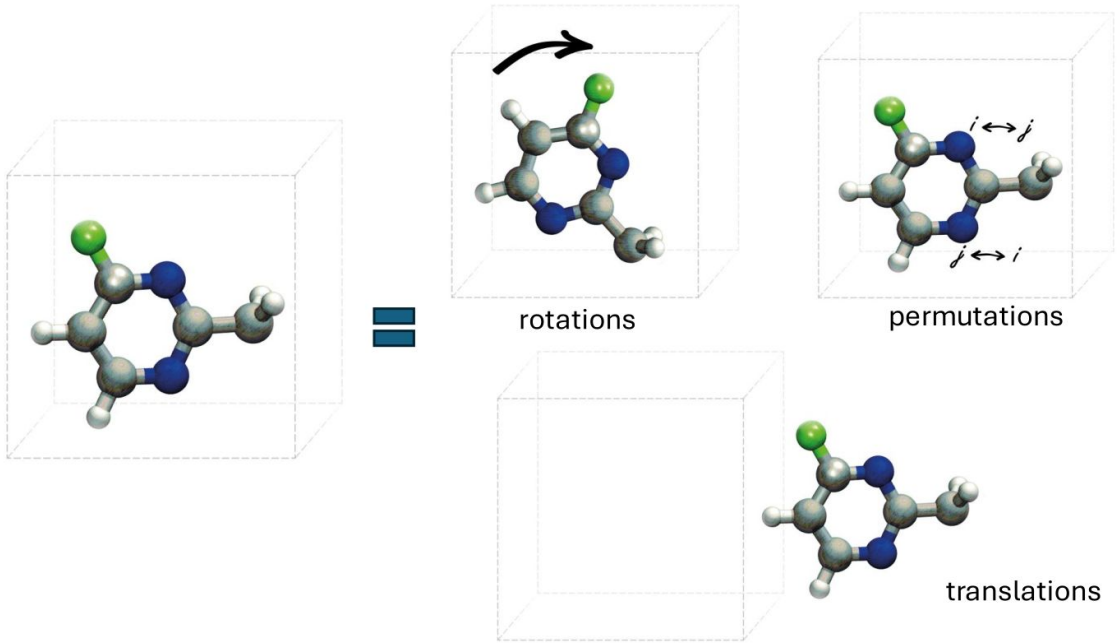
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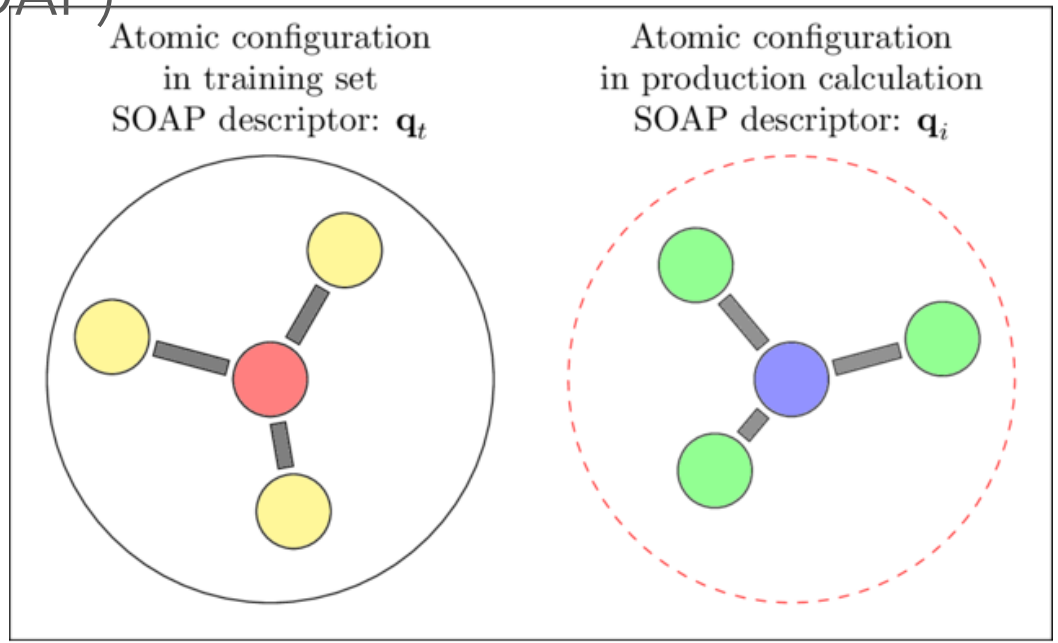
What are atomic representations?

- Mathematical description of atomic environments
- The representation should capture the general symmetries of the atomic structures



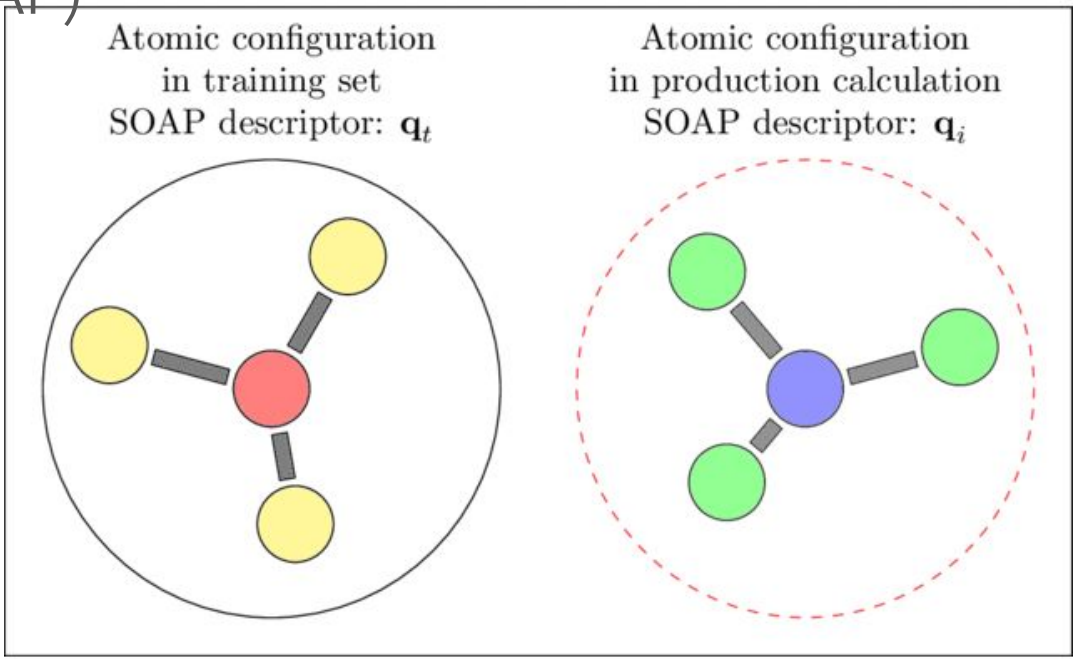
Many-body descriptors

Smooth Overlap of Atomic Positions (SOAP)



Many-body SOAP descriptors

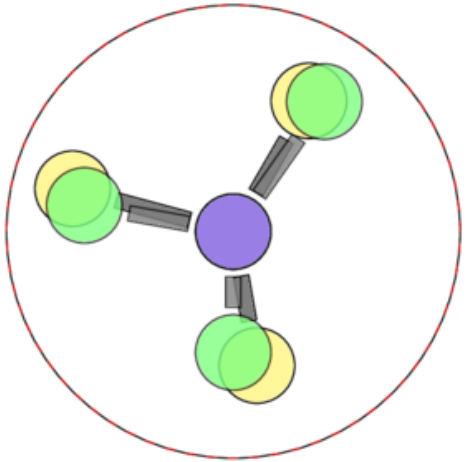
Smooth Overlap of Atomic Positions (SOAP)



Many-body SOAP descriptors

Smooth Overlap of Atomic Positions (SOAP)

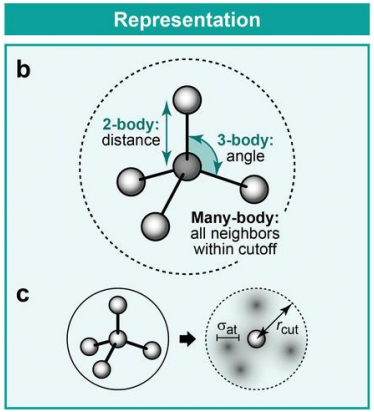
Atomic configuration in training set
SOAP descriptor: $\mathbf{q}_t$



Atomic configuration in production calculation
SOAP descriptor: $\mathbf{q}_i$

Rotationally-invariant similarity between environments is given by the kernel:
$K(\mathbf{q}_t, \mathbf{q}_i) \in [0, 1]$

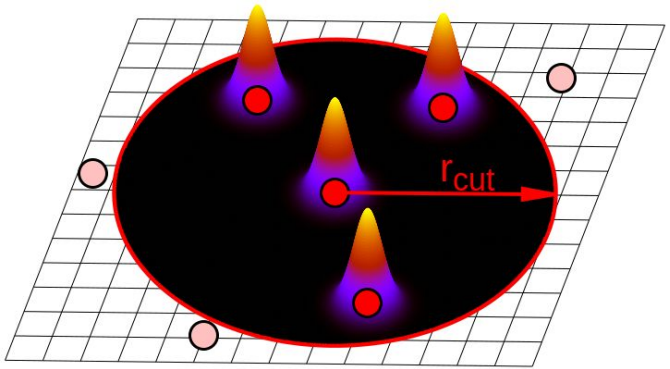
Representation for ML: Smooth Overlap of Atomic Positions



Atomic environment expanded as neighbor density:

$$\rho_i^j(\mathbf{r}) = \exp\left(-\frac{|\mathbf{r}_j - \mathbf{r}_i|^2}{2\sigma_{\text{atom}}^2}\right) \qquad |\mathbf{r}_j - \mathbf{r}_i| < r_{\text{cutoff}}$$

Build a kernel, which is similarity measure:

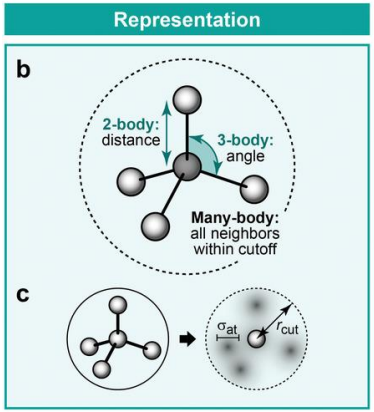


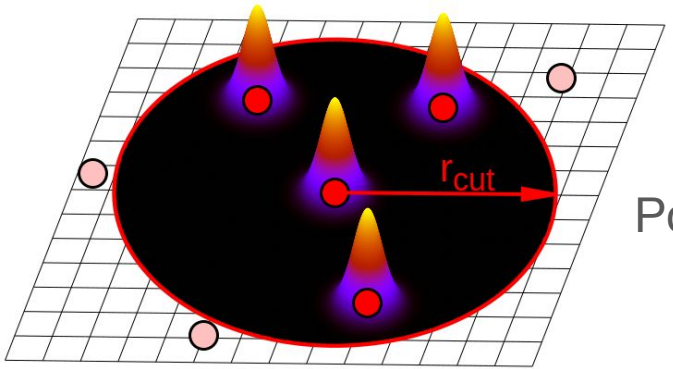
$$k^{(\text{mb})}(i,j) \propto \int \mathrm{d}\hat{R} \left| \int \mathrm{d}\mathbf{r}\, \rho_i^*(\mathbf{r}) \rho_j(\hat{R}\mathbf{r}) \right|^2$$

k = 0 completely different
k = 1 completely identical (up to cutoff)

A. P. Bartók, R. Kondor, and G. Csányi, Phys. Rev. B 87, 184115 (2013)

Representation for ML: Smooth Overlap of Atomic Positions





Atomic environment expanded on a local basis and spherical harmonics:

$$\rho(\mathbf{r}) = \sum_{nlm} c_{nlm}\, g_n(r)\, Y_l^m(\hat{\mathbf{r}})$$

Construct rotationally invariant power spectrum:

$$k^{(\mathrm{mb})}(i,j) \propto \sum_{nn'lmm'} c^i_{nlm}(c^i_{n'lm})^* c^j_{n'lm'}(c^j_{nlm'})^*$$

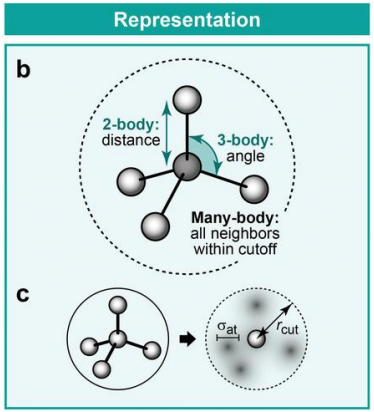
$$= \sum_{nn'l} p_{nn'l}(i)\, p_{nn'l}(j)$$

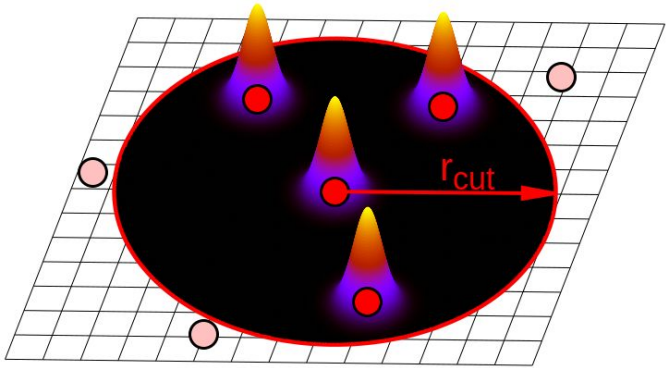
Power spectrum vector is a SOAP descriptor:

$$p_{nn'l}(i) = \sum_m c^i_{nlm}(c^i_{n'lm})^*$$

A. P. Bartók, R. Kondor, and G. Csányi, Phys. Rev. B 87, 184115 (2013)

Representation for ML: Smooth Overlap of Atomic Positions





The SOAP kernel is given as a dot product of the normalized SOAP vectors:

$$k^{(\mathrm{mb})}(i,j) = \mathbf{q}^{(\mathrm{mb})}(i) \cdot \mathbf{q}^{(\mathrm{mb})}(j)$$

A. P. Bartók, R. Kondor, and G. Csányi, Phys. Rev. B 87, 184115 (2013)

Kernel-based ML model

$$\bar{\epsilon}_i = \delta^2 \sum_{t \in T} \alpha_t k(i,t) + e_0.$$

$k(i,t)$ is the kernel

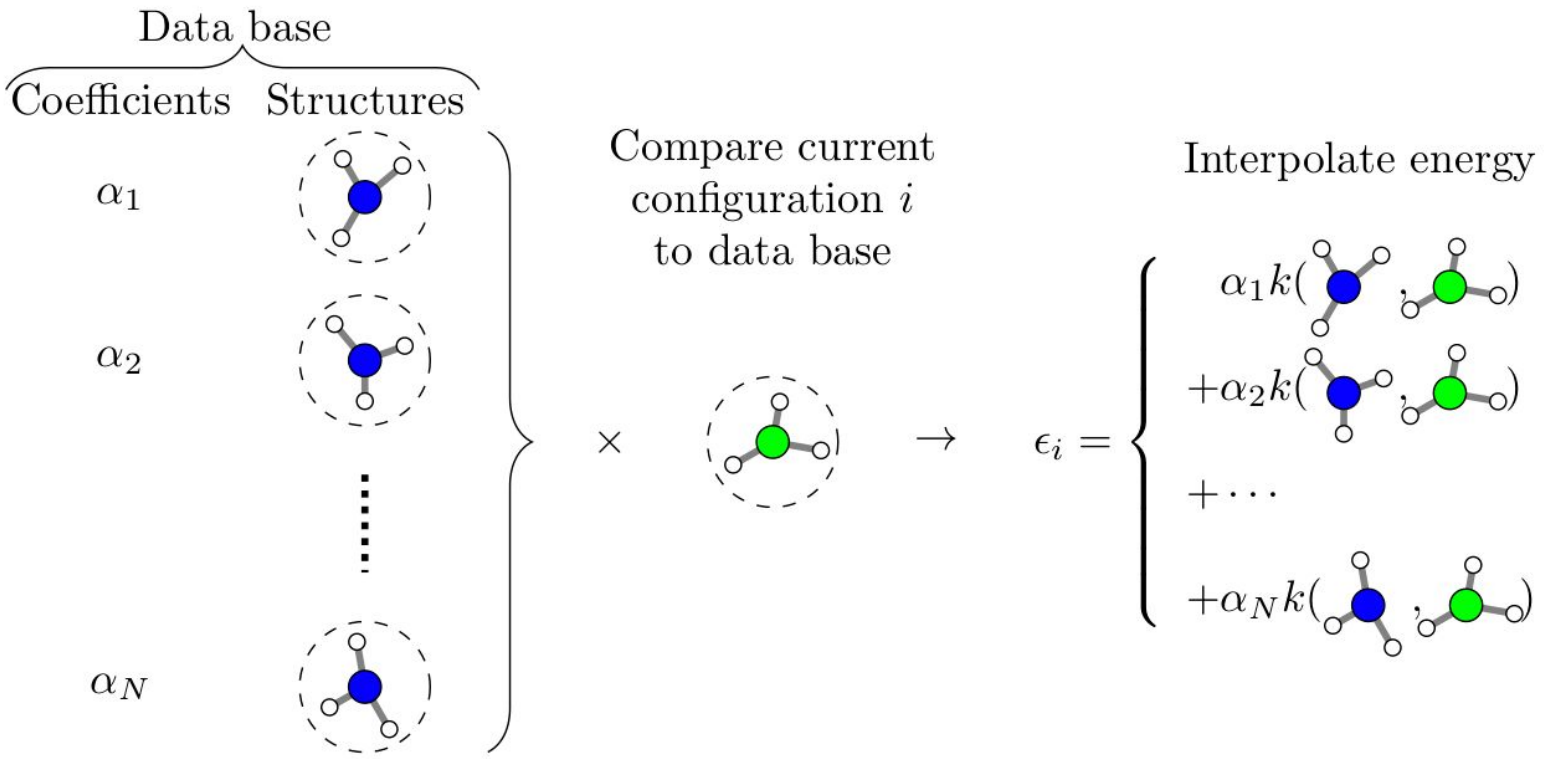
$0 < k(i,t) < 1$

α_t [eV^{-1}] are fitting coefficients (from least-squares regression)

δ [eV^2] determines energy scale (related to std of input data)

e_0 [eV] is the reference atomic energy

Kernel-based ML model



Fitting coefficients

$$\begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_N \end{pmatrix} = \delta^2 \begin{pmatrix} k_{11} & k_{12} & \dots & k_{1N} \\ k_{21} & k_{22} & \dots & k_{2N} \\ \vdots & \vdots & & \vdots \\ k_{N1} & k_{N2} & \dots & k_{NN} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_N \end{pmatrix},$$

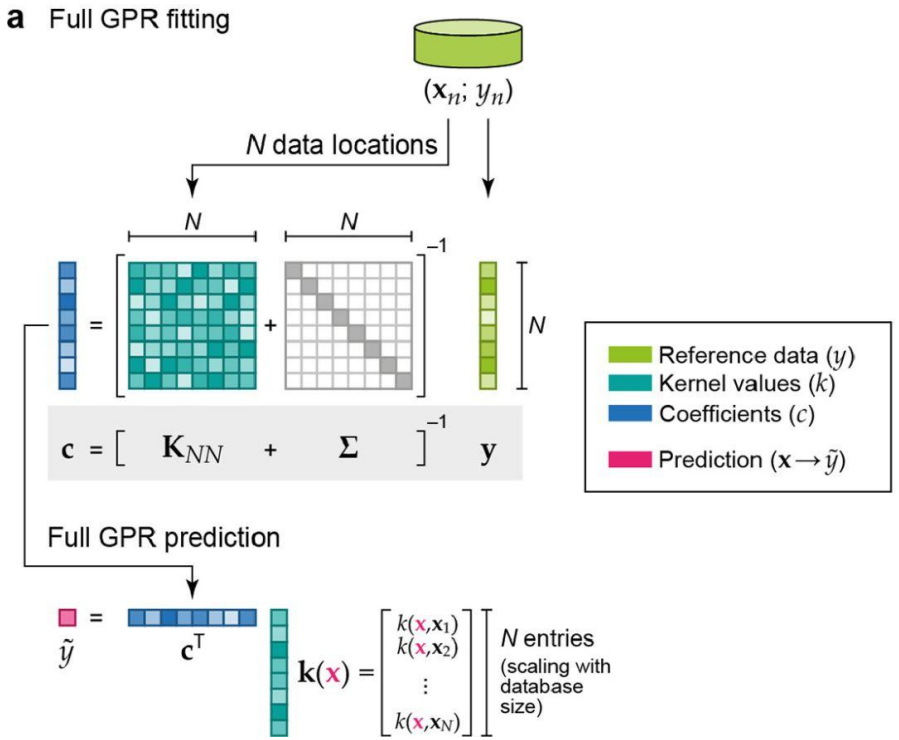
In matrix form:

$$\boldsymbol{\epsilon} = \delta^2 \boldsymbol{K} \boldsymbol{\alpha}$$

The analytical solution is given by:

$$\boldsymbol{\alpha} = \delta^{-2} \boldsymbol{K}^{-1} \boldsymbol{\epsilon}$$

$$\boldsymbol{\alpha} = \underset{\boldsymbol{\alpha} \in \mathcal{R}^N}{\operatorname{argmin}} \| \delta^2 \boldsymbol{K} \boldsymbol{\alpha} - \boldsymbol{\epsilon} \|^2$$



Total energies *vs* local energies

From QC calculations we usually get total energies of the structure:

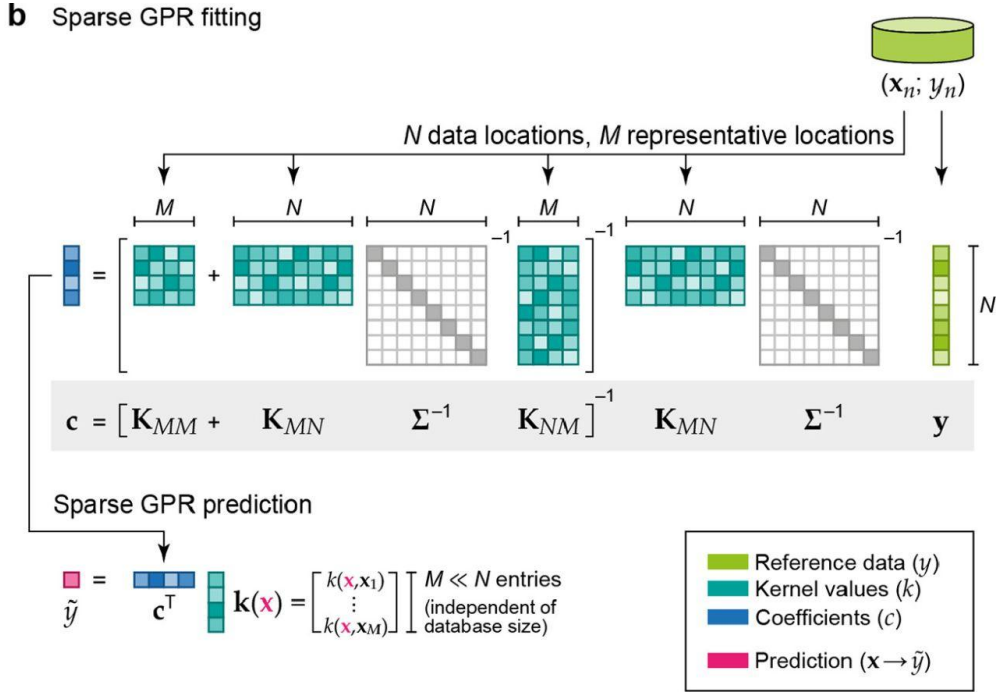
$$E_i = \sum_{j \in T_i} \epsilon_j$$

If we rewrite the total energy in terms of the kernels and fitting coefficients:

$$E_i = \delta^2 \sum_{t_i} \sum_{t} \alpha_t k(t_i, t) = \delta^2 \sum_{t} \alpha_t \underbrace{\sum_{t_i} k(t_i, t)}_{k_s(T_i, t)}$$

The linear least square problem would be expressed as:

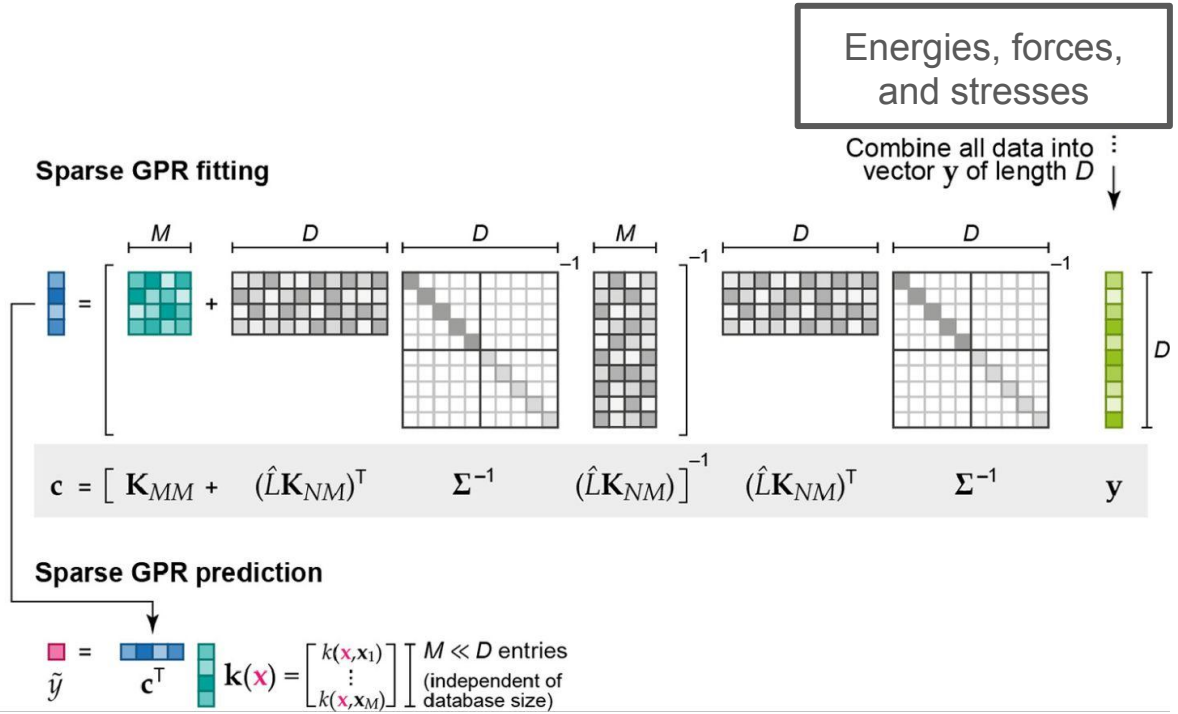
$$\boldsymbol{\alpha} = \underset{\boldsymbol{\alpha} \in \mathcal{R}^N}{\operatorname{argmin}} \| \delta^2 \boldsymbol{K}_s \boldsymbol{\alpha} - \mathbf{E} \|^2$$



The summed kernel matrix is not square anymore and has M x N

Other observables

- We need forces for molecular dynamics
- Computing them directly is impractical
- Learning forces within GAP is the extension of learning energies
- We obtain forces from our reference data, however, the algebra gets much more nasty



Regularization

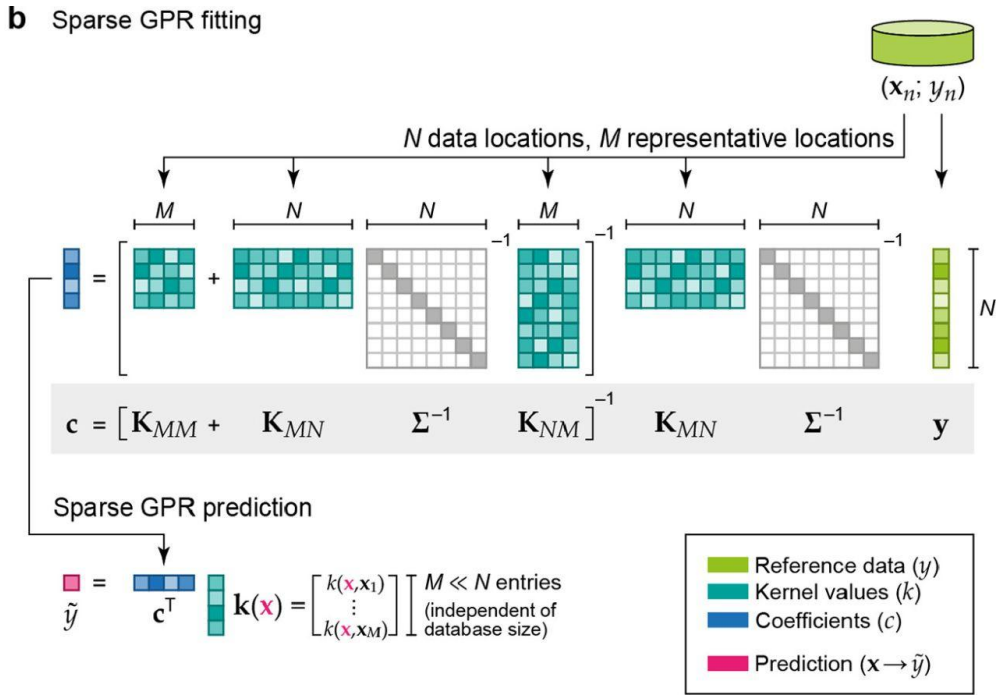
In GAP regularization is done via Tikhonov regularization (L2 regularization)

$$\boldsymbol{\alpha}_{\text{opt}} = \underset{\boldsymbol{\alpha}}{\operatorname{argmin}} \left(\left\| \delta^2 \mathbf{K}\boldsymbol{\alpha} - \boldsymbol{\epsilon} \right\|^2 + \left\| \sigma^2 \boldsymbol{\alpha} \right\|^2 \right),$$

$$\boldsymbol{\alpha} = \delta^2 \left(\delta^4 \mathbf{K}^T \mathbf{K} + \sigma^4 I \right)^{-1} \mathbf{K}^T \boldsymbol{\epsilon}$$

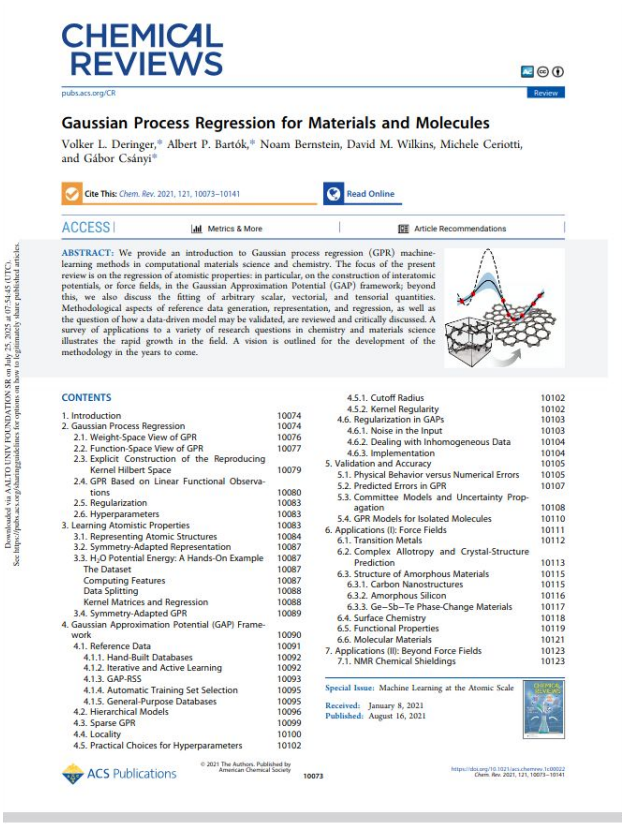
Avoids individual weights from contributing too much and dominating the fit:

- You can use regularization per config. type (e.g., high for melts, low for harmonic distortions)
- You can regularize forces individually



Volker L. Deringer, Albert P. Bartók, Noam Bernstein, David M. Wilkins, Michele Ceriotti, and Gábor Csányi Chemical Reviews **2021**

Gaussian Process Regression



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Review

Gaussian Process Regression for Materials and Molecules

Volker L. Deringer,* Albert P. Bartók,* Noam Bernstein, David M. Wilkins, Michele Ceriotti, and Gábor Csányi*

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ABSTRACT: We provide an introduction to Gaussian process regression (GPR) machine-learning methods in computational materials science and chemistry. The focus of the present review is on the regression of atomistic properties: in particular, on the construction of interatomic potentials, or force fields, in the Gaussian Approximation Potential (GAP) framework; beyond this, we also discuss the fitting of arbitrary scalar, vectorial, and tensorial quantities. Methodological aspects of reference data generation, representation, and regression, as well as the question of how a data-driven model may be validated, are reviewed and critically discussed. A survey of applications to a variety of research questions in chemistry and materials science illustrates the rapid growth in the field. A vision is outlined for the development of the methodology in the years to come.

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Special Issue: Machine Learning at the Atomic Scale

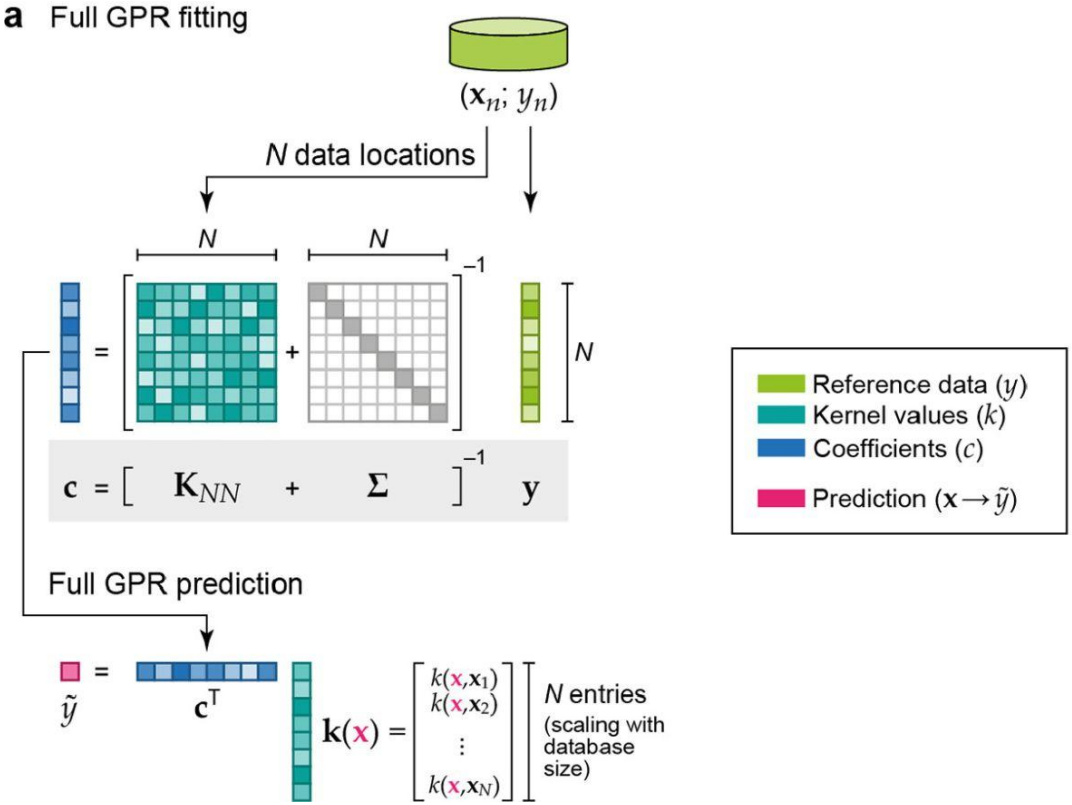
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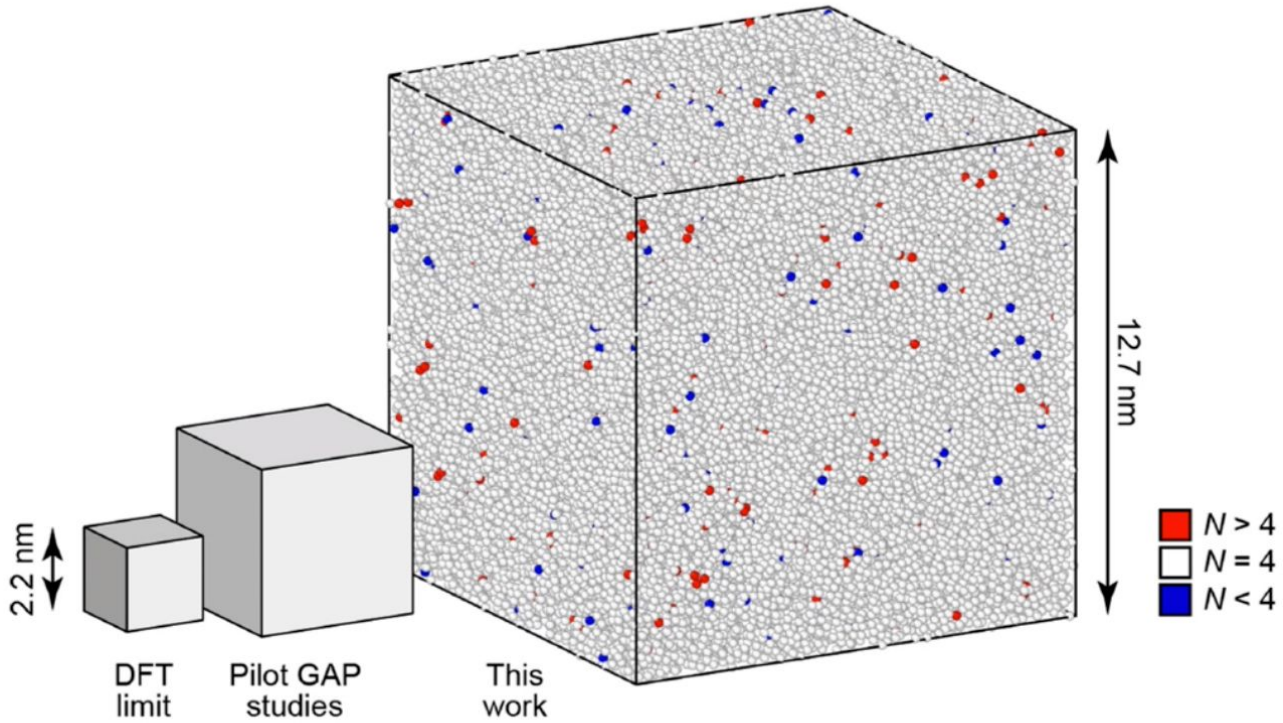
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https://doi.org/10.1021/acs.chemrev.1c00022
Chem. Rev. 2021, 121, 10073−10141



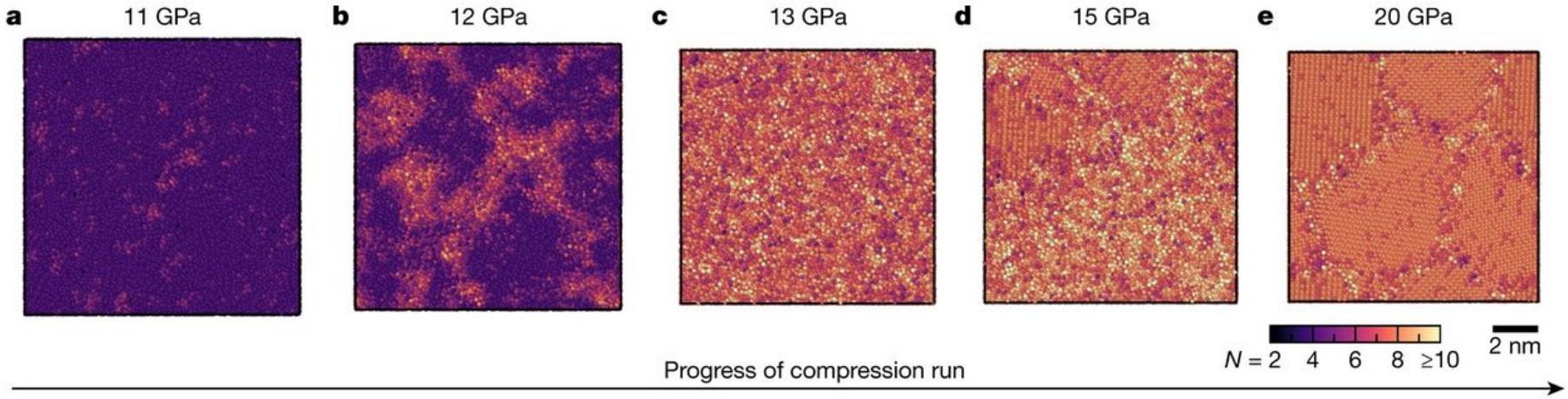
Volker L. Deringer, Albert P. Bartók, Noam Bernstein, David M. Wilkins, Michele Ceriotti, and Gábor Csányi Chemical Reviews **2021**

Larger system, same accuracy, lower cost



Deringer, V.L., Bernstein, N., Csányi, G. *et al.* Origins of structural and electronic transitions in disordered silicon. *Nature* **589**, 59–64 (2021)

Silicon example



Phase transitions in disordered silicon up to crystallization

Deringer, V.L., Bernstein, N., Csányi, G. *et al.* Origins of structural and electronic transitions in disordered silicon. *Nature* **589**, 59–64 (2021)

MLIP safety guide

ML interatomic potentials don’t “know” chemistry!

- They mimic it through data-driven interpolation

ML interatomic potentials don’t “know” physics!

- They mimic it through data-driven interpolation

ML interatomic potentials don’t “know” Schrödinger equation!

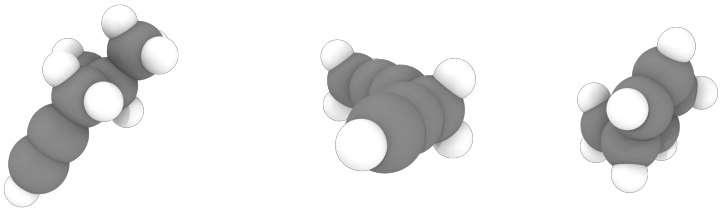
- They mimic it through data-driven interpolation

ML interatomic potentials only “know” about DATA

MLIP safety guide

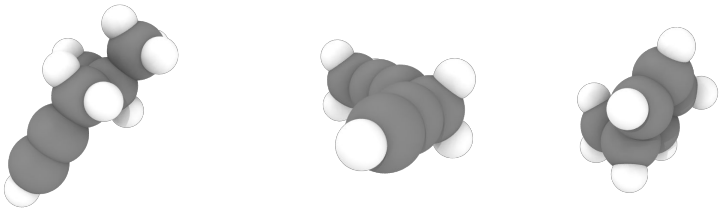
QM9 database contains many C, H, O molecules

Ground-state molecules



Fit GAP using only ground-state molecules

Rattled molecules

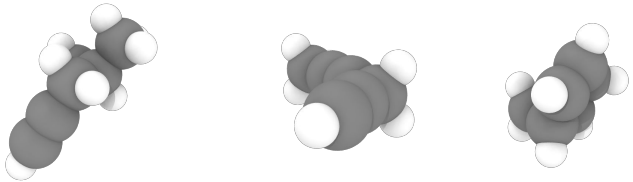


Fit GAP using only rattled molecules

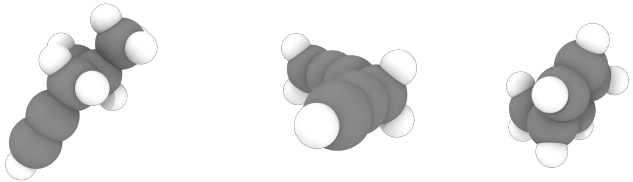
[1]R. Ramakrishnan, P. O. Dral, M. Rupp, and O. A. von Lilienfeld, Scientific Data 1 (2014)

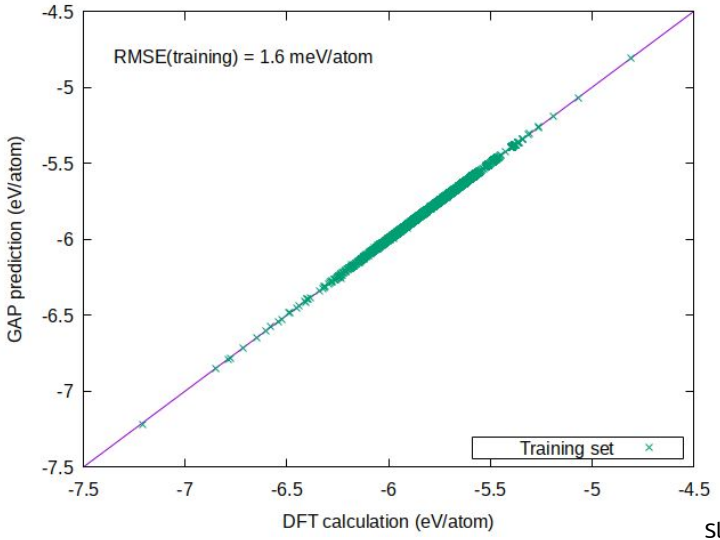
MLIP safety guide

Ground-state molecules



Rattled molecules

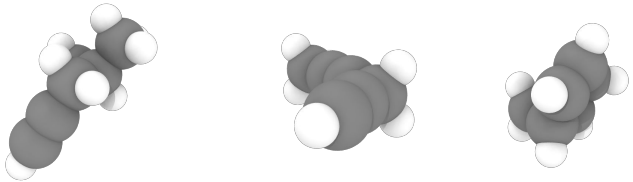


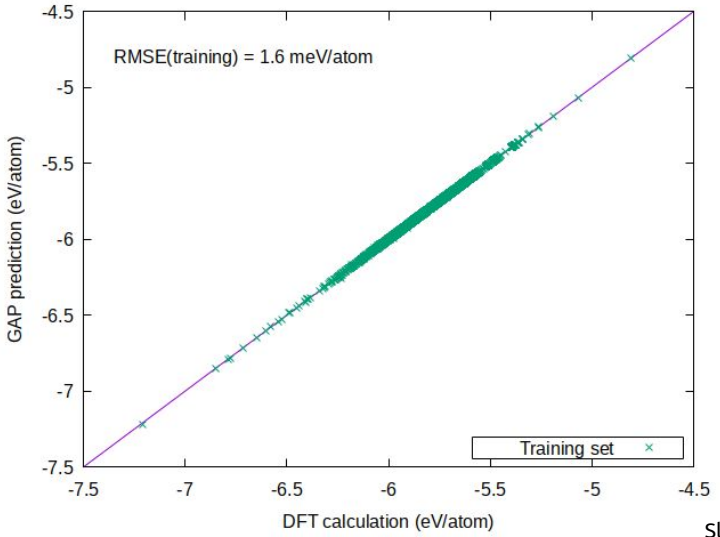


Slide from Miguel Caro

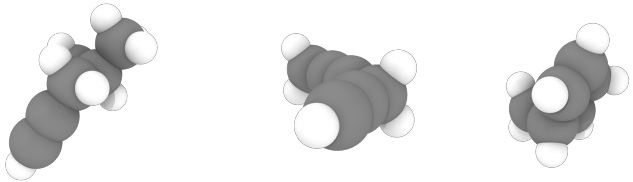
MLIP safety guide

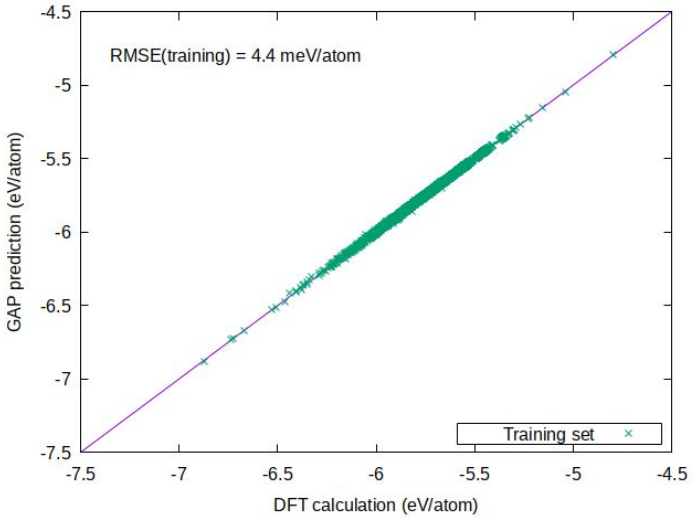
Ground-state molecules





Rattled molecules

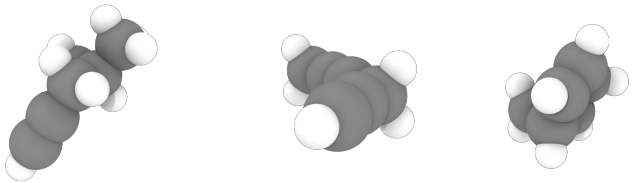




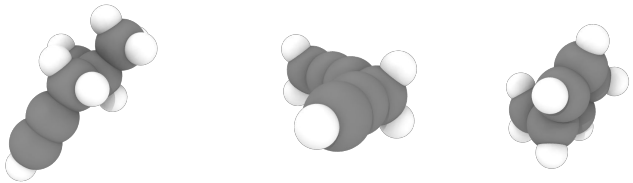
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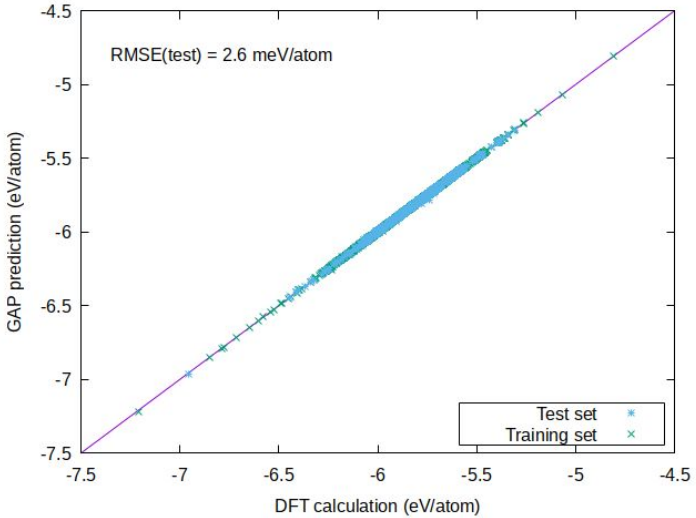
MLIP safety guide

Ground-state molecules



Rattled molecules

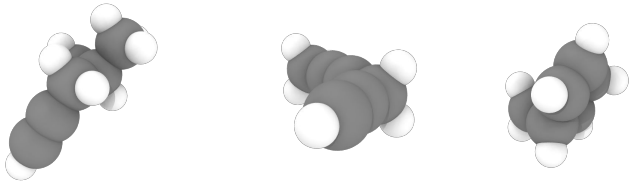


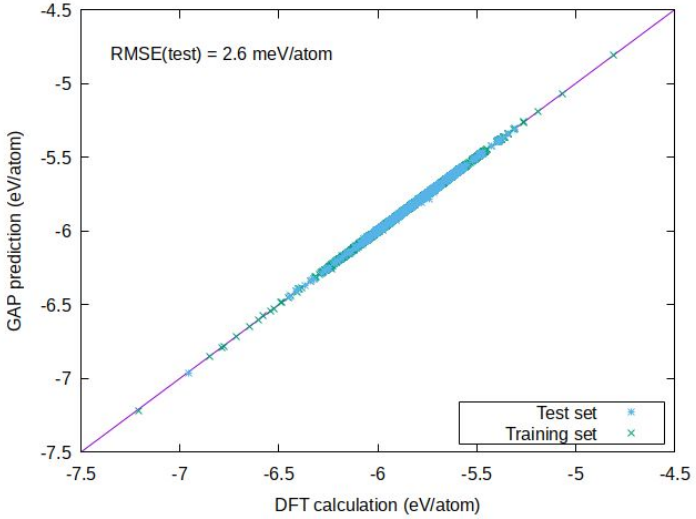


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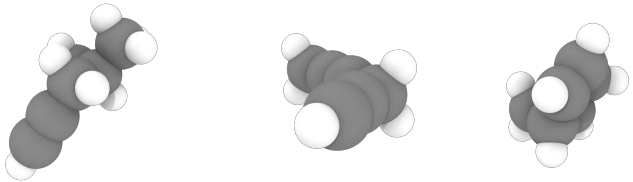
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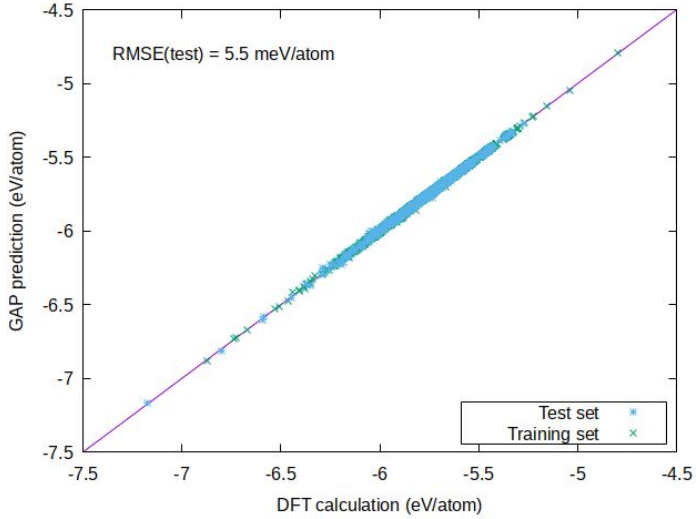
Ground-state molecules





Rattled molecules

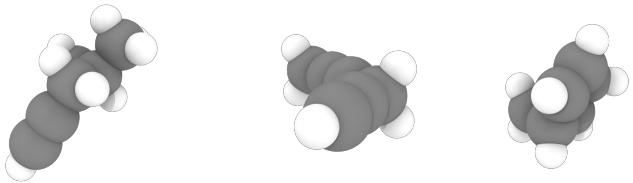




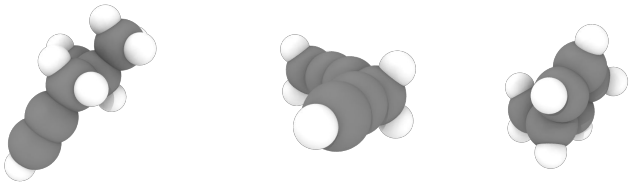
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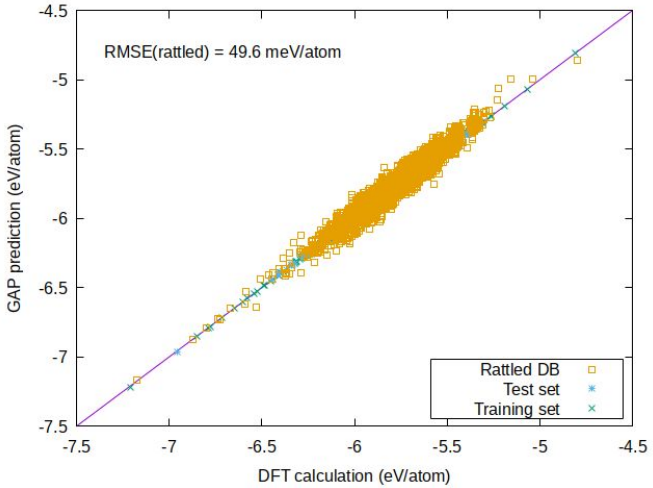
MLIP safety guide

Ground-state molecules



Rattled molecules

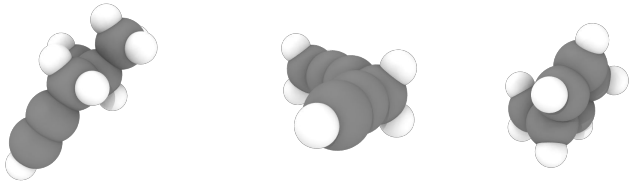




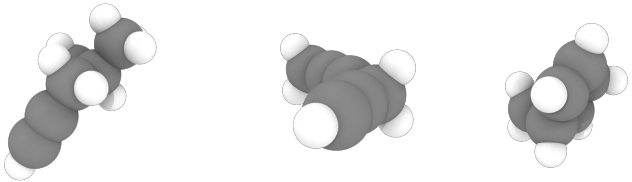
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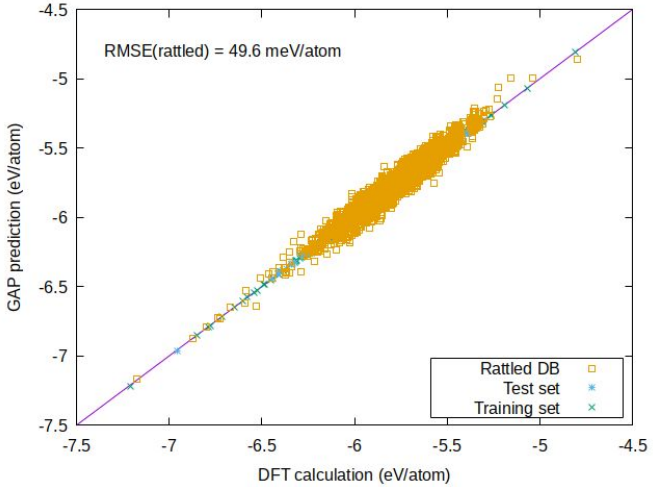
MLIP safety guide

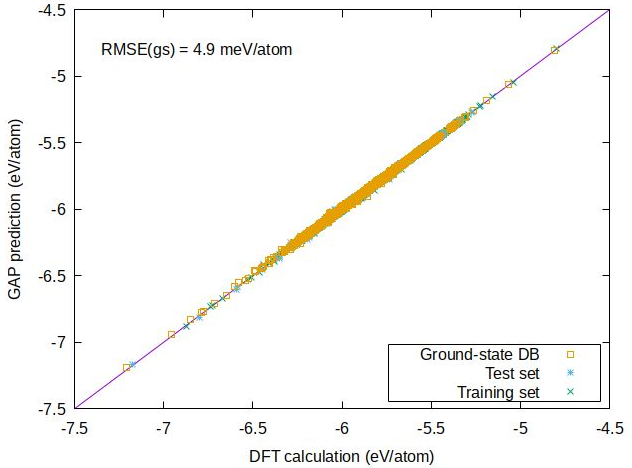
Ground-state molecules



Rattled molecules







Slide from Miguel Caro

Build your database

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Where to start:

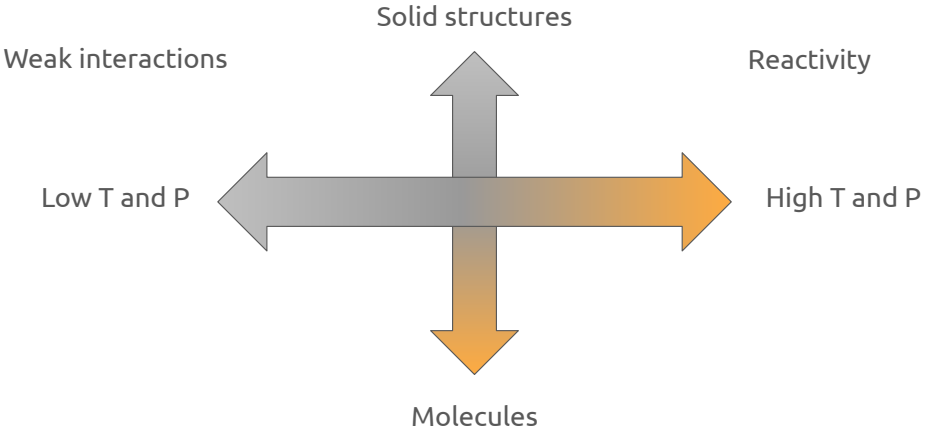
- Large datasets are available (Materials Project, Alexandria, Nomad, QM7, QM9 etc)
- Ground-state configurations

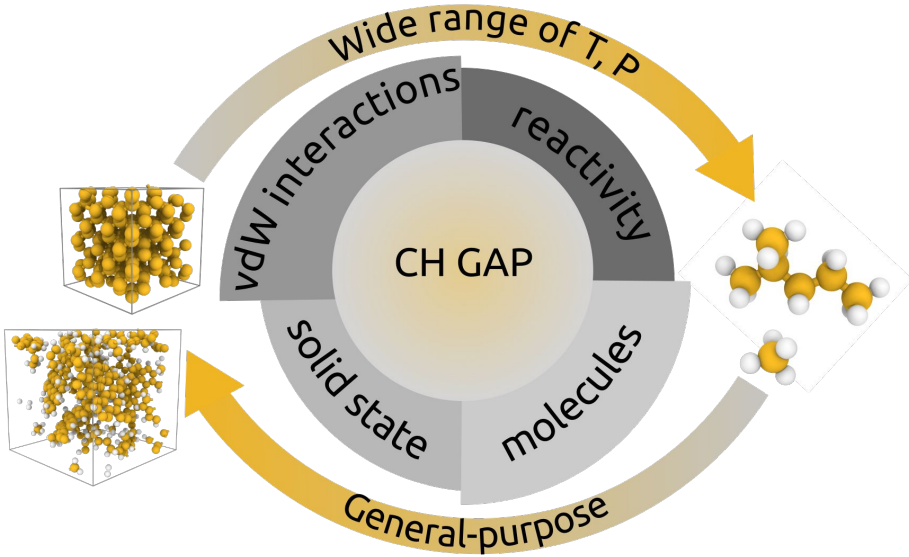
However, we need much more configurations!

Techniques for better representing your configuration space:

- Iterative training
- Active learning

How to fit MLIP: General-purpose CH GAP case

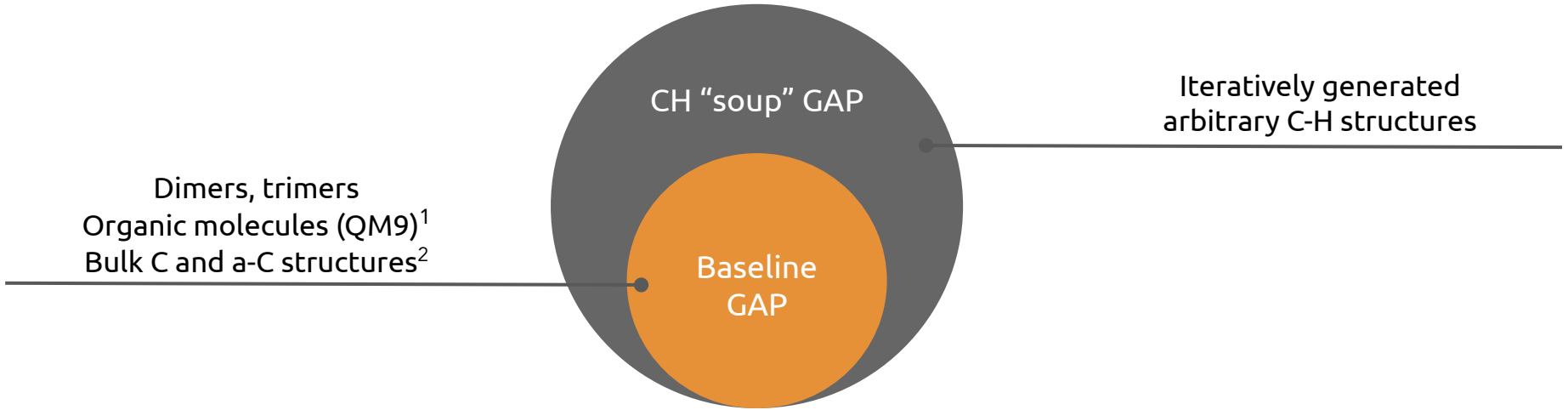




Unifying the description of hydrocarbons and hydrogenated carbon materials

Build your database

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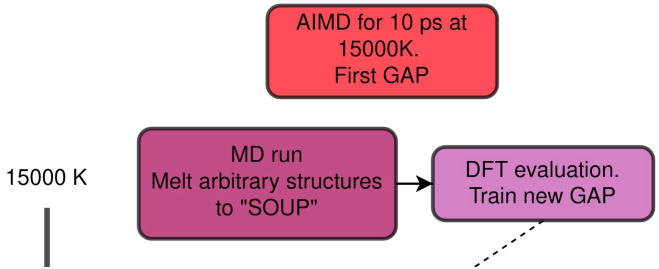
[1]R. Ramakrishnan, P. O. Dral, M. Rupp, and O. A. von Lilienfeld, Scientific Data 1 (2014)
[2]V.L. Deringer and G. Csányi. Phys. Rev. B (2017)

Iterative training

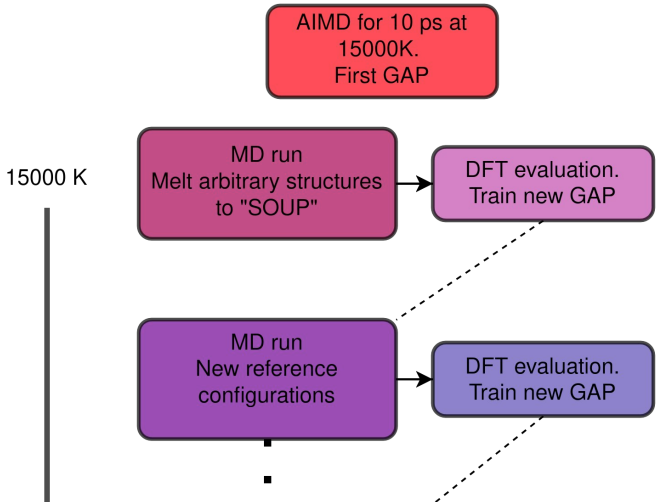
AIMD for 10 ps at 15000K.
First GAP

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Iterative training

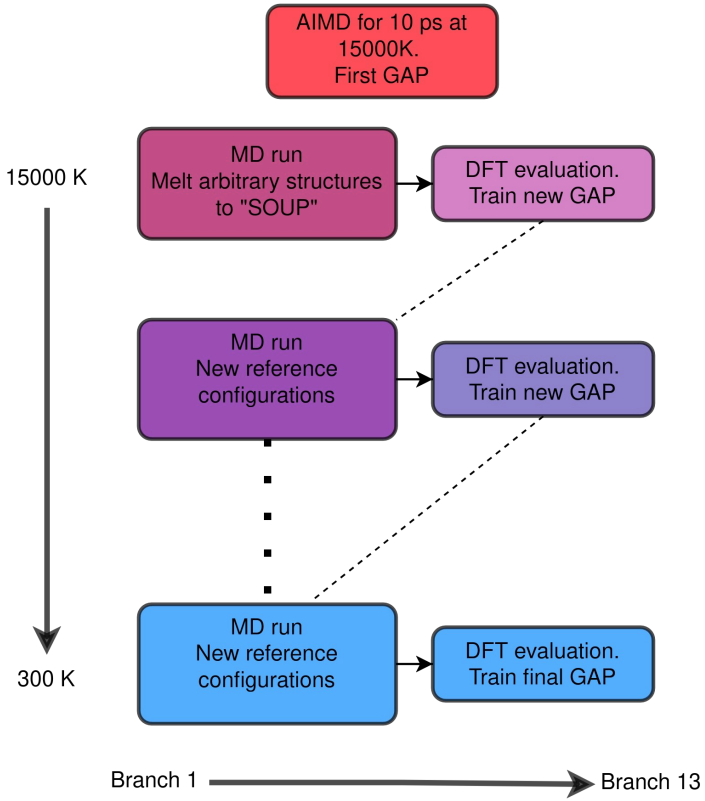


Iterative training



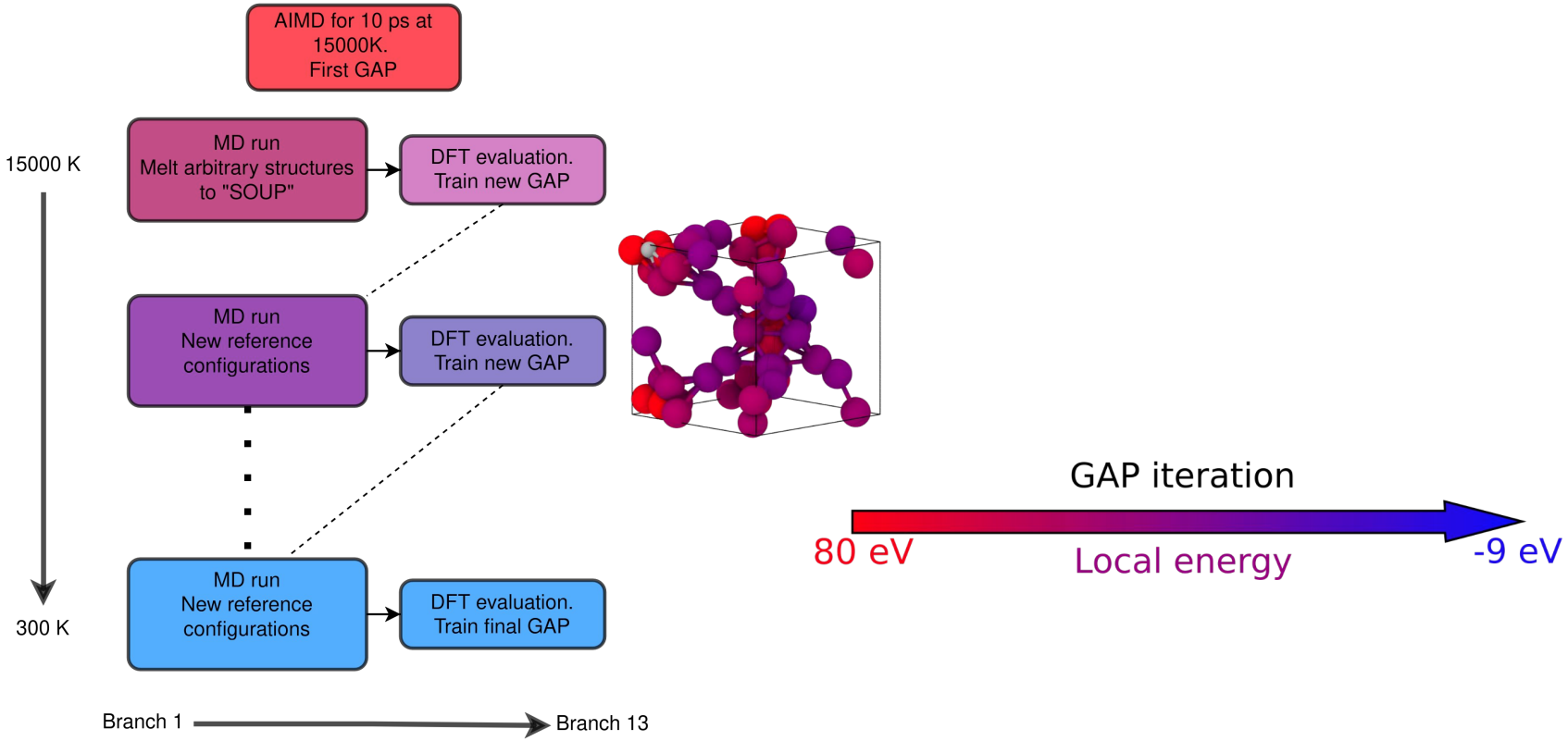
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Iterative training



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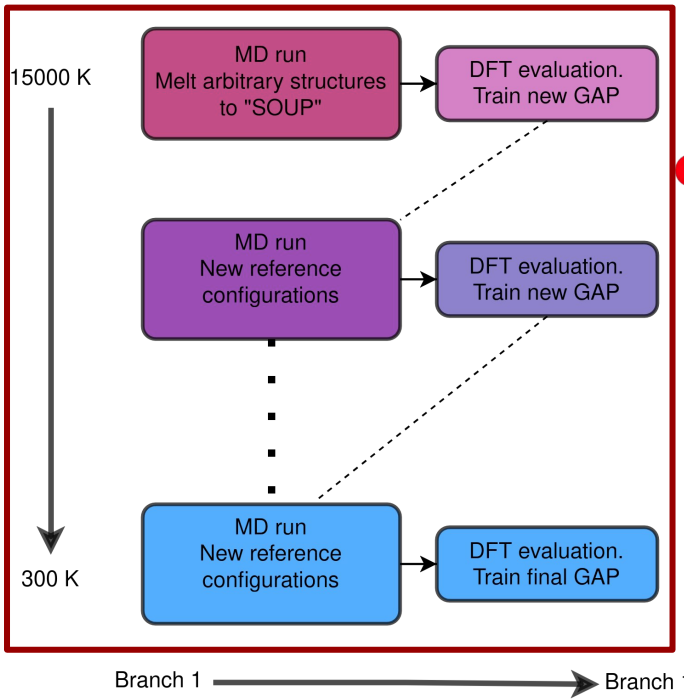
Iterative training

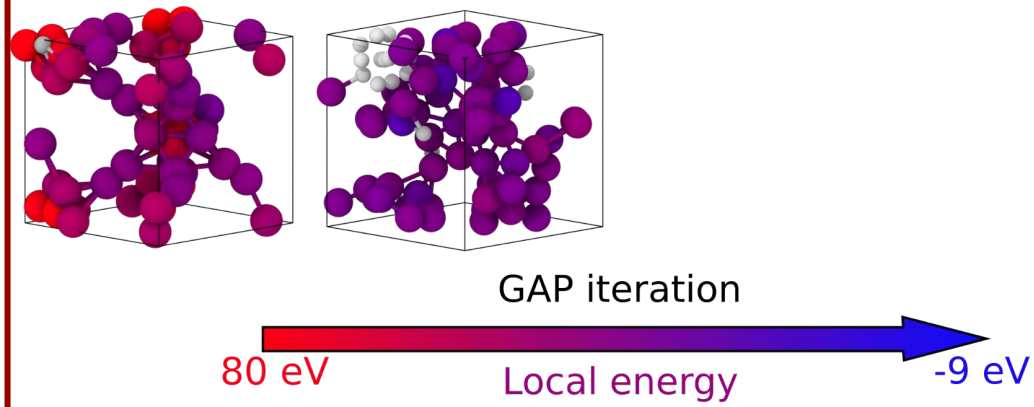


Iterative training

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Repeat *N* times

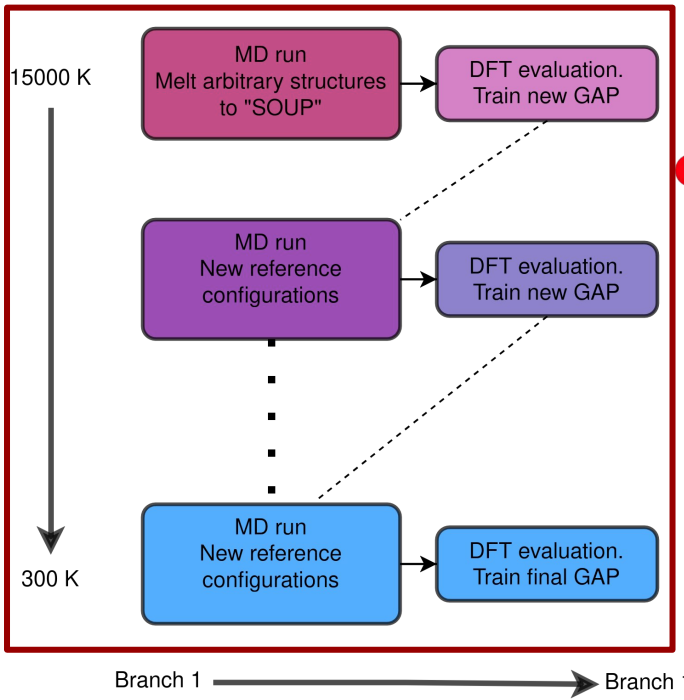


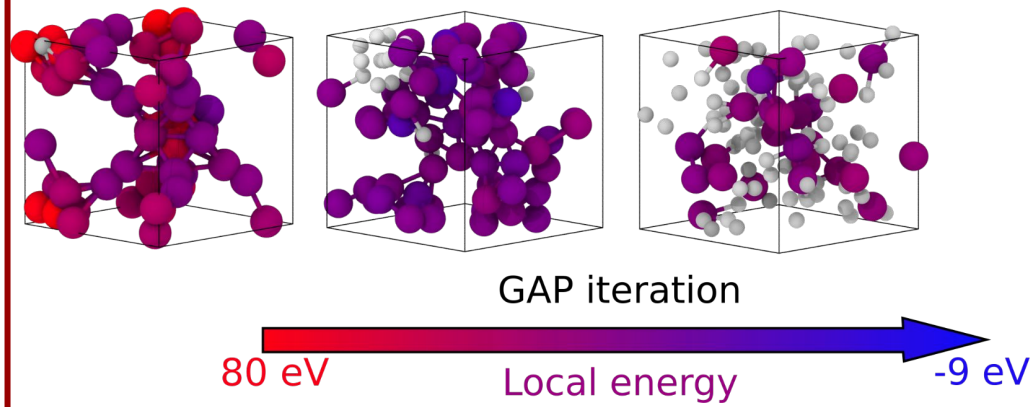


Iterative training

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Repeat *N* times

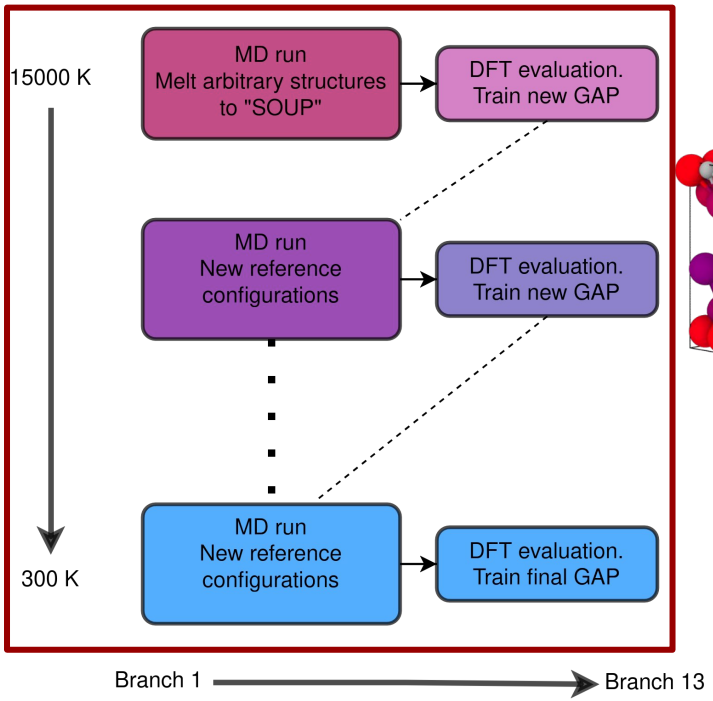


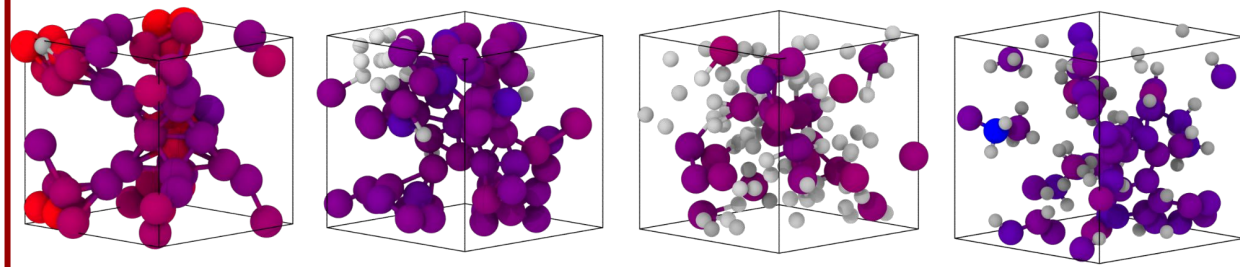


Iterative training

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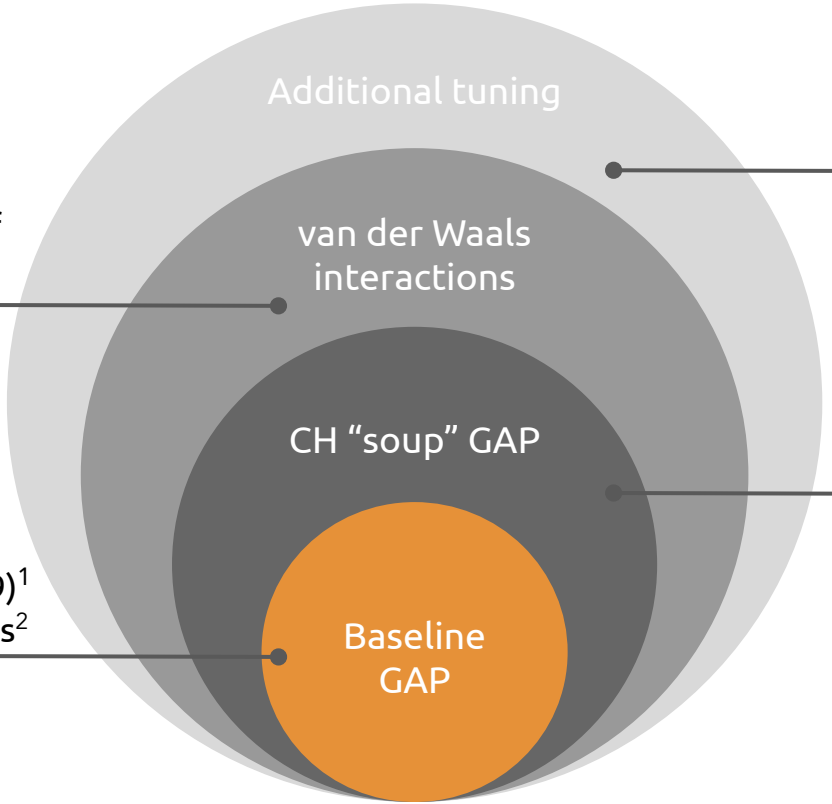
Repeat *N* times





General-purpose CH GAP

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High P and T structures, interacting molecules

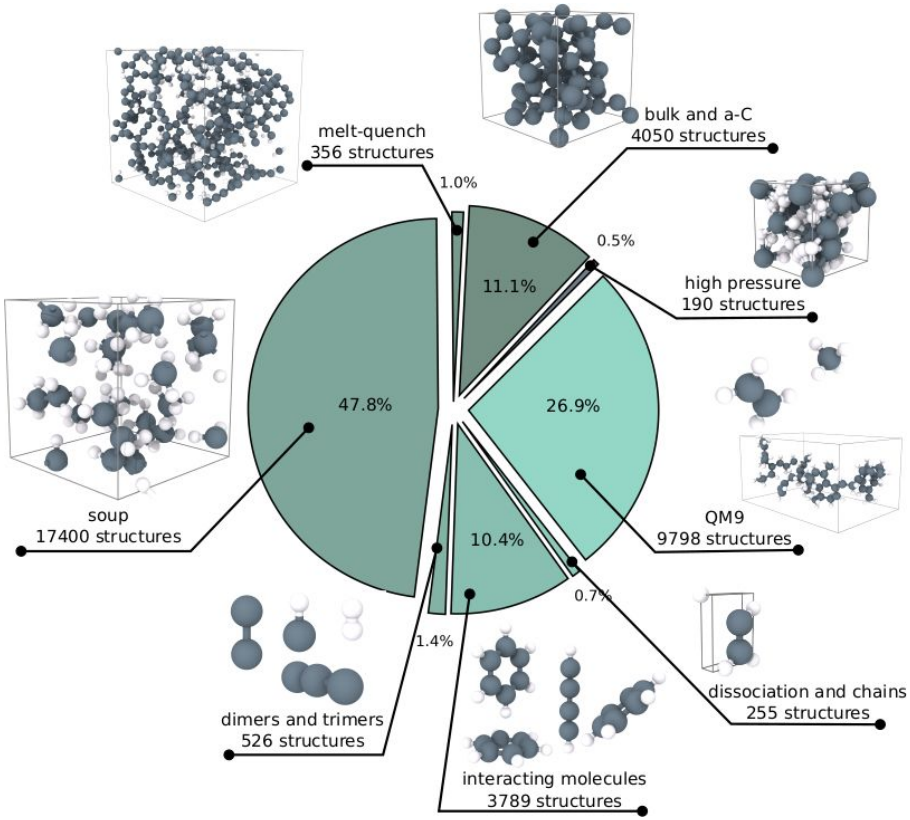
Local vdW parametrization of the data subset

Iteratively generated arbitrary C-H structures

Dimers, trimers
Organic molecules (QM9)[1]
Bulk C and a-C structures[2]

[1]R. Ramakrishnan, P. O. Dral, M. Rupp, and O. A. von Lilienfeld, Scientific Data 1 (2014)
[2]V.L. Deringer and G. Csányi. Phys. Rev. B (2017)

Database structure



Dataset contains ~40k structures

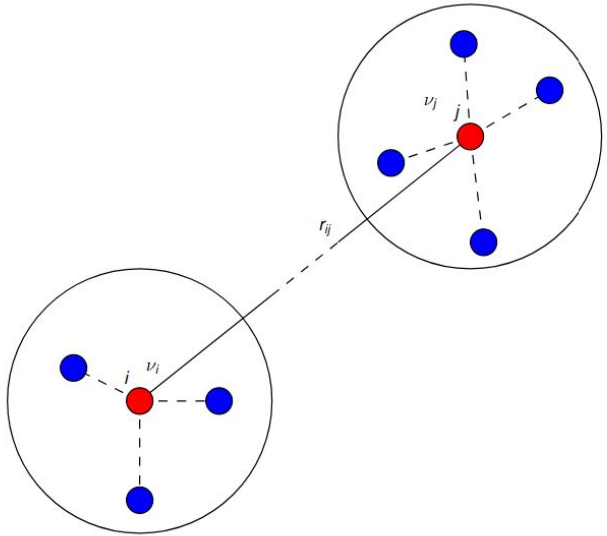
R. Ibragimova, M. Kuklin, T. Zarrouk, M. A. Caro, Chemistry of Materials 37 (2025)

Van der Waals interactions

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- Partitioning the electronic density through local effective volumes of the molecules from QM9, quenched molecules and separate molecules calculated with TS[1] corrections
- The local effective volumes can be predicted with ML[2]
- Energy calculated by summing two-body interactions:

$$E_{\text{disp}} = -\frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}\frac{C_{6,ij}}{r_{ij}^{6}} f_{\text{damp}}(r_{ij})$$

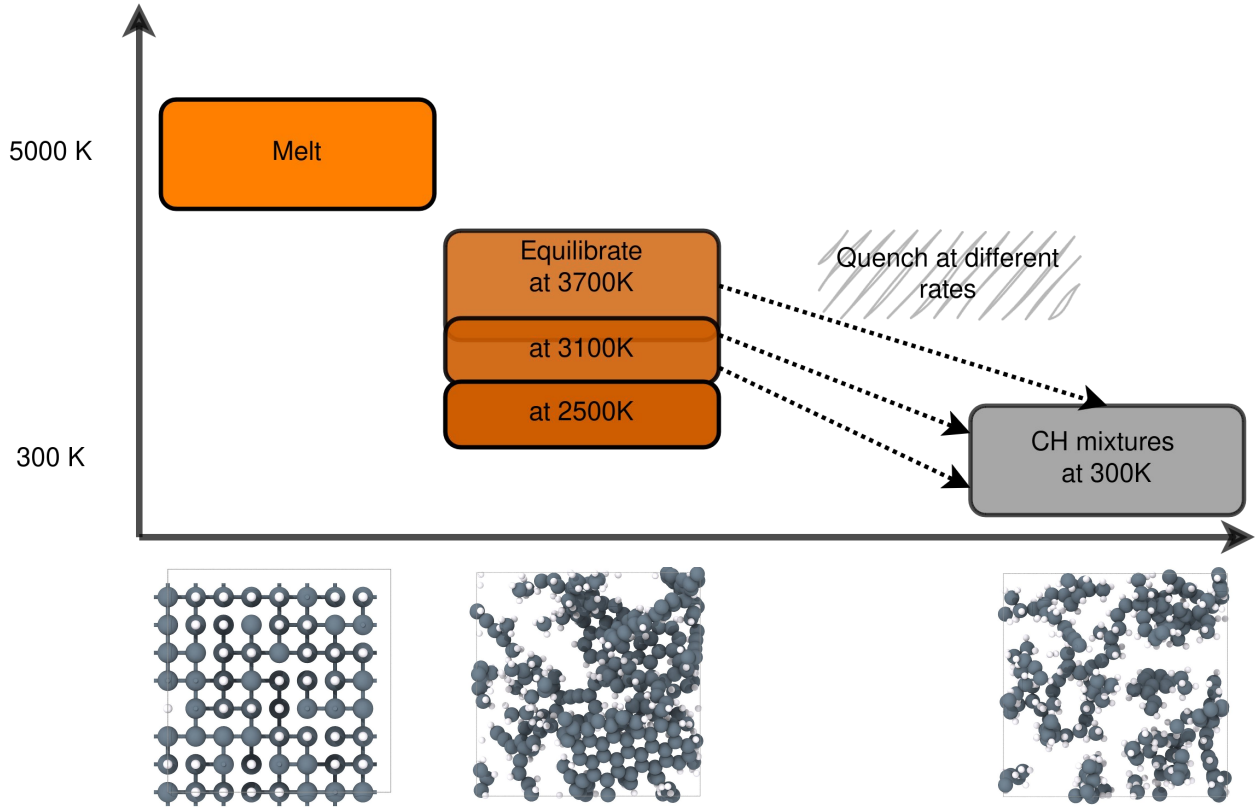


TurboGAP
Data-driven atomistic simulation

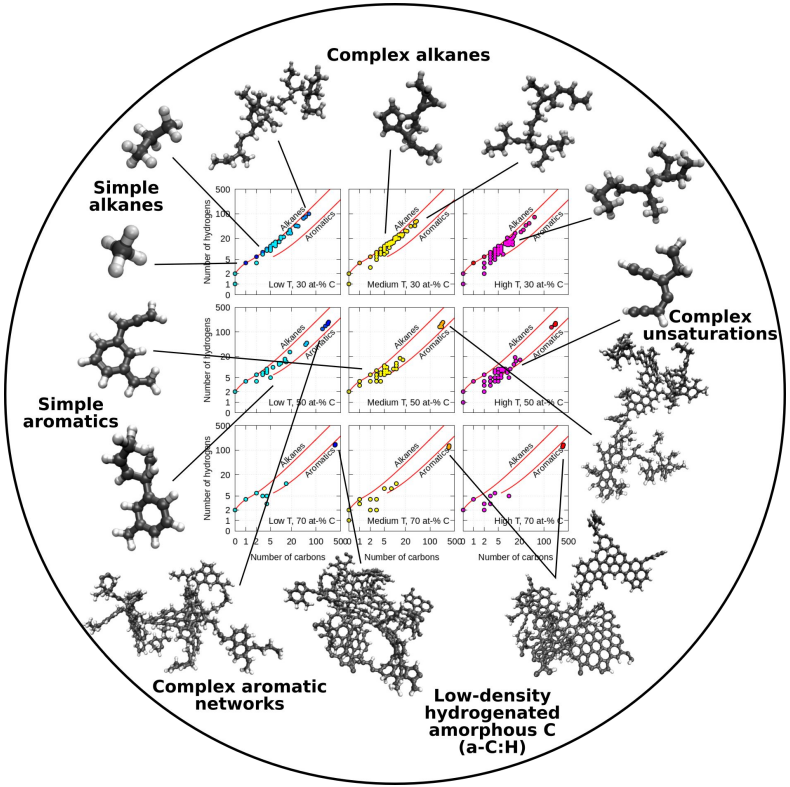
[1]Tkatchenko, M. Scheffler, Phys. Rev. Lett (2009)
[2]H. Muhli et. al., Phys. Rev. B (2021)

Generative melt-quench simulations of hydrocarbons and a-C:H

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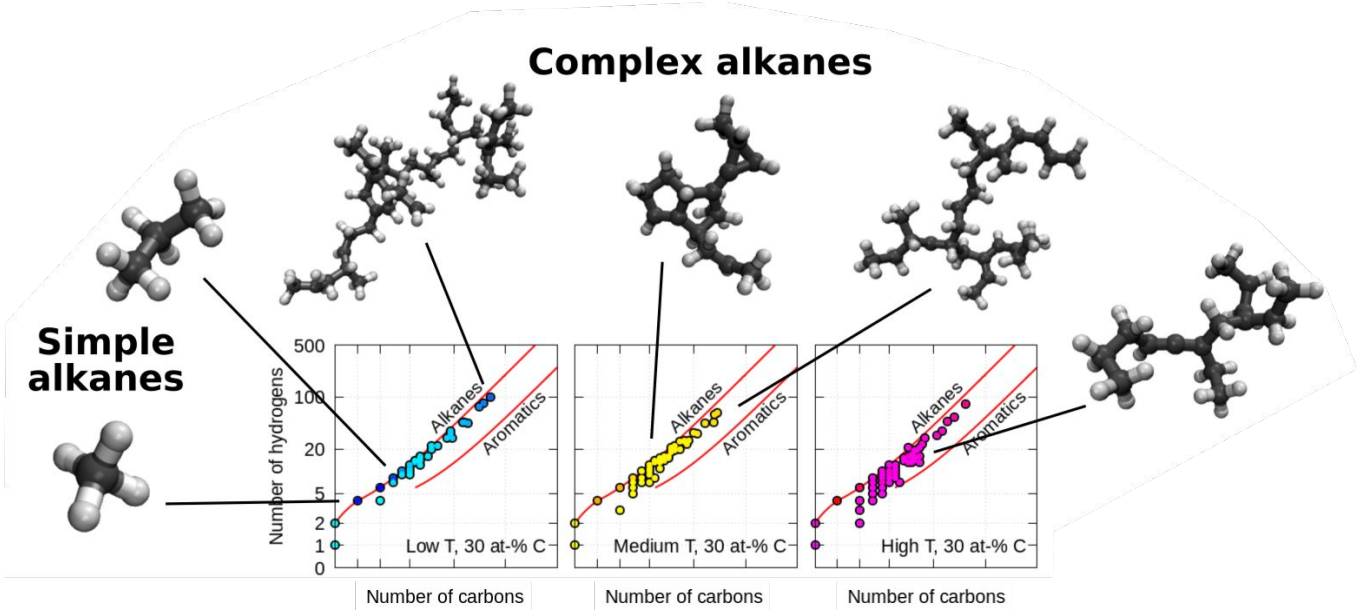
Generative melt-quench simulations of hydrocarbons and a-C:H



R. Ibragimova, M. Kuklin, T. Zarrouk, M. A. Caro, Chemistry of Materials 37 (2025)

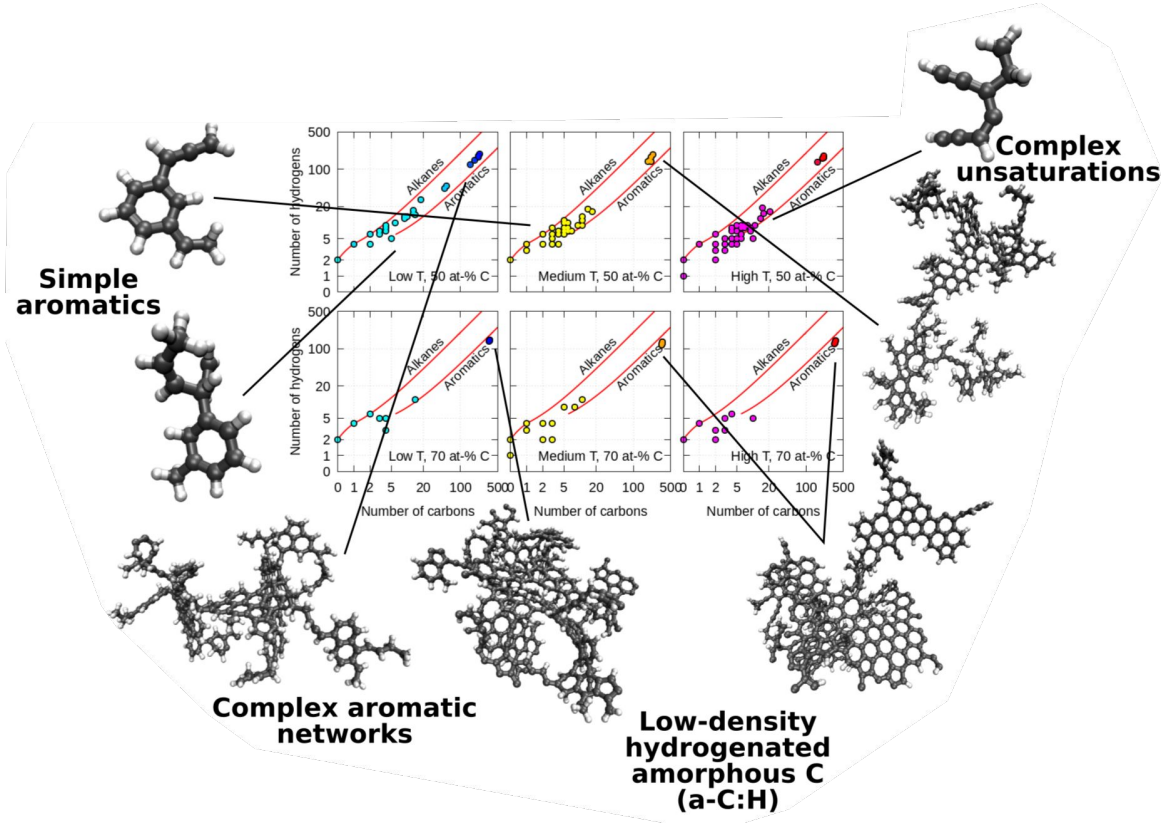
Generative melt-quench simulations of hydrocarbons and a-C:H

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R. Ibragimova, M. Kuklin, T. Zarrouk, M. A. Caro, Chemistry of Materials 37 (2025)

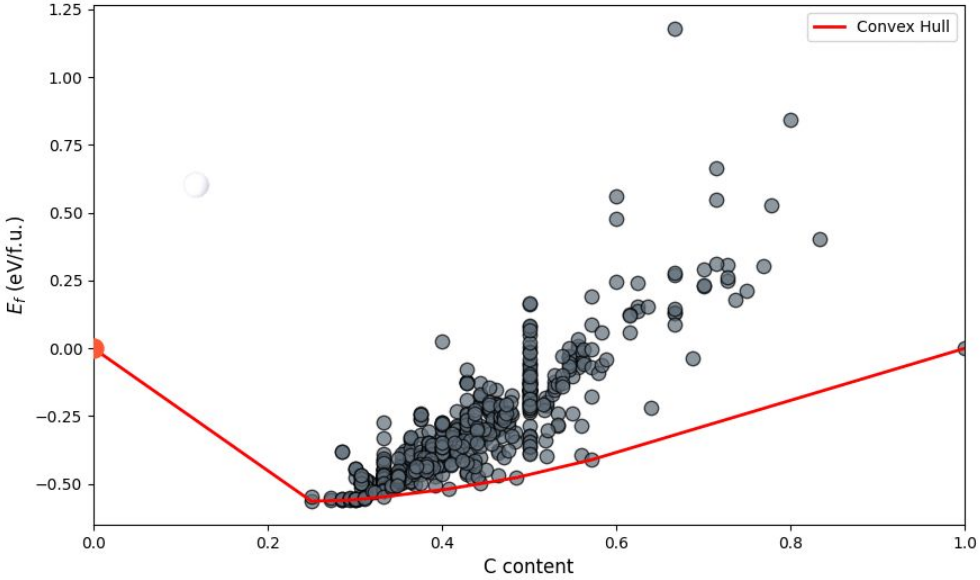
Generative melt-quench simulations of hydrocarbons and a-C:H



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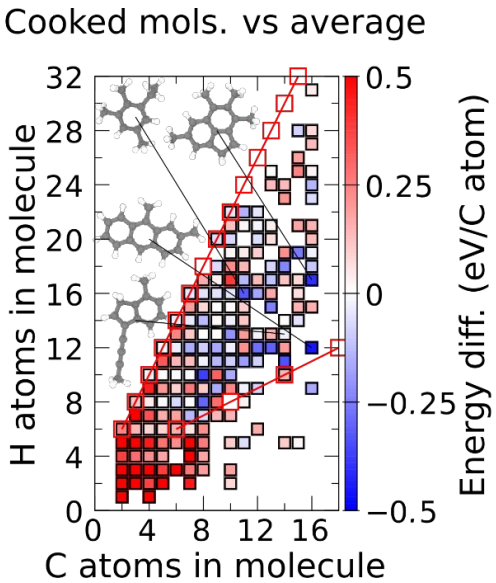
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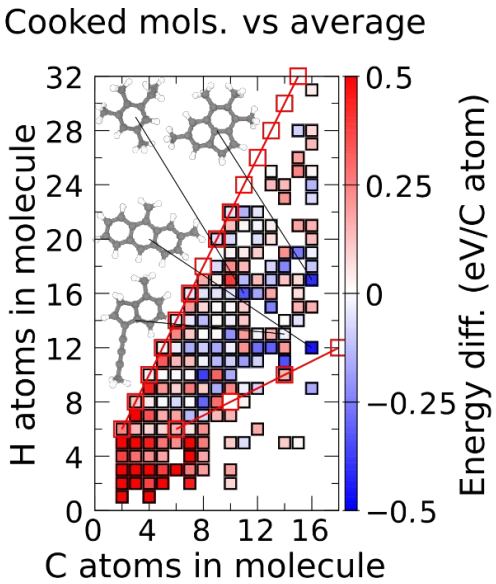
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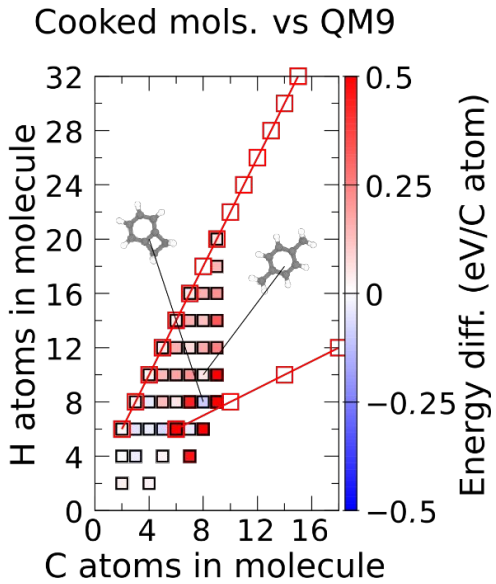


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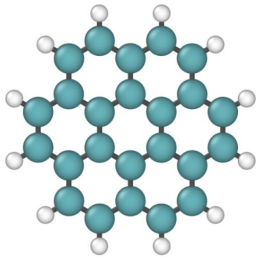


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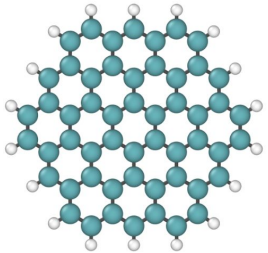
C-H compounds under extreme conditions

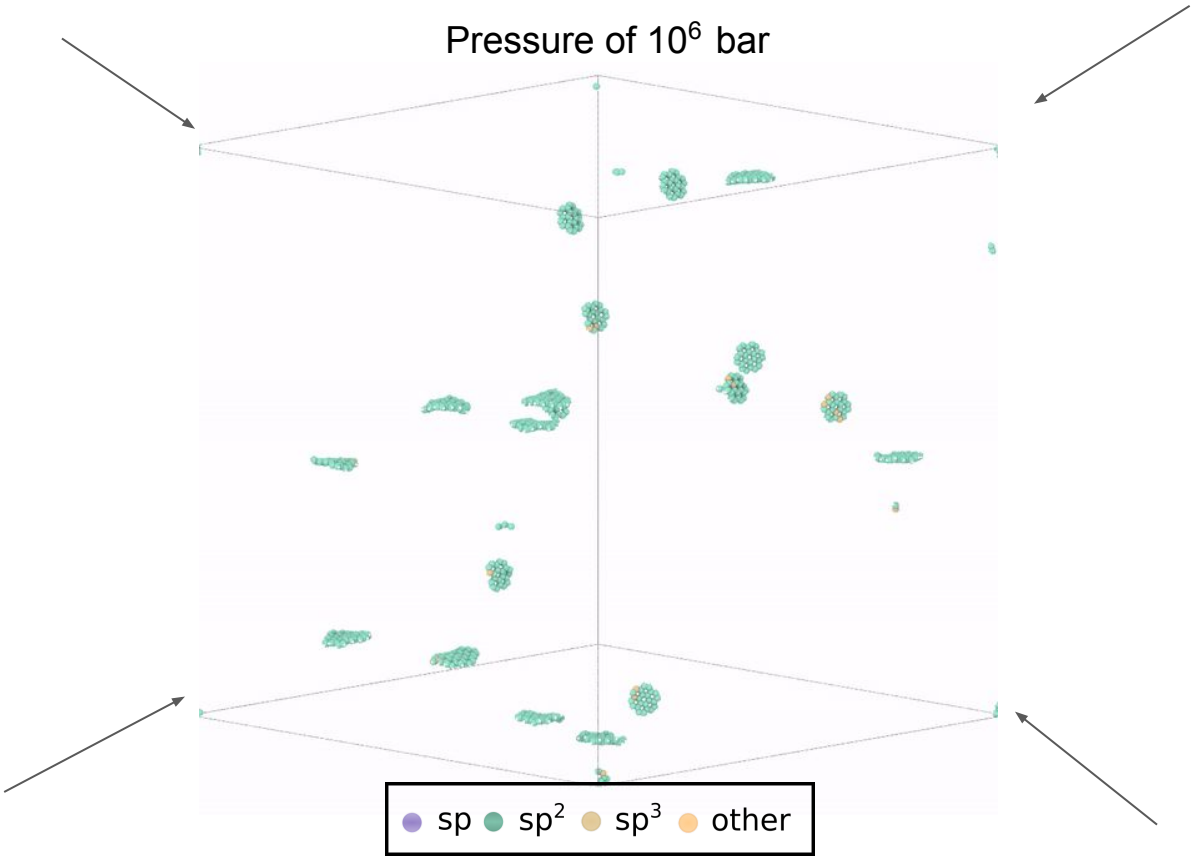
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Coronene



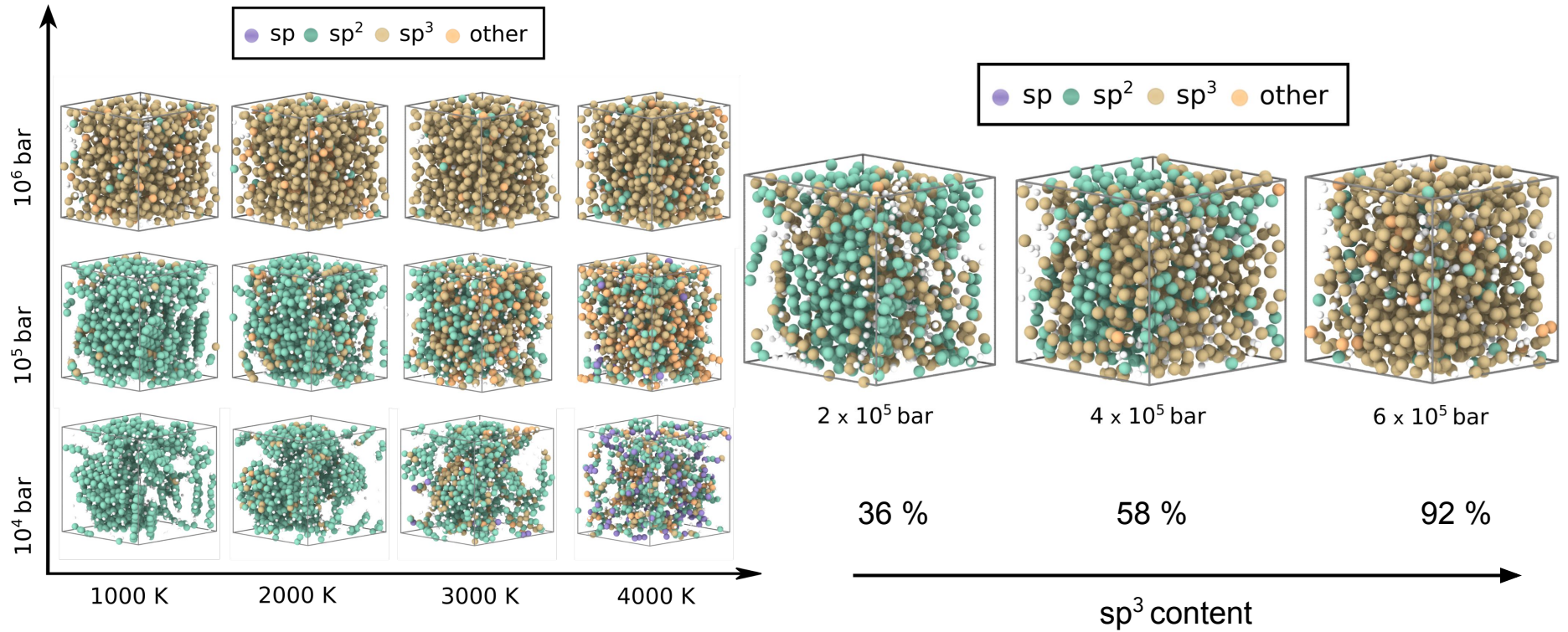
Circumcoronene





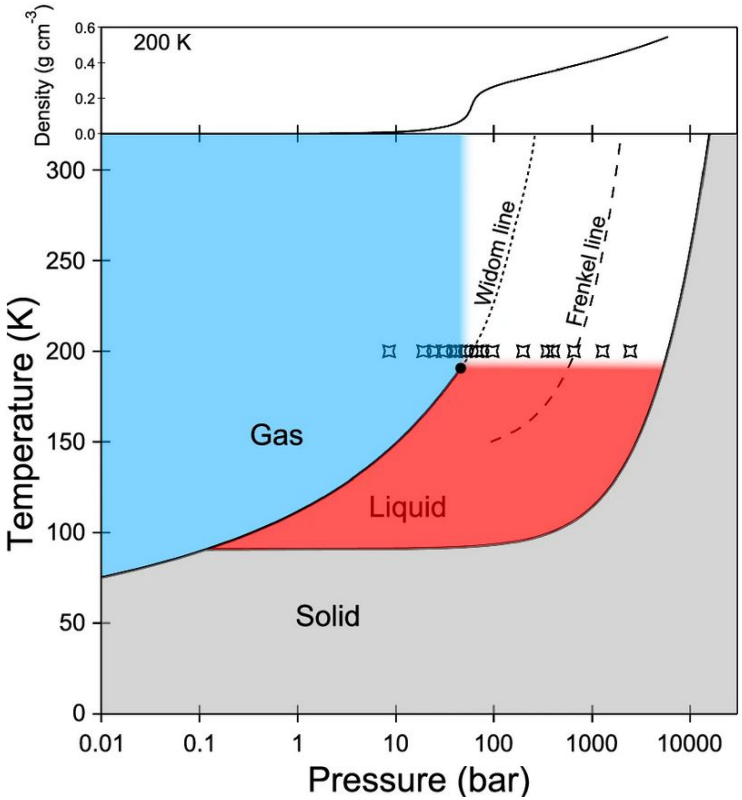
C-H compounds under extreme conditions

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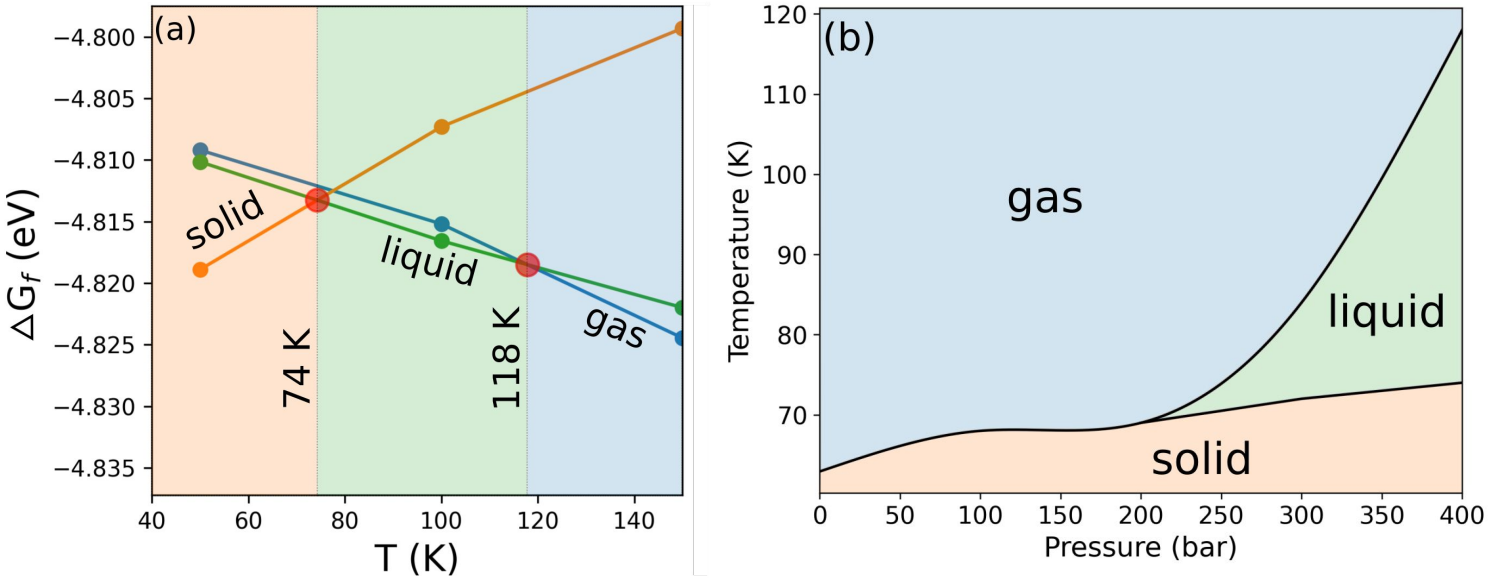
R. Ibragimova, M. Kuklin, T. Zarrouk, M. A. Caro, Chemistry of Materials 37 (2025)

Methane at low temperature



Ranieri, U., Formisano, F., Gorelli, F.A. et al., Nat Commun 15 (2024)

Methane at low temperature



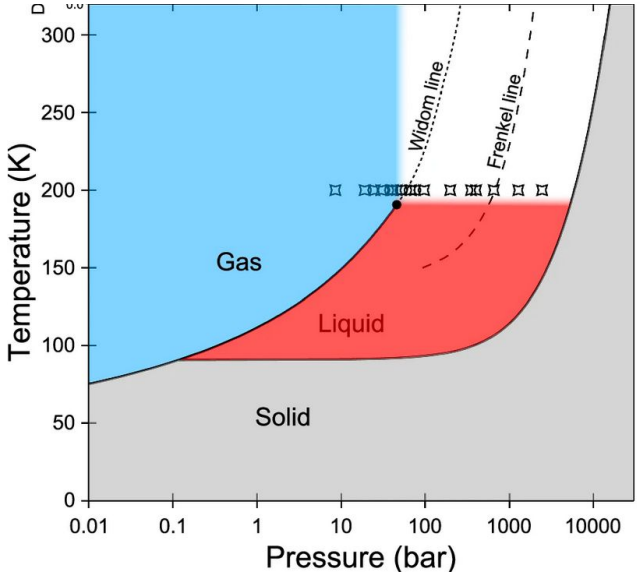
Gibbs free energies calculated for solid, liquid, and gas phases using 2PT method and DoSPT code

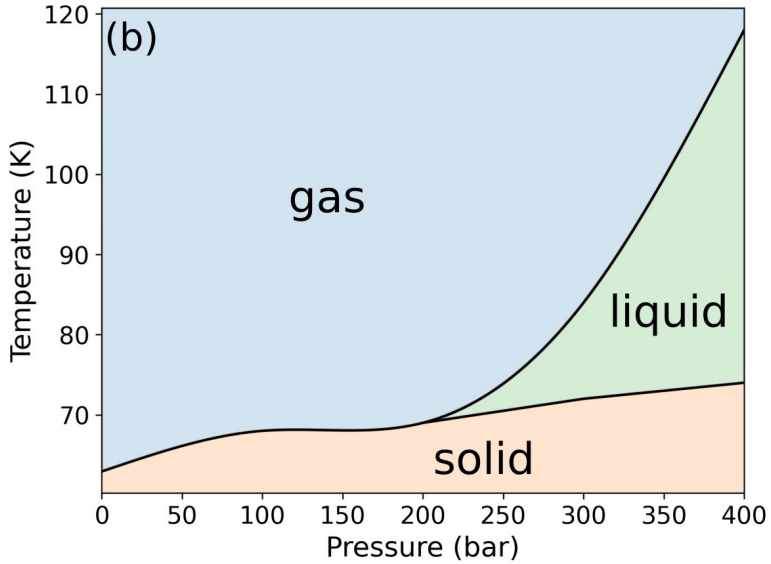
S.-T. Lin, M. Blanco, and W. A. Goddard III, J. Chem. Phys. 119 (2003)

M. A. Caro, O. Lopez-Acevedo, and T. Laurila, Journal of Chemical Theory and Computation 13 (2017)

R. Ibragimova, M. Kuklin, T. Zarrouk, M. A. Caro, Chemistry of Materials 37 (2025)

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Available on Zenodo

General-purpose CH GAP

https://doi.org/10.5281/zenodo.10925279

CH database

https://doi.org/10.5281/zenodo.10925480

Machine learning models for interatomic potentials

Kernel-Based and linear methods

- GAP (Gaussian Approximation Potentials) – uses SOAP descriptors.
- Spectral Neighbor Analysis Potential (SNAP) – uses bispectrum components.
- Moment Tensor Potentials (MTP) – uses moment tensor descriptors.
- Atomic Cluster Expansion (ACE) – generalized body-order expansion; both linear and neural variants exist.

Neural Network Potentials (NNPs)

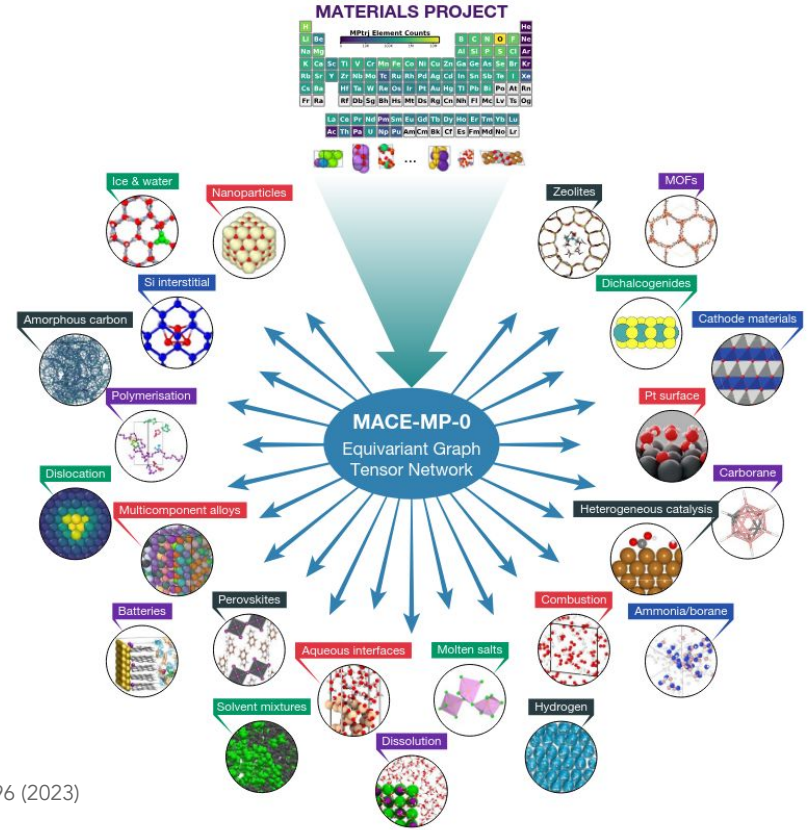
- Behler–Parrinello Neural Network (BPNN) – early neural network using symmetry functions.
- SchNet – continuous-filter convolutional network.
- NequIP (Neural Equivariant Interatomic Potential) – SE(3)-equivariant Graph Neural Networks (GNN).
- MACE (Message Passing ACE) – combines message passing with the body-order expansion idea from ACE.

Foundation models and transferable MLIPs

Universal (Foundation) Models:

- Trained on large, diverse datasets
- Capture general atomic interaction principles
- Transfer learning
- Generalize across materials, phases, and compositions

However, fine tuning is needed!



Preprint at arXiv:2401.00096 (2023)

MACE foundation model

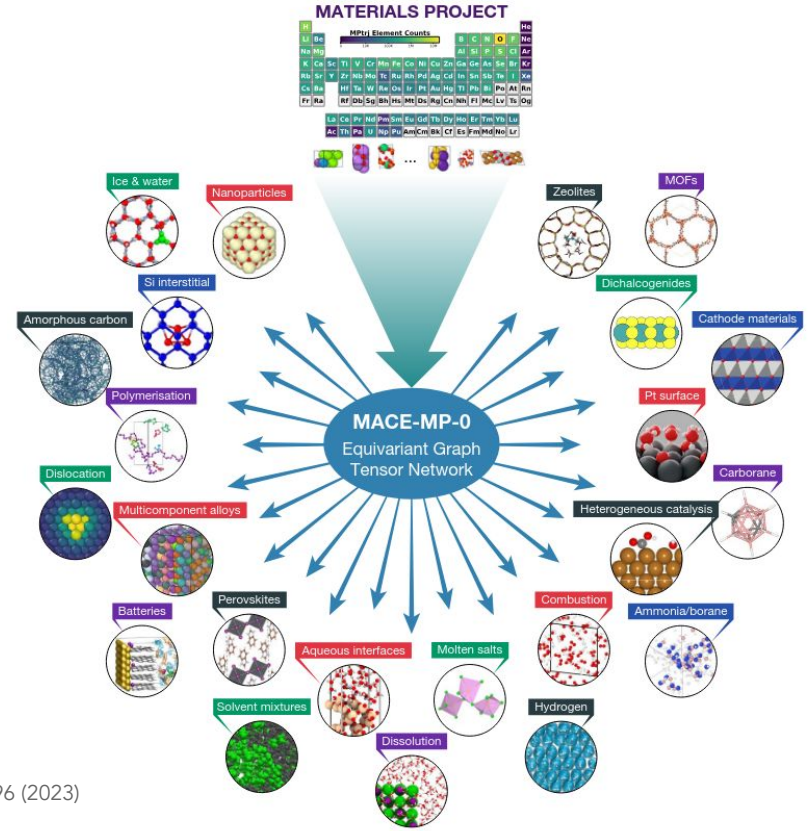
arXiv:2401.00096v2 [physics.chem-ph] 1 Mar 2024

A foundation model for atomistic materials chemistry

Ilyes Batatia[!1], Philipp Benner[!2], Yuan Chiang[!3,4], Alin M. Elena[!17], Dávid P. Kovács[!1], Janosh Riebesell[!4,13], Xavier R. Advincula[12,13], Mark Asta[3,4], Matthew Avaylon[30], William J. Baldwin[1], Fabian Berger[12], Noam Bernstein[11], Arghya Bhowmik[25], Samuel M. Blau[10], Vlad Cărare[1,13], James P. Darby[1], Sandip De[18], Flaviano Della Pia[12], Volker L. Deringer[16], Rokas Elijošius[1], Zakariya El-Machachi[16], Fabio Falcioni[31], Edvin Fako[18], Andrea C. Ferrari[26], Annalena Genreith-Schriever[12], Janine George[2,6], Rhys E. A. Goodall[15], Clare P. Grey[12], Petr Grigorev[27], Shuang Han[18], Will Handley[13,19], Hendrik H. Heenen[9], Kersti Hermansson[23], Christian Holm[22], Stephan Hofmann[1], Jad Jaafar[1], Konstantin S. Jakob[9], Hyunwook Jung[9], Venkat Kapil[12, 21], Aaron D. Kaplan[4], Nima Karimitari[20], James R. Kermode[28], Namu Kroupa[13,19,1], Jolla Kullgren[23], Matthew C. Kuner[3,4], Domantas Kuryla[12], Guoda Liepuoniute[1,26], Johannes T. Margraf[8], Ioan-Bogdan Magdău[24], Angelos Michaelides[12], J. Harry Moore[1], Aakash A. Naik[2,6], Samuel P. Niblett[12], Sam Walton Norwood[25], Niamh O'Neill[12,13], Christoph Ortner[5], Kristin A. Persson[3,4,7], Karsten Reuter[9], Andrew S. Rosen[3,4], Lars L. Schaaf[1], Christoph Schran[13], Benjamin X. Shi[12], Eric Sivonxay[10], Tamás K. Stenczel[1], Viktor Svahn[23], Christopher Sutton[20], Thomas D. Swinburne[27], Jules Tilly[31], Cas van der Oord[1], Santiago Vargas[29], Eszter Varga-Umbrich[1], Tejs Vegge[25], Martin Vondrák[8,9], Yangshuai Wang[5], William C. Witt[14], Fabian Zills[22], and Gábor Csányi[*1]

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Matbench “explosion”

Model	r_{cut}	Date Added	Targets	Params	Training Set	RMSD ↓	κ_{SRME} ↓	R^2 ↑	MAE ↓	Prec ↑	DAF ↑	F1 ↑	Acc ↑	CPS ↑
eSEN-30M-OAM	6 Å	2025-03-17	EFSG	30.2M	6.6M (113M) OMat24+MPtrj+sAlex	0.061	0.170	0.866	0.018	0.928	6.069	0.925	0.977	0.888
ORB v3	6 Å	2025-04-05	EFSG	25.5M	6.47M (133M) MPtrj+Alex+OMat24	0.075	0.210	0.821	0.024	0.904	5.912	0.905	0.971	0.861
SevenNet-MF-ompa	6 Å	2025-03-13	EFSG	25.7M	6.6M (113M) OMat24+sAlex+MPtrj	0.064	0.317	0.867	0.021	0.890	5.825	0.901	0.969	0.845
GRACE-2L-OAM	6 Å	2025-02-06	EFSG	12.6M	6.6M (113M) OMat24+sAlex+MPtrj	0.067	0.294	0.862	0.023	0.883	5.774	0.880	0.963	0.837
AlphaNet-v1-OMA	5 Å	2025-05-12	EFSG	4.65M	6.6M (113M) OMat24+sAlex+MPtrj	0.032	0.644	0.868	0.020	0.883	5.777	0.909	0.971	0.804
DPA-3.1-3M-FT	6 Å	2025-06-05	EFSG	3.27M	163M OpenLAM	0.069	0.469	0.869	0.023	0.866	5.667	0.884	0.963	0.802
eSEN-30M-MP	6 Å	2025-03-17	EFSG	30.1M	146k (1.58M) MPtrj	0.075	0.340	0.822	0.033	0.804	5.260	0.831	0.946	0.797
MACE-MPA-0	6 Å	2024-12-09	EFSG	9.06M	3.37M (12M) MPtrj+sAlex	0.073	0.412	0.842	0.028	0.853	5.582	0.852	0.954	0.795
MatterSim v1 5M	5 Å	2024-12-16	EFSG	4.55M	17M MatterSim	0.073	0.574	0.863	0.024	0.895	5.852	0.862	0.959	0.767
GRACE-1L-OAM	6 Å	2025-02-06	EFSG	3.45M	6.6M (113M) OMat24+sAlex+MPtrj	0.072	0.516	0.842	0.031	0.803	5.255	0.824	0.944	0.761
Eqnorm MPtrj	6 Å	2025-05-26	EFSG	1.31M	146k (1.58M) MPtrj	0.084	0.408	0.799	0.040	0.741	4.844	0.786	0.929	0.756
DPA-3.1-MPtrj	6 Å	2025-06-05	EFSG	4.81M	146k (1.58M) MPtrj	0.080	0.650	0.812	0.037	0.768	5.024	0.803	0.936	0.718
SevenNet-l3i5	5 Å	2024-12-10	EFSG	1.17M	146k (1.58M) MPtrj	0.085	0.550	0.776	0.044	0.708	4.629	0.760	0.920	0.714
HIENet	5 Å	2025-07-01	EFSG	7.51M	146k (1.58M) MPtrj	0.080	0.642	0.793	0.041	0.754	4.932	0.777	0.929	0.707
MatRIS v0.5.0 MPtrj	6 Å	2025-03-13	EFSGM	5.83M	146k (1.58M) MPtrj	0.077	0.861	0.803	0.037	0.772	5.049	0.809	0.938	0.681
GRACE-2L-MPtrj	6 Å	2024-11-21	EFSG	15.3M	146k (1.58M) MPtrj	0.090	0.525	0.741	0.052	0.636	4.163	0.691	0.896	0.681
MACE-MP-0	6 Å	2023-07-14	EFSG	4.69M	146k (1.58M) MPtrj	0.091	0.647	0.697	0.057	0.577	3.777	0.669	0.878	0.644
eqV2 M	12 Å	2024-10-18	EFSD	86.6M	3.37M (102M) OMat24+MPtrj	0.069	1.771	0.848	0.020	0.924	6.047	0.917	0.975	0.558
ORB v2	10 Å	2024-10-11	EFSD	25.2M	3.25M (32.1M) MPtrj+Alex	0.097	1.732	0.824	0.028	0.924	6.041	0.880	0.965	0.529
eqV2 S DeNS	12 Å	2024-10-18	EFSD	31.2M	146k (1.58M) MPtrj	0.076	1.676	0.788	0.036	0.771	5.042	0.815	0.941	0.522
ORB v2 MPtrj	10 Å	2024-10-14	EFSD	25.2M	146k (1.58M) MPtrj	0.101	1.725	0.756	0.045	0.719	4.702	0.765	0.922	0.470
M3GNet	5 Å	2022-09-20	EFSG	228k	62.8k (188k) MPF	0.112	1.412	0.585	0.075	0.441	2.882	0.569	0.813	0.428
CHGNet	5 Å	2023-03-03	EFSGM	413k	146k (1.58M) MPtrj	0.095	1.717	0.689	0.063	0.514	3.361	0.613	0.851	0.400
GNoME	5 Å	2024-02-03	EFG	16.2M	6M (89M) GNoME	n/a	n/a	0.785	0.035	0.844	5.523	0.829	0.955	NaN

https://matbench-discovery.materialsproject.org/

How to navigate

(some) Considerations

- Know your application
- Data
- Accuracy requirements: general accuracy *vs* application specific accuracy
- How well MLIP is scaling up
- Robustness and transferability
- Hardware resources: CPU *vs* GPU availability

Recap

- Gaussian Approximation Potential is a robust, well-established ML framework to build accurate and transferable interatomic potentials
- No matter how sophisticated is the ML architecture: MLIP needs DATA
- A wide selection of training data is important for transferability: select basic data and complement with application-specific data
- Application specific validation is necessary
- Different pre-trained MLIPs are available to use
- Universal (foundation) MLIPs are emerging

Thank you

Acknowledgements

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• COST (European Cooperation in Science & Technology) is a funding agency for research and innovation networks. Our Actions help connect research initiatives across Europe and enable scientists to grow their ideas by sharing them with their peers. This boosts their research, career and innovation.

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