AI-Assisted Physical Modeling in the Cloud-Native Era

Linfeng Zhang, DP Technology

Nov. 10, 2021

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Outline

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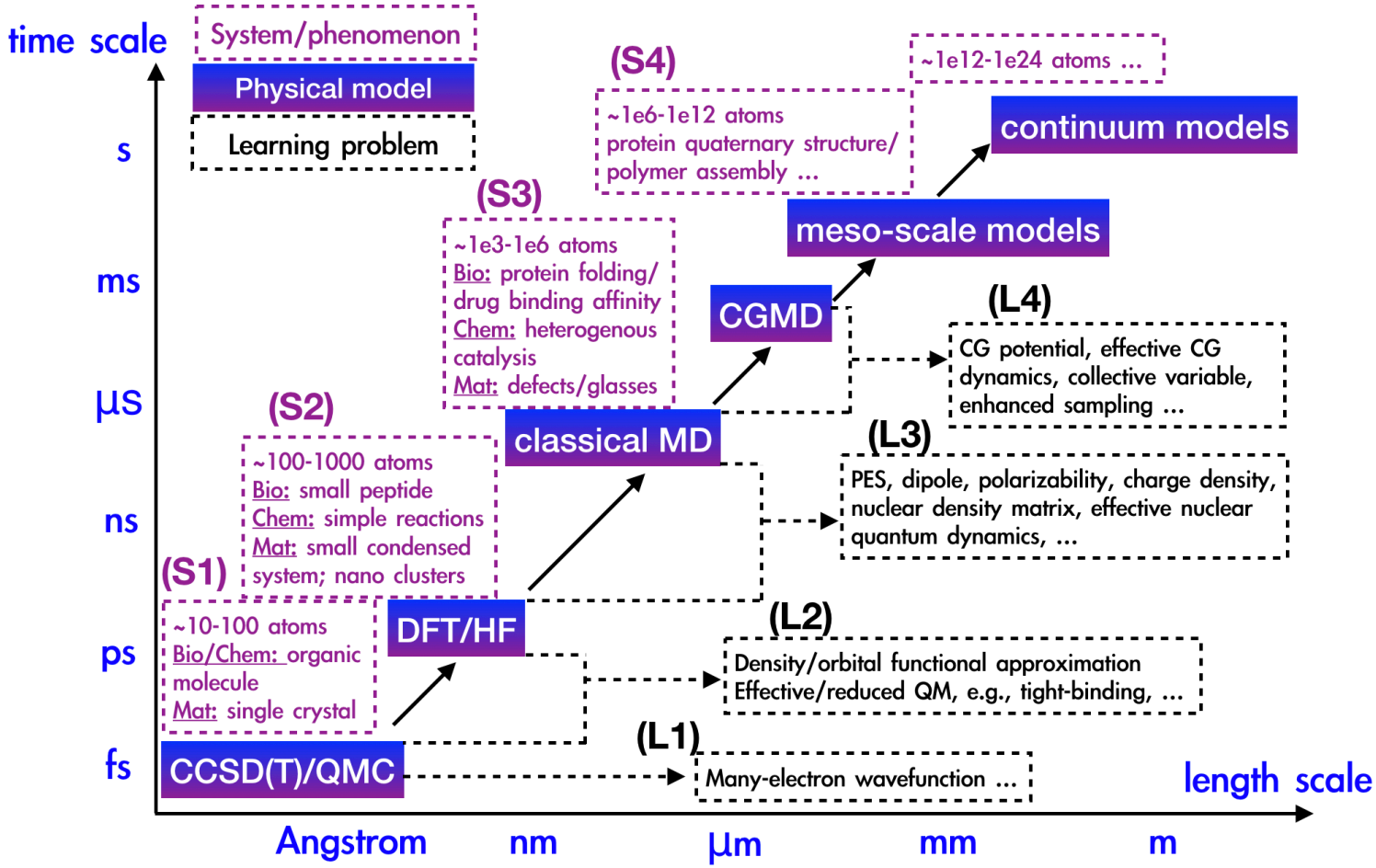
Multi-scale modeling and machine learning



Opportunity: to use machine learning to bridge different scales.

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Requirement for a reliable physics-based ML model

- **Accuracy**
  e.g. uniformly accurate in relevant physical space
- **Efficiency**
  e.g. linear scaling
- **Locality**
  model learned from small-size data can be used for large-size systems
- **Physical constraints**
  e.g. extensive property, symmetry, asymptotic behavior
- **No human intervention/ end-to-end.**

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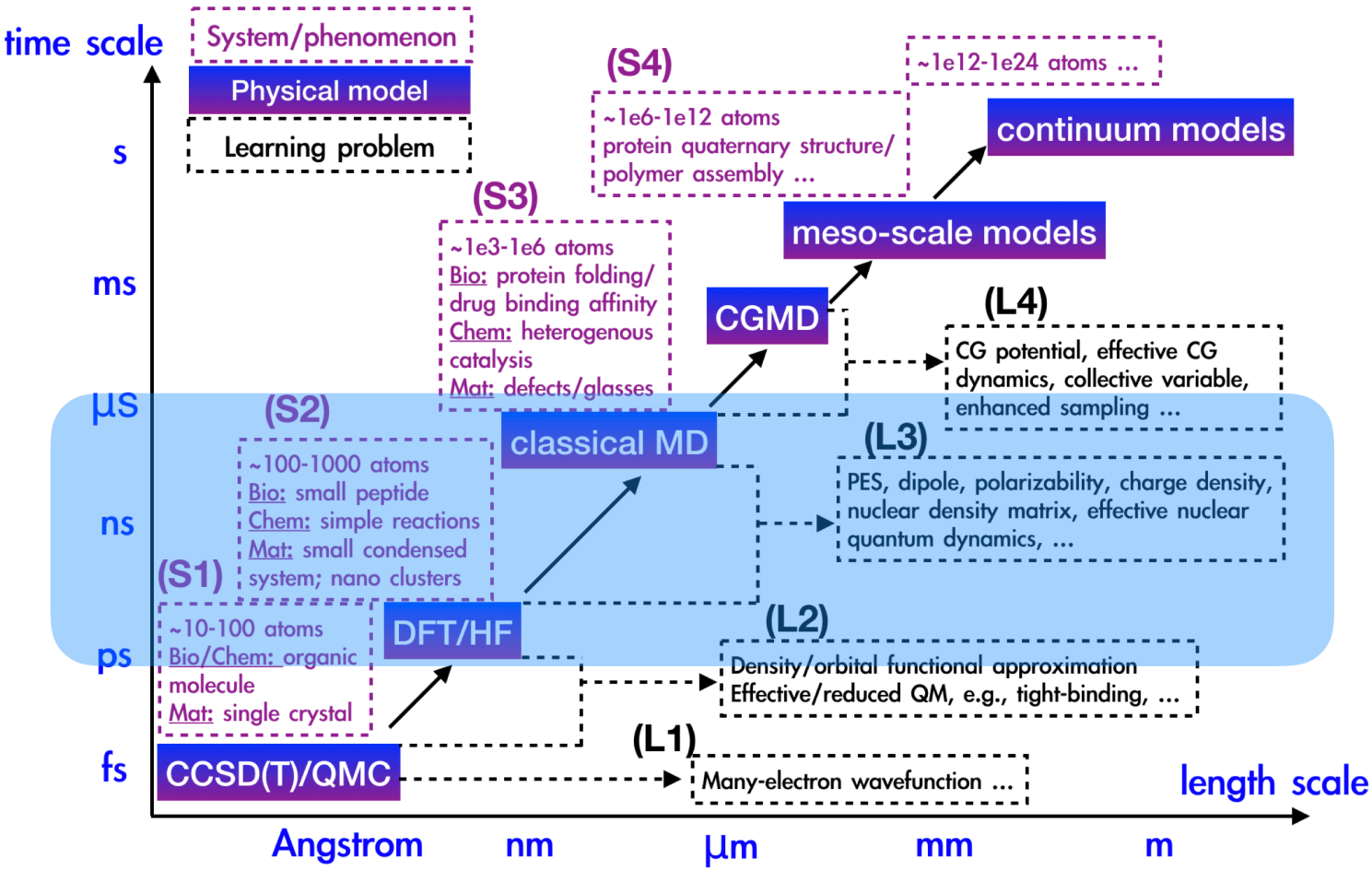
Problem 1: from QM to MD



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Problem 1: from QM to MD

- **Microscopic model: QM**, e.g., the Car-Parrinello (CP) scheme within the Kohn-Sham (KS) density functional theory:

$$\mu\ddot{\psi}_i(\boldsymbol{x},t) = -\delta E_{KS}/\delta\psi_i^*(\boldsymbol{x},t) + \sum_k \Lambda_{ik}\psi_k(\boldsymbol{x},t);$$

$$M_I\ddot{\boldsymbol{R}}_I = -\nabla_I E_{KS}.$$

  Accurate but expensive, $\sim$ 100-1000 atoms, $\sim$ 10-100 ps.

- **Macroscopic model: MD**, e.g., Newton's equation of motion driven by the Lennard-Jones (LJ) potential

$$E_{LJ} = \frac{1}{2}\sum_{i\neq j} V_{ij}, \quad V_{ij} = 4\epsilon[(\frac{\sigma}{r_{ij}})^{12} - (\frac{\sigma}{r_{ij}})^{6}];$$

$$M_I\ddot{\boldsymbol{R}}_I = -\nabla_I E_{LJ}.$$

  Fast but limited, $\sim$ 100-1000 K atoms, $\sim$ 10-100 μs.

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Important quantities at the scales between QM/MD

- Potential energy surface (PES) $E(\boldsymbol{R})$:
  - Locality: $E(\boldsymbol{R}) = \sum_I E_I(\boldsymbol{R}_I, \boldsymbol{R}_J, J \in \mathcal{N}_I(r_c))$;
  - Symmetry: translation (T), rotation (R), permutation (P) invariant.
- Electric polarization $\boldsymbol{M}(\boldsymbol{R})$:
  - Locality: $\boldsymbol{M}(\boldsymbol{R}) = \sum_I \boldsymbol{M}_I(\boldsymbol{R}_I, \boldsymbol{R}_J, J \in \mathcal{N}_I(r_c))$;
  - Symmetry: TP-invariant, R-covariant $(\boldsymbol{M}(\mathcal{U}\boldsymbol{R}) = \mathcal{U}\boldsymbol{M}(\boldsymbol{R}))$
- Electric polarizability $\boldsymbol{\alpha}(\boldsymbol{R}) = \frac{\delta \boldsymbol{M}(\boldsymbol{R})}{\delta \boldsymbol{E}}$:
  - Locality: $\boldsymbol{\alpha}(\boldsymbol{R}) = \sum_I \boldsymbol{\alpha}_I(\boldsymbol{R}_I, \boldsymbol{R}_J, J \in \mathcal{N}_I(r_c))$;
  - Symmetry: TP-invariant, R-covariant $(\boldsymbol{\alpha}(\mathcal{U}\boldsymbol{R}) = \mathcal{U}\boldsymbol{\alpha}(\boldsymbol{R})\mathcal{U}^T)$

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A general demand: approximation of high dimensional tensorial functions

$\boldsymbol{T}_I$ of degree (p, q), taking as input the relative coordinates between atoms I and $J \in \mathcal{N}_I^{r_c}$:

$$\boldsymbol{T}_I \equiv (T_I)^{t_1,\ldots,t_q}_{s_1,\ldots,s_p}(\{r^k_{JI}\}),\ \{r^k_{JI}\} \equiv \{r^1_{JI}, r^2_{JI}, r^3_{JI}\} = \boldsymbol{r}_{JI} = \boldsymbol{r}_J - \boldsymbol{r}_I$$

Rotational *covariance* and *contravariance* :

$$(T_I)^{t_1,\ldots,t_q}_{s_1,\ldots,s_p}(U^k_{k'} r^{k'}_{JI}) = U^{t_1}_{t'_1} \cdots U^{t_q}_{t'_q} \cdot (T_I)^{t'_1,\ldots,t'_q}_{s'_1,\ldots,s'_p}(r^k_{JI}) \cdot (U^{-1})^{s'_1}_{s_1} \cdots (U^{-1})^{s'_p}_{s_p},$$

Permutational invariance:

$$\boldsymbol{T}_I(\ldots, \boldsymbol{r}_{JI}, \ldots, \boldsymbol{r}_{KI}, \ldots) = \boldsymbol{T}_I(\ldots, \boldsymbol{r}_{JI}, \ldots, \boldsymbol{r}_{KI}, \ldots),\ \text{if } \alpha(J) = \alpha(K).$$

($\alpha(J)$: chemical species of atom J.)

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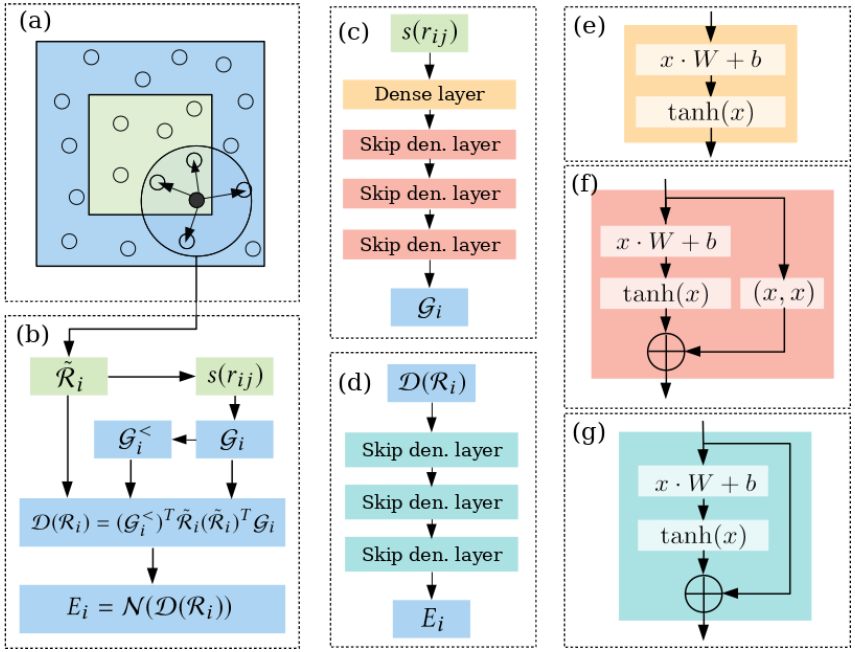
Extended Deep Potential (DP) approach

- **Embedding network**: $(\mathcal{G}_I)^m_J = \left(\delta^\beta_{\alpha_I}\delta^{\beta_1}_{\alpha_J} G^m_{\beta,\beta_1}(s(r_{JI}))\right)$,
- **Symmetrized coordinates**: $\mathcal{Q}_I = \mathcal{G}_I^\dagger \cdot \tilde{\mathcal{R}}_I$,
- **Feature matrix** $\mathcal{D}_I$: $\mathcal{D}_I = \tilde{\mathcal{Q}}_I^\dagger \cdot \mathcal{Q}_I = \tilde{\mathcal{G}}_I^\dagger \cdot \tilde{\mathcal{R}}_I \cdot \tilde{\mathcal{R}}_I^\dagger \mathcal{G}_I$,
- **Fitting network**: $\mathcal{N}^{n_1,\ldots,n_q}_{m_1,\ldots,m_p}(\mathcal{D}_I)$,
- **Symmetry adaptation**:

$$(T_I)^{t_1,\ldots,t_q}_{s_1,\ldots,s_p} = (\mathcal{Q}_I)^{t_1}_{n_1} \cdots (\mathcal{Q}_I)^{t_q}_{n_q} \cdot (\mathcal{Q}_I^T)^{m_1}_{s_1} \cdots (\mathcal{Q}_I^T)^{m_p}_{s_p} \cdot \mathcal{N}^{n_1,\ldots,n_q}_{m_1,\ldots,m_p}(\mathcal{D}_i).$$



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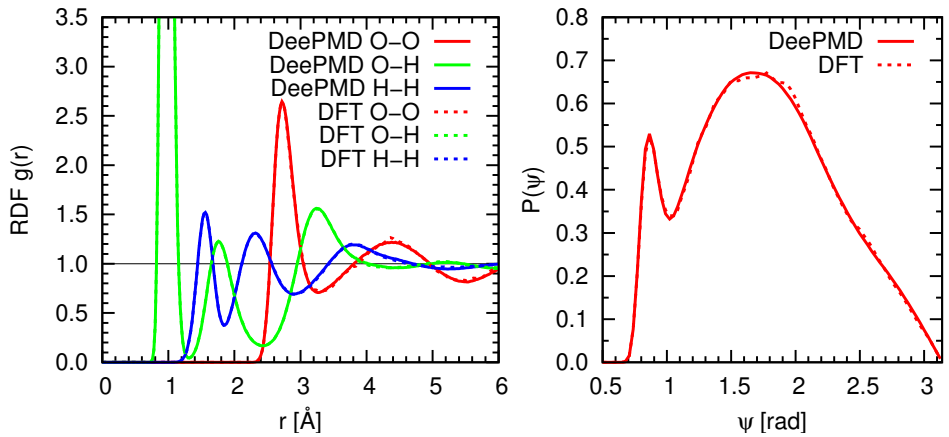
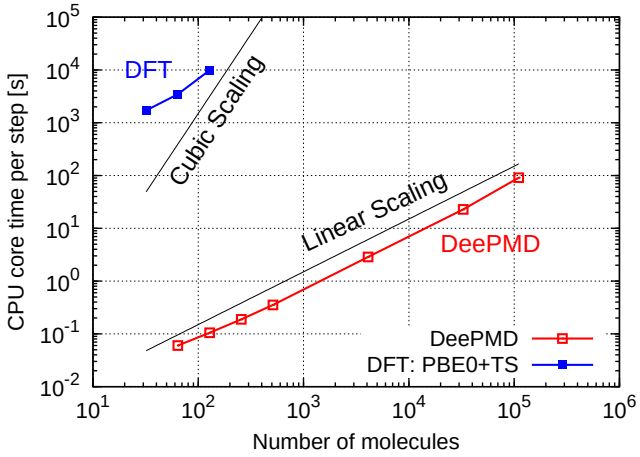
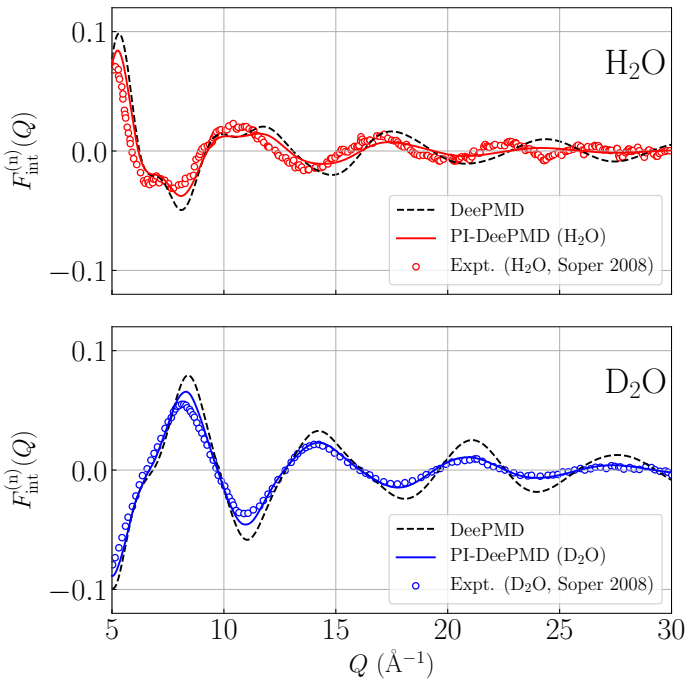
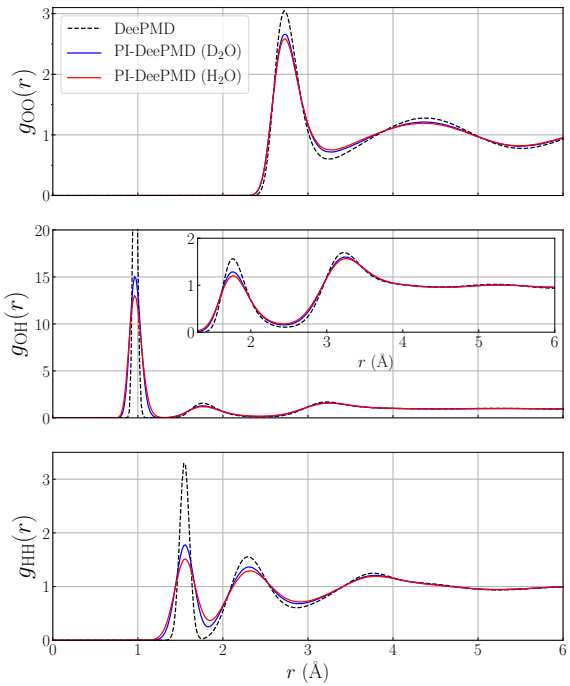
Water as an example: Structural properties









$g(r)$: radial distribution function;

$P(\phi)$: angular distribution function;

$F_{\text{int}}^{(n)}(Q)$: interference diff. cro. sec.

L. Zhang, J. Han, H. Wang, R. Car, W. E, PRL, 120, 143001 (2018);

H.-Y. Ko, L. Zhang, B. Santra, H. Wang, W. E, R. DiStasio, R. Car, Mol. Phys. 117(22): 3269-81 (2019).

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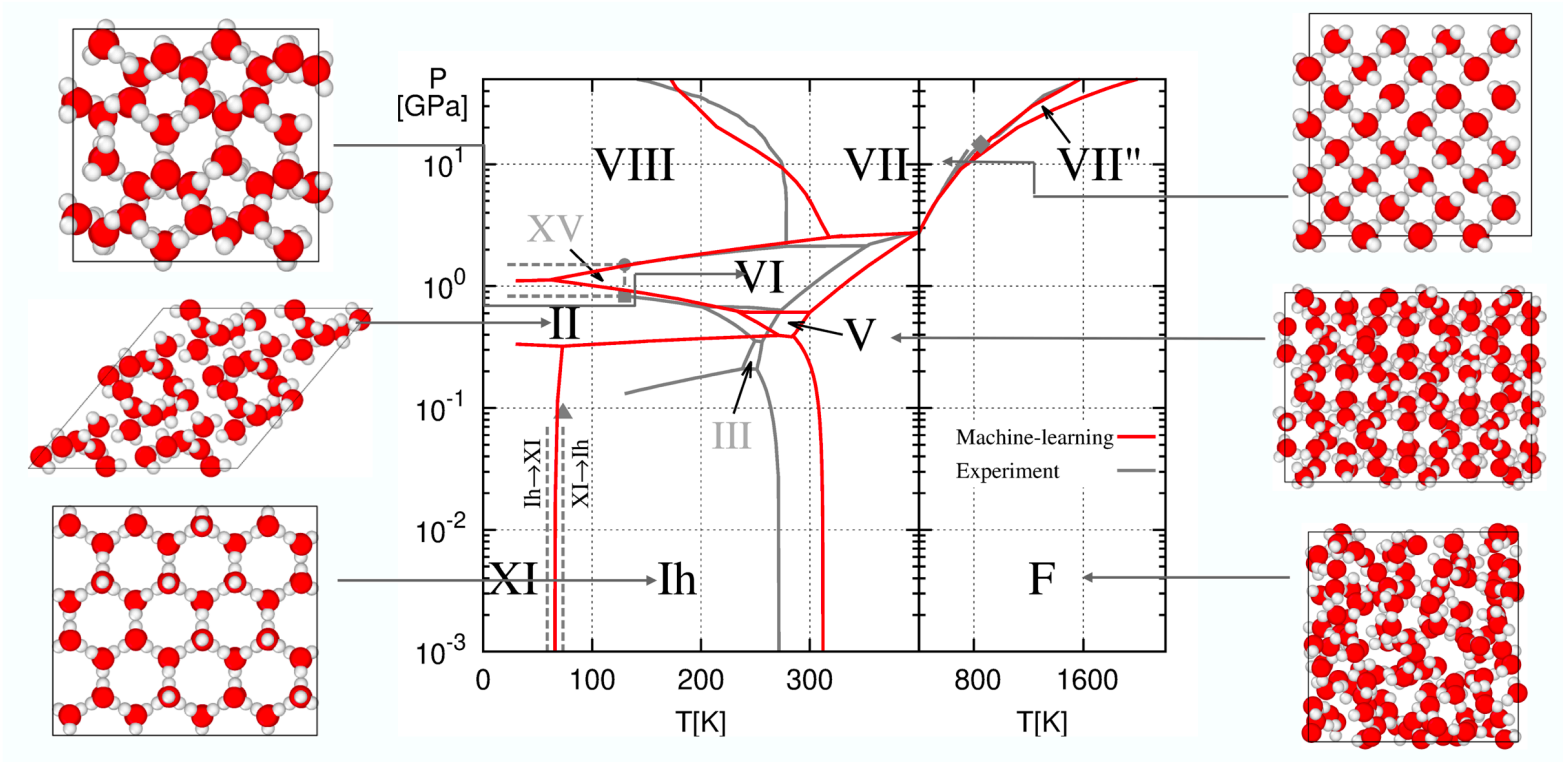
Water as an example: phase diagram

Featured in Physics | Editors' Suggestion

Phase Diagram of a Deep Potential Water Model

Linfeng Zhang, Han Wang, Roberto Car, and Weinan E
Phys. Rev. Lett. **126**, 236001 – Published 9 June 2021

Physics See synopsis: An Efficient Way to Predict Water's Phases



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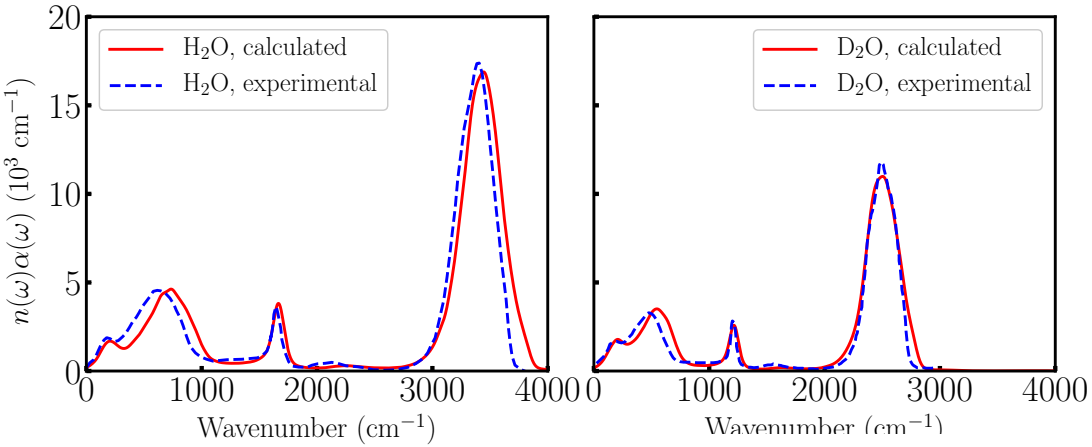
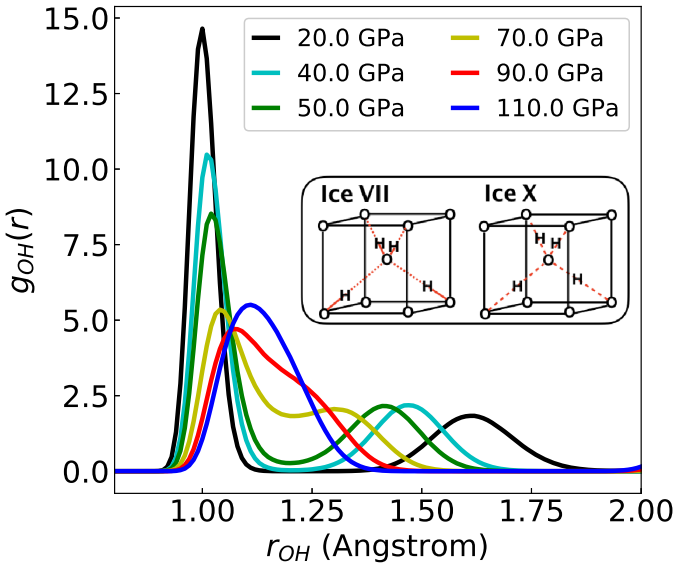
Water as an example: Infrared spectra

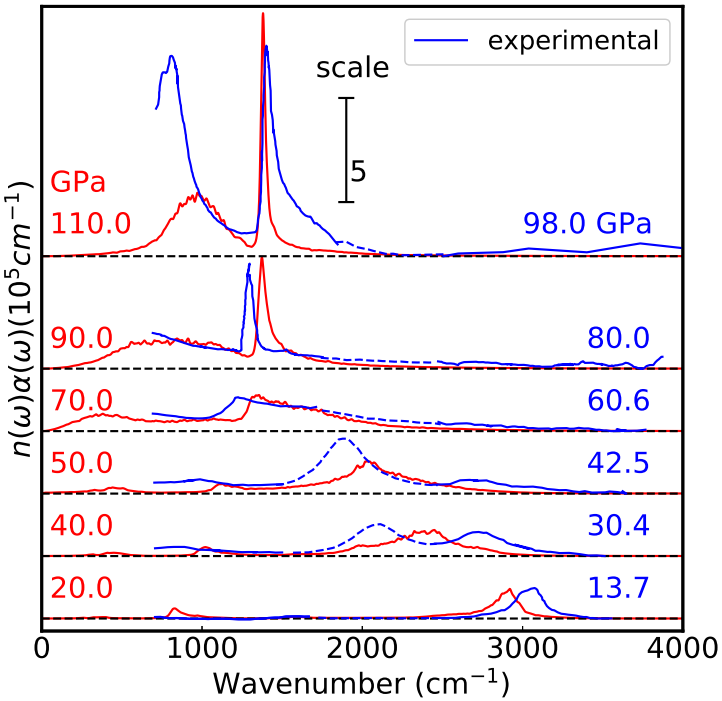


$$\alpha(\omega)n(\omega) = \frac{2\pi\beta}{3cV}\int dt e^{-i\omega t}\langle \dot{\boldsymbol{M}}(0)\cdot\dot{\boldsymbol{M}}(t)\rangle.$$

← IR spectra of light and heavy water at 300 K (at the level of PBE0+TS).



↑ O-H RDF calculated at T=300 K.



←

IR spectra calculated at T=300 K.

L. Zhang, M. Chen, X. Wu. H. Wang, W. E, R. Car, PRB, 102(2020) No. 4, 041121.

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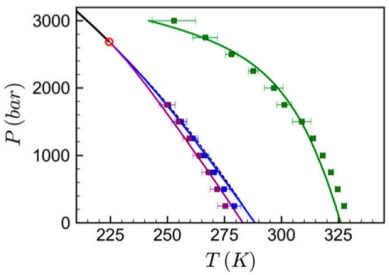
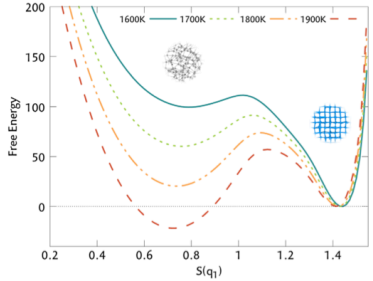
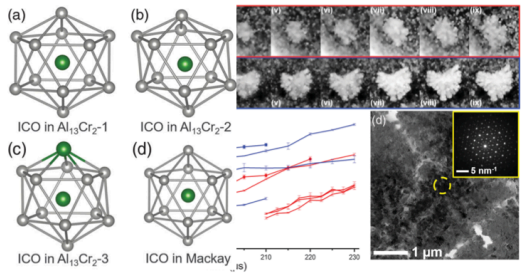
More applications



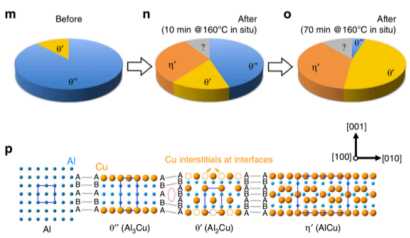
Liquid-liquid phase transition
Gartner III et al, PNAS, 117, 42 (2020)



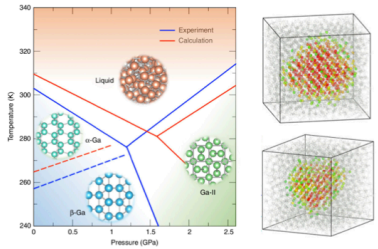
Nucleation in silicon
Bonati et al, PRL 121, 265701 (2018)



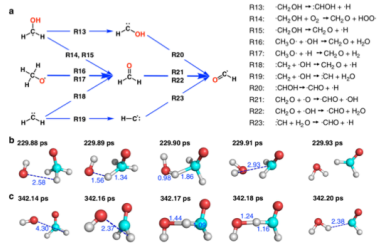
Structure in quasicrystal growth
Han et.al, PRL 125, 195503 (2020)



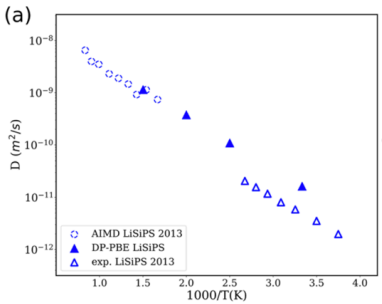
Nucleation of strengthening precipitates
Bourgeois et al, Nat Comm, 11 1248 (2020)



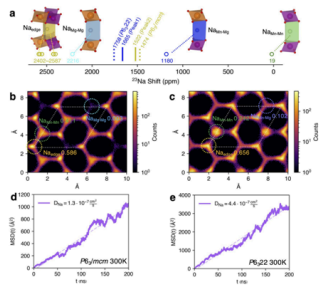
Phase diagram of gallium
Niu et al, Nat Comm, 11 2654 (2020)



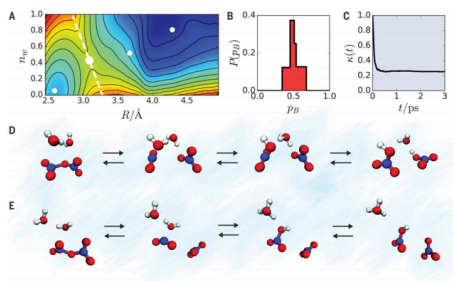
Complex reactions in combustion
Zeng et al, Nat Comm, 11 5713 (2020)



Diffusion property of superionic solids
Huang, et al, JCP 154, 094703 (2021)



Alkali-Ion Dynamics in Battery Materials
Lin, et al, Angew.Chem. Int. Ed. 2021, 60



Reactive uptake of N2O5
Galib et al., Science 371, 921–925 (2021)

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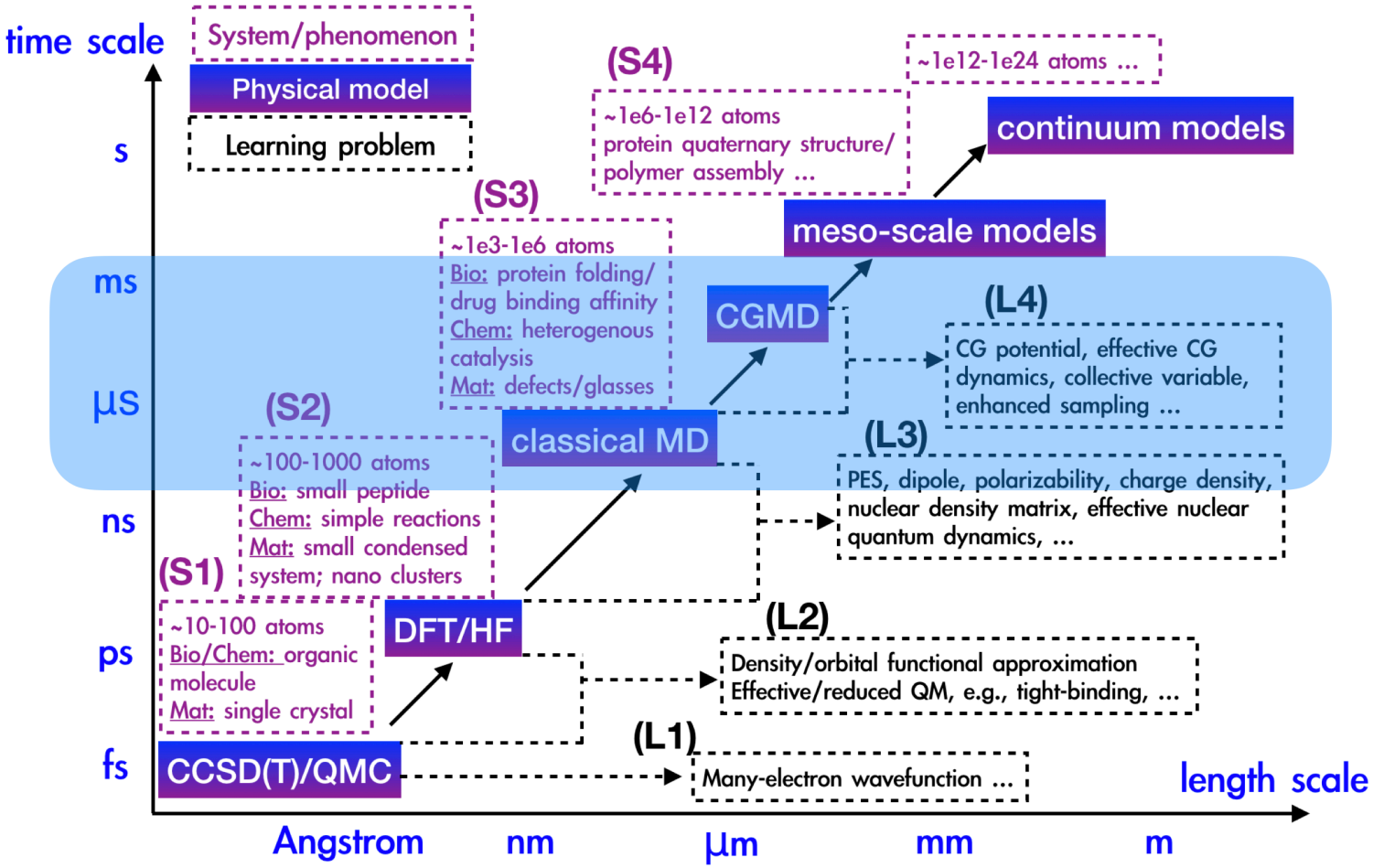
Problem 2: from atoms to coarse-grained particles



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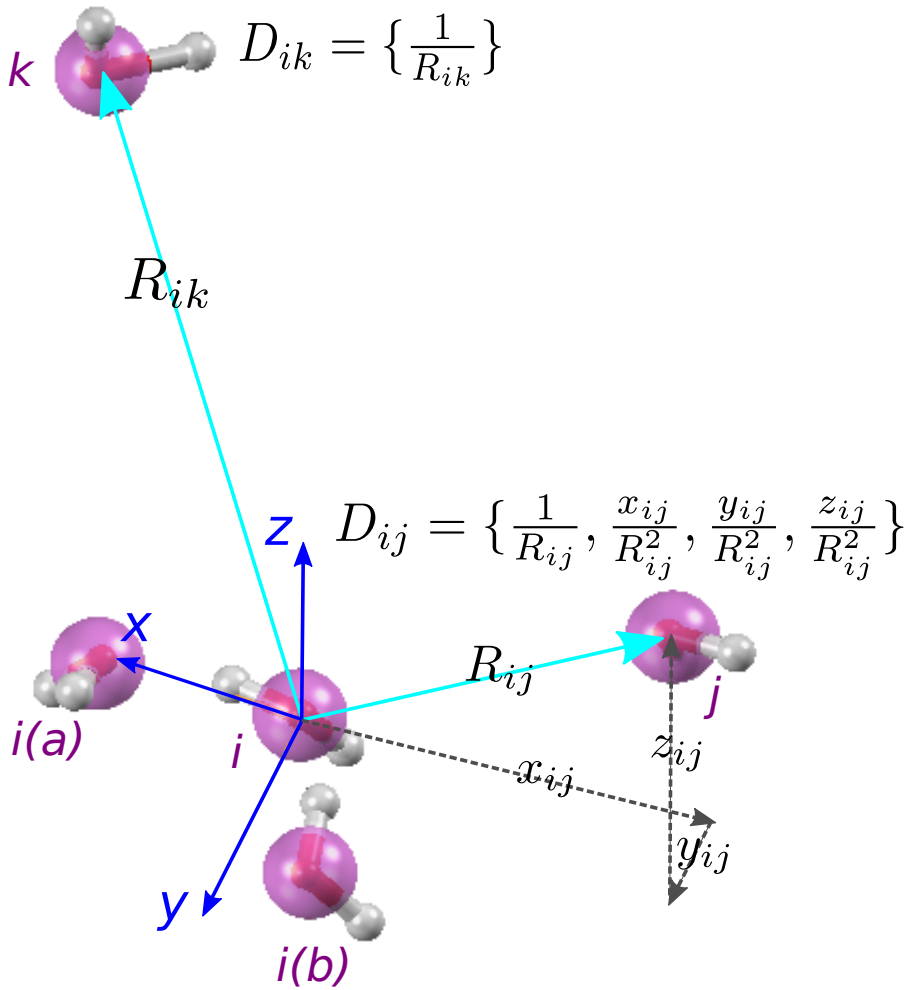
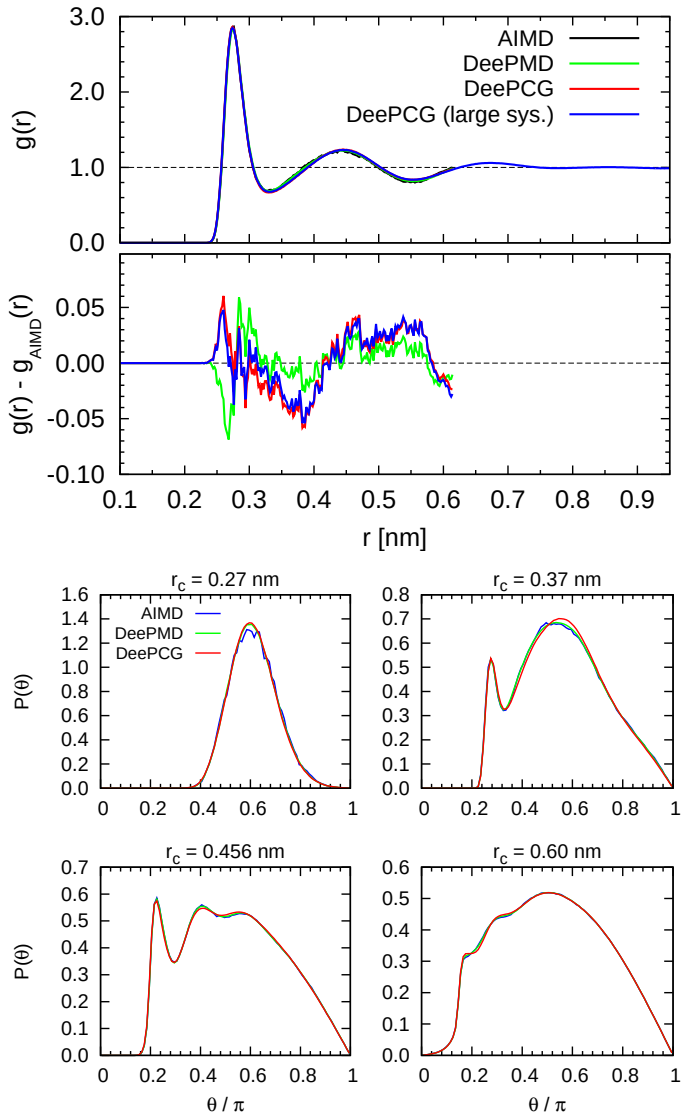
Problem 2: from atoms to coarse-grained particles





Zhang et.al. J. Chem. Phys., 149, 034101 (2018)

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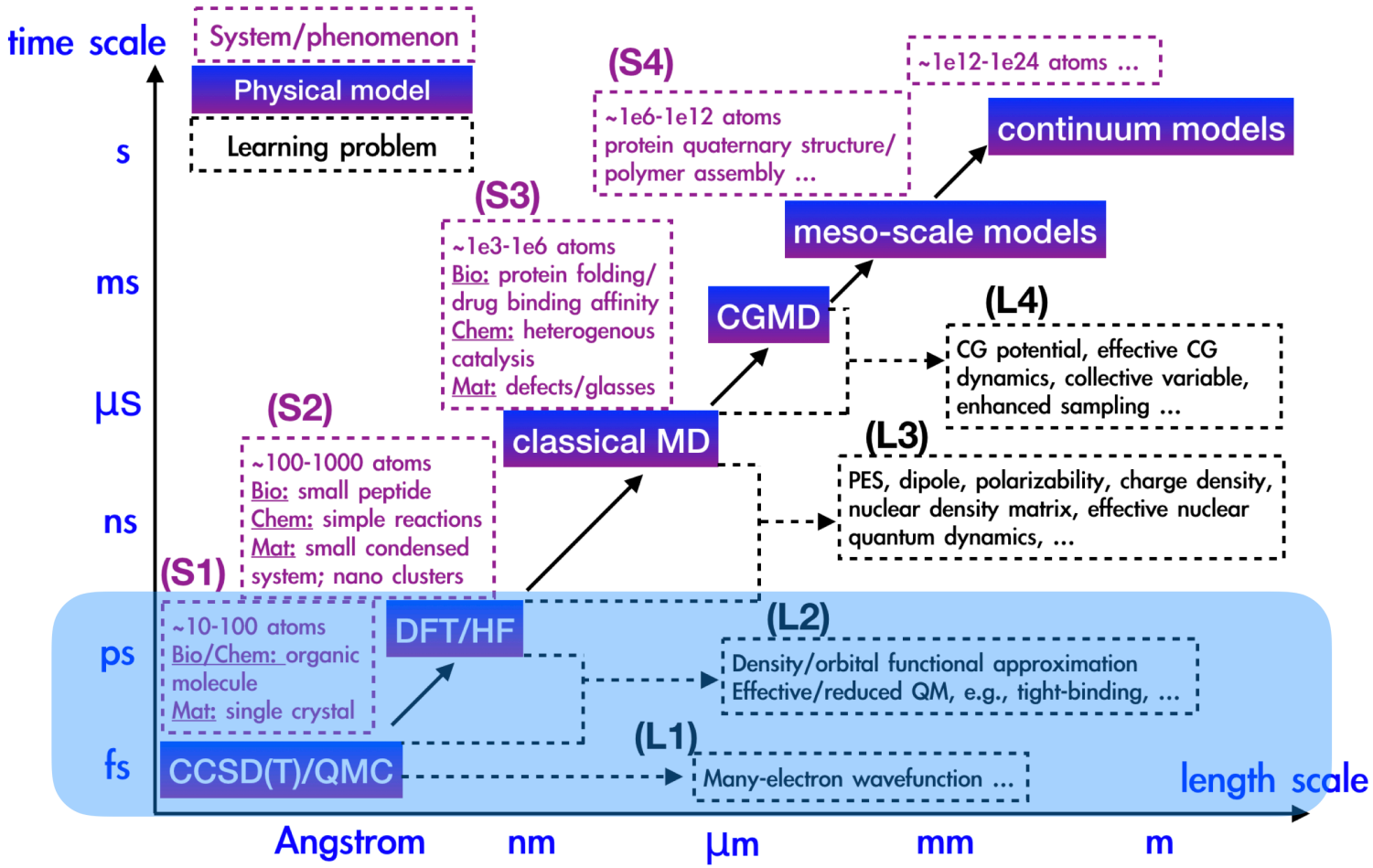
Problem 3: from QM to DFT



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Problem 3: from QM to DFT

1. **Energy Model (Deep post-HF, DeePHF)**:
   $E_{\mathrm{tot}} = E_{\mathrm{HF}}\left[\{\psi_i^0\}\right] + E_c\left[\{\psi_i^0\}|\omega\right]$
   input: HF orbitals $\{\psi_i^0\}$;
   output: "correlation" energy E_c.

2. **Self Consistent Model (Deep Kohn Sham, DeePKS)**:
   $E_{\mathrm{tot}} = \min_{\langle\psi_i|\psi_j\rangle=\delta_{ij}} E_{\mathrm{HF/KS}}\left[\{\psi_i\}\right] + E_c\left[\{\psi_i\}|\omega\right]$;
   input: atomic coordinates and nuclear charges;
   output: ground-state energy and electron density.

DeePHF: Y. Chen, et al, J. Phys. Chem. A, 2020, 124(2020) No. 35, 7155-7165

DeePKS: Y. Chen, et al, J. Chem. Theory Comput. 2021, 17, 1, 170-181

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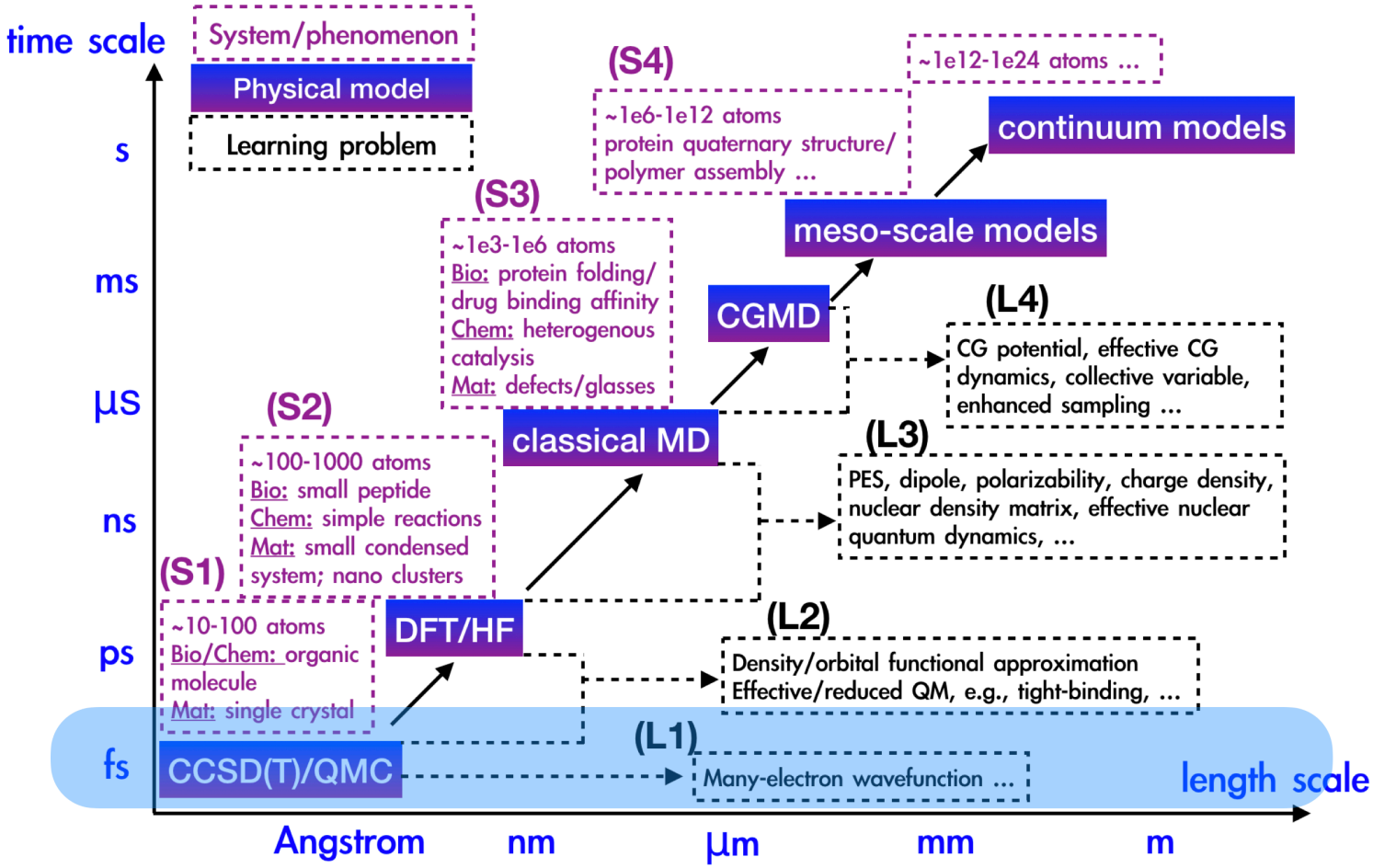
Problem 4: Many-electron Schrödinger equation



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NN-based algorithms for Schrödinger equation

- Carleo and Troyer (2016): RBM for spin problem
- Han, Zhang and E (2018): NN-based models for electron problem improving the Jastrow factor, simple ansatz for the anti-symmetric part
- dealing with the backflow:
  - Luo and Clark (2018): Additive

$$\hat{\phi}^{\sigma}_{\mu,i}(\mathbf{R}) = \phi^{\sigma}_{\mu}(\mathbf{r}_i) + f^{\sigma}_{\theta,\mu,i}(\mathbf{R})$$

  - PauliNet (Hermann et al 2019): multiplicative

$$\hat{\phi}^{\sigma}_{\mu,i}(\mathbf{R}) = \phi^{\sigma}_{\mu}(\mathbf{r}_i) f^{\sigma}_{\theta,\mu,i}(\mathbf{R})$$

  - FermiNet (Pfau et al. 2020): compositional

$$\hat{\phi}^{\sigma}_{\mu,i}(\mathbf{R}) = \phi^{\sigma}_{\mu}(f^{\sigma}_{\theta,\mu,i}(\mathbf{R}))$$

still lack systematic approaches!

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The optimization problem

Data generation (Labeling) is important.
It is expensive to calculate the labels $f(\boldsymbol{x}_i)$.

$$\min_{\boldsymbol{w}} \frac{1}{\|\mathcal{D}\|} \sum_{i \in \mathcal{D}} l(f^{\boldsymbol{w}}(\boldsymbol{x}_i), f(\boldsymbol{x}_i))$$

What are the best data sets, which result in a uniformly accurate model upon training?

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The EELT procedure for concurrent learning

Start with only a micro-scale model and repeat the following steps:

- **Exploration**: explore the configuration space
- **Examination**: decide which configurations need to be labeled;
- **Labeling**: compute the micro-scale solutions for the configurations that need to be labeled. This is our data set;
- **Training**: train the macro-scale model, and use it to help the exploration.

How to explore?
Judiciously employ the currently learned ML model.

How to decide?
Need good error indicators.

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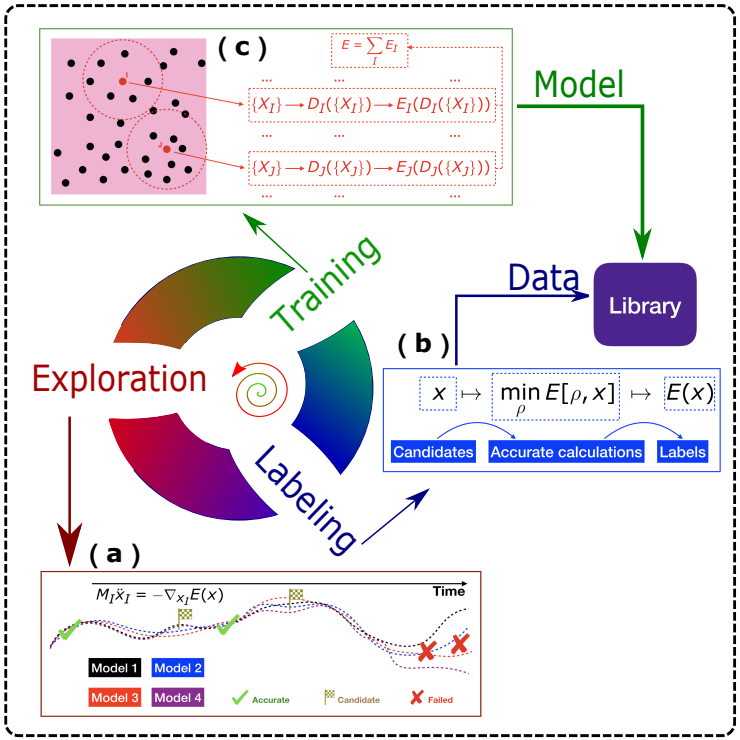
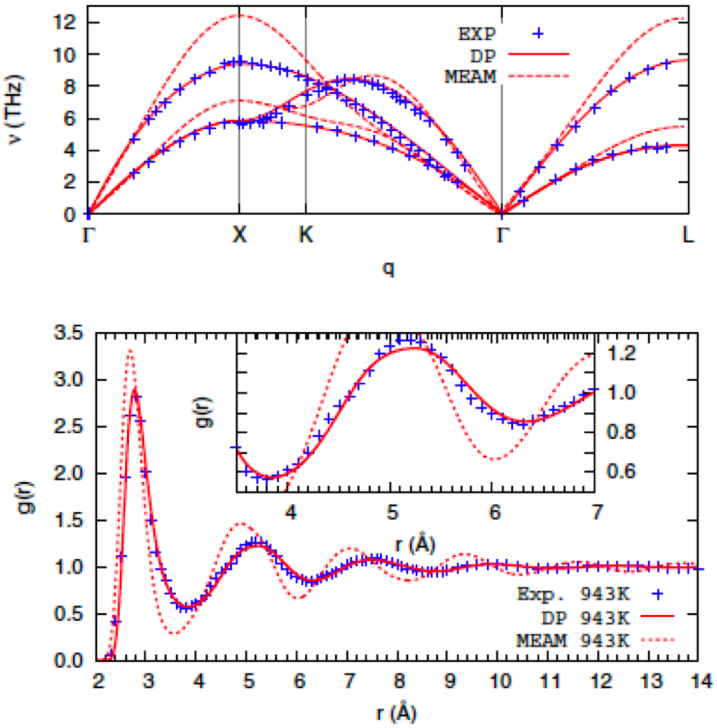
Deep Potential Generator (DP-GEN)





Labeling when model deviation is large: $\epsilon = \max_i \sqrt{\langle \|\boldsymbol{f}_i - \langle \boldsymbol{f}_i \rangle\|^2 \rangle}$.

See, e.g. principle of maximal disagreement in "Query by Committee" by Seung, Opper, Sompolinsky (1992).

Deep Potential Generator (DP-GEN), L. Zhang, D. Lin, H. Wang, R. Car, W. E, Phys. Rev. Mat. 3, 023804 (2019)

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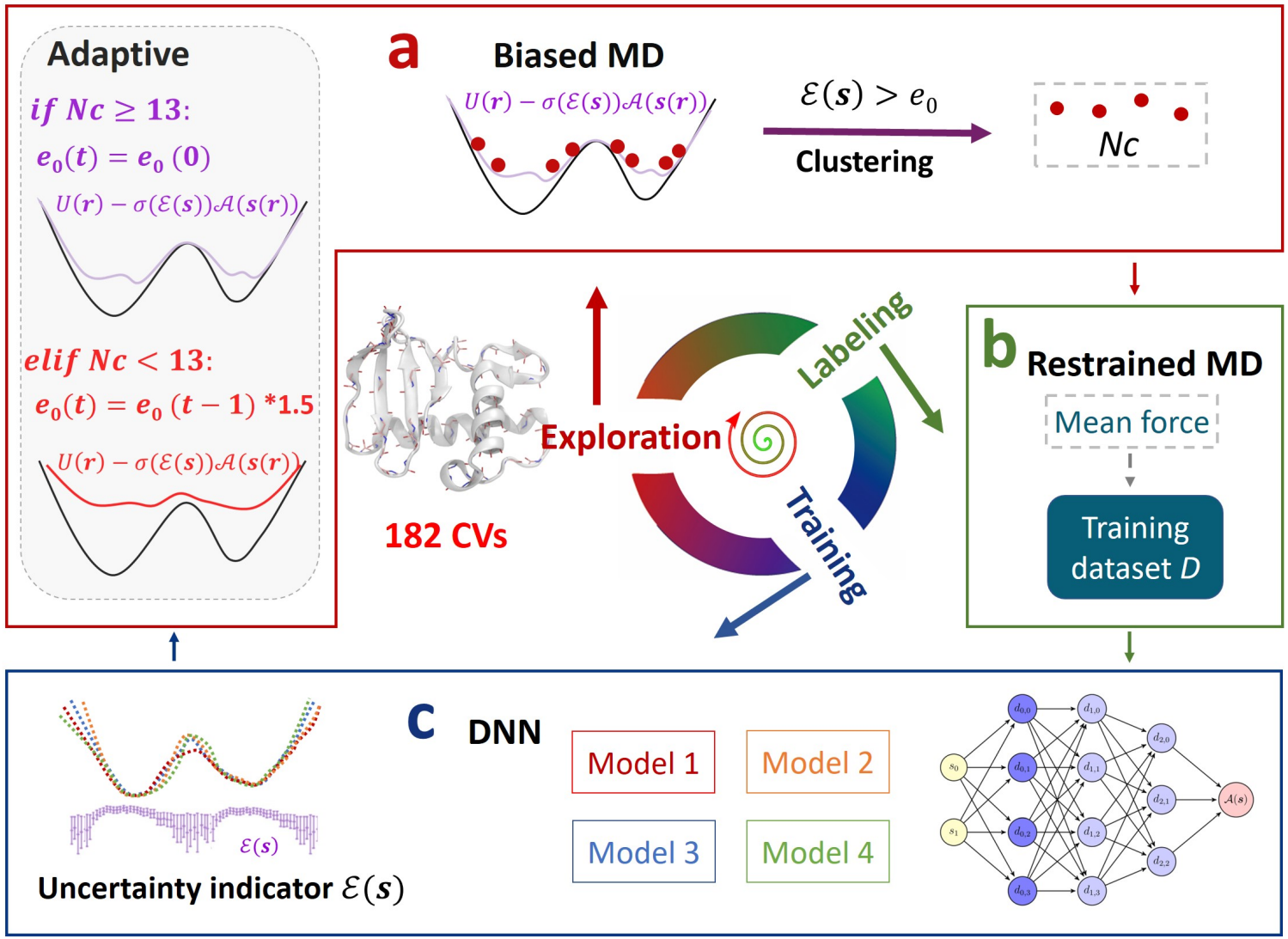
Reinforced dynamics (RiD) for protein structure refinement



L. Zhang, H. Wang, W. E, J. Chem. Phys. 148, 124113 (2018).

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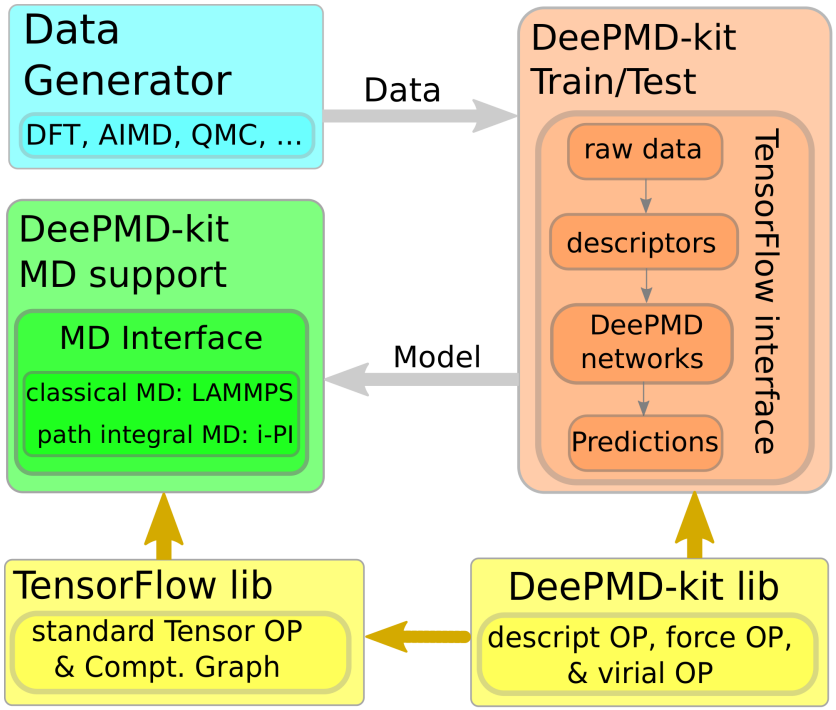
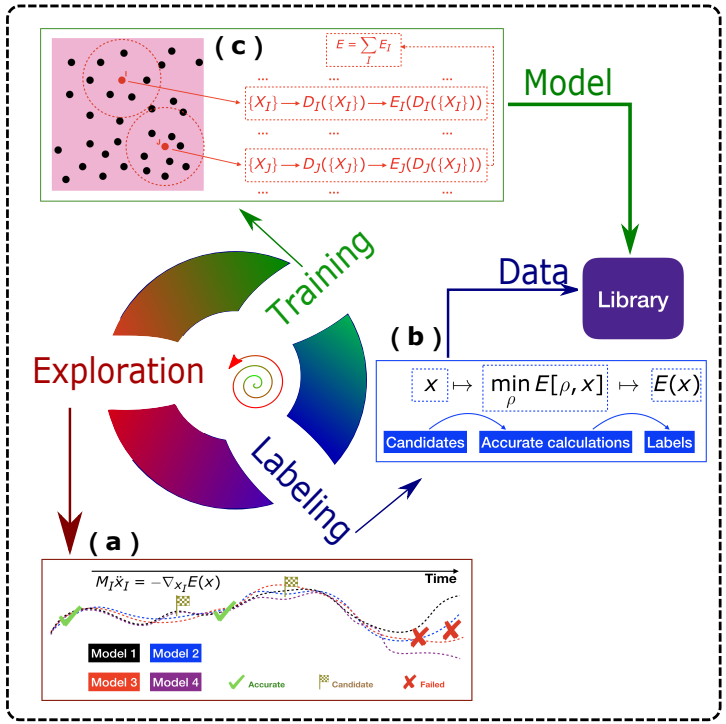
Open-source softwares: DeePMD-kit, DeePKS-kit, DP-GEN, etc.





Free download from https://github.com/deepmodeling/

H. Wang, et al, Comp. Phys. Comm., 0010-4655 (2018); Y. Zhang, et al, Comp. Phys. Comm. (2020): 107206.

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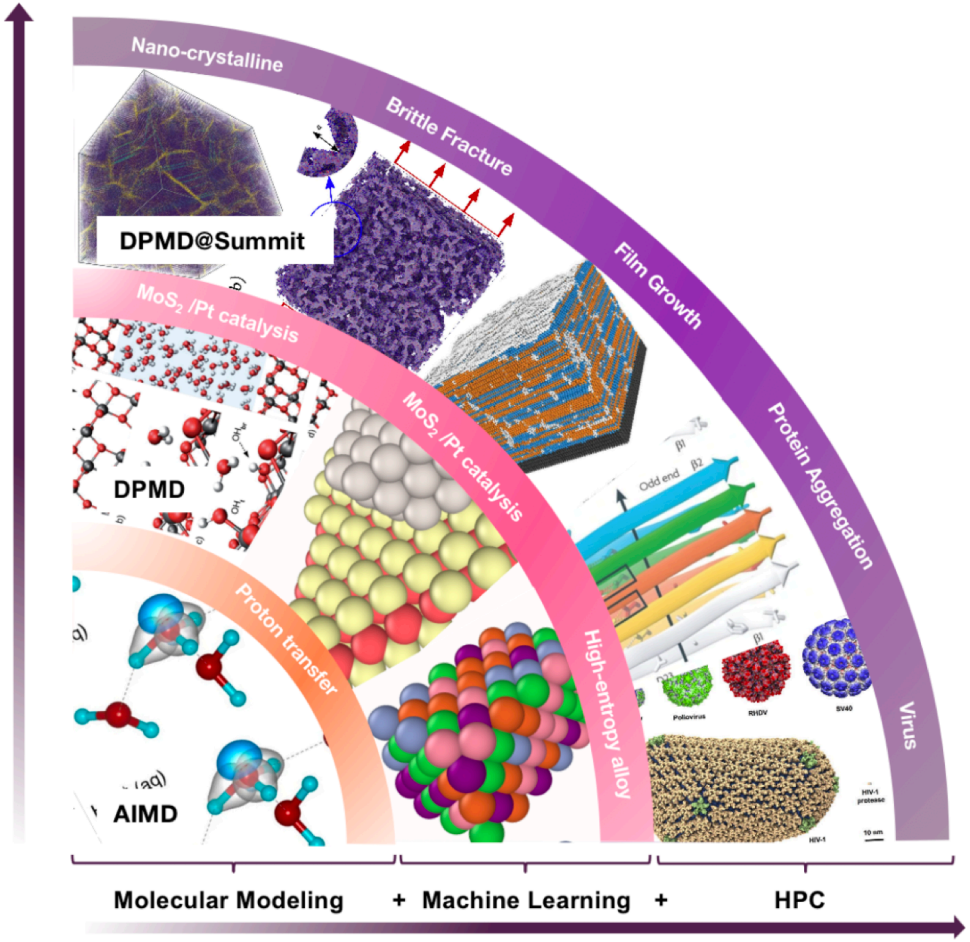
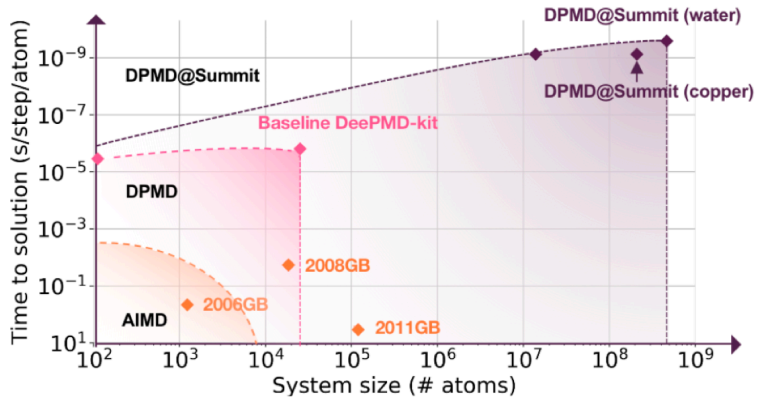
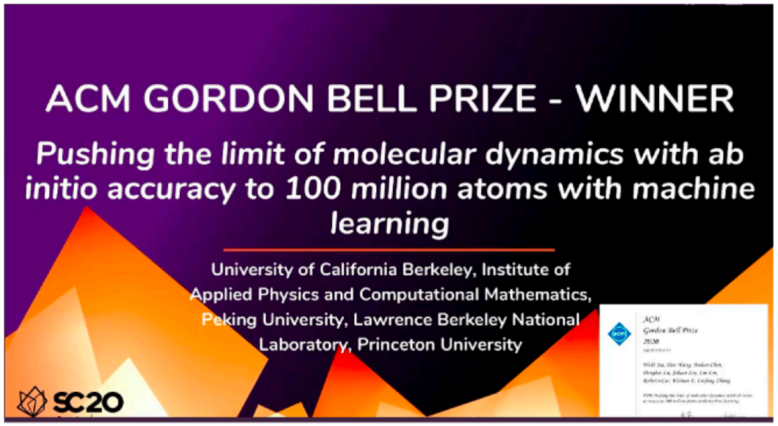
Pushing MD with *ab initio* accuracy to 10^8 atoms







Weile Jia, et al, SC20: International Conference for High Performance Computing, Networking, Storage and Analysis

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The next-generation infrastructures

New paradigm:
a seamless integration: **MM+ML+HPC**.

New challenges:

- **hardware**: heterogeneous performance and scale;
- **software**: different code styles/conventions;
- **expertise**: need people from very different backgrounds.

Joint effort needed!

- **general-purpose platform**: DP series for learning-assisted molecular simulation;
- **problem-oriented platform**: Hermite for drug design.

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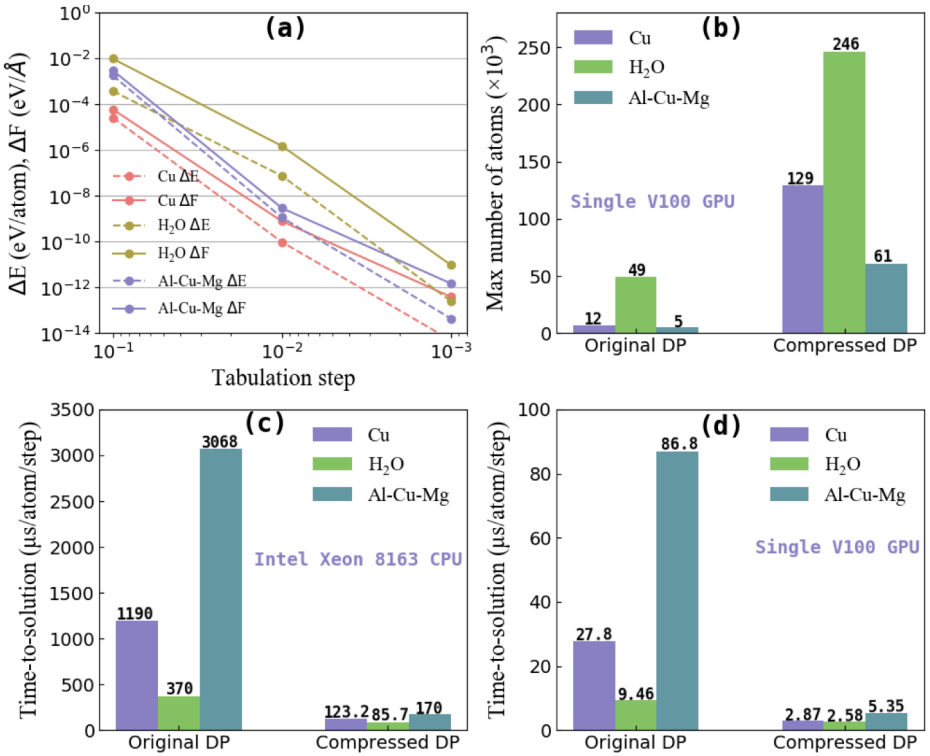
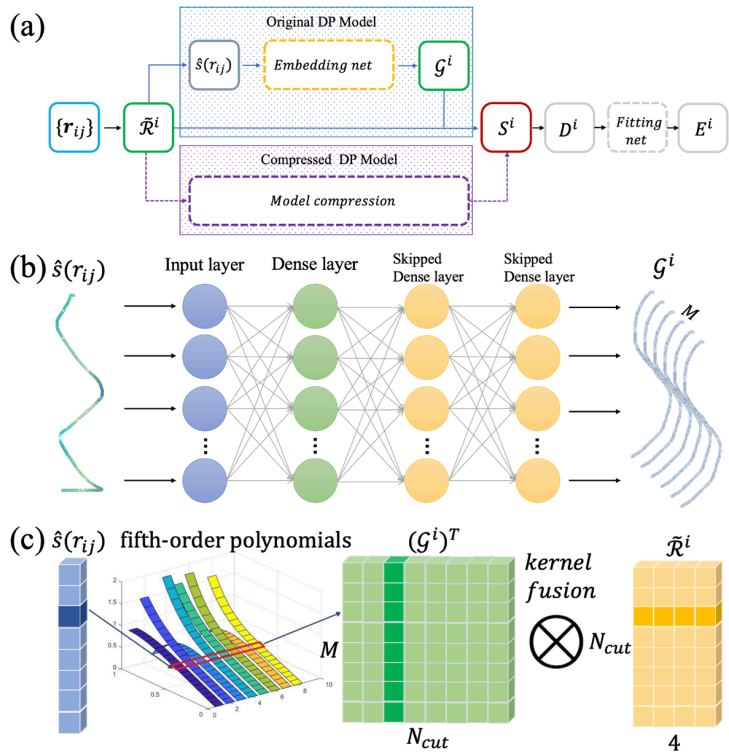
DP model compression





Denghui Lu, et al, DP Train, then DP Compress: Model Compression in DeePMD, arXiv:2107.02103

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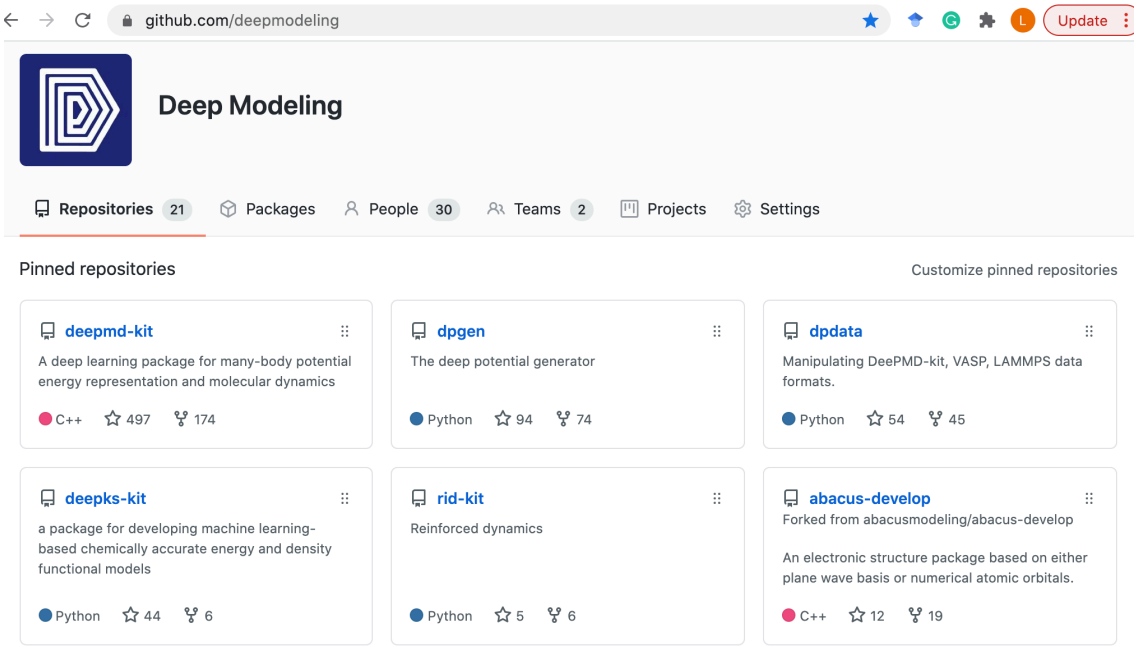
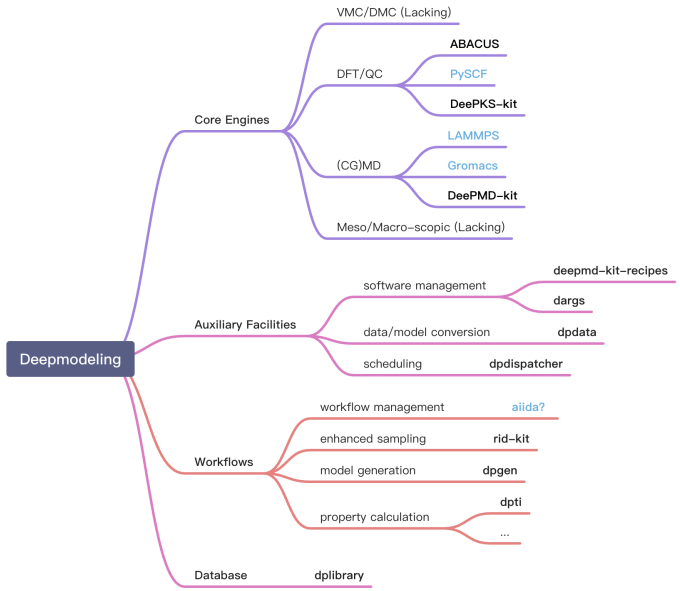
DeepModeling open-source community





See our DeepModeling Manifesto here:
https://github.com/deepmodeling/community

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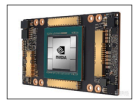
The engineerization process of "AI+Science"

	Scale Engineering: Computing Oriented	Data Engineering: Physics Oriented	Performance Engineering: Algorithm Oriented
Past Practice	Spark, kubernetes, slurm workload manager Big Data; Internet Service; High Performance Computing	IMAGENET, Open SLR, RCSB PDB PROTEIN DATA BANK Image Database; **Speech Database**; **Laboratory Database**	   DeePMD on Summit; GPU for AI; Anton for MD
New Demand	☐Large-scale parallel simulation ; ☐Large-scale concurrent offline computing ; ☐Merge calls of multiple computing resource ; ☐Transregional data transfer, storage, and access ; ☐...	☐Effective data generation and collection; ☐Automated testing of data quality; ☐Pre-training Model based on scientific computing; ☐Models across migration scenarios; ☐...	☐Automated performance testing framework; ☐Ultimate optimization of algorithms; ☐Hardware-Software Co-design; ☐……

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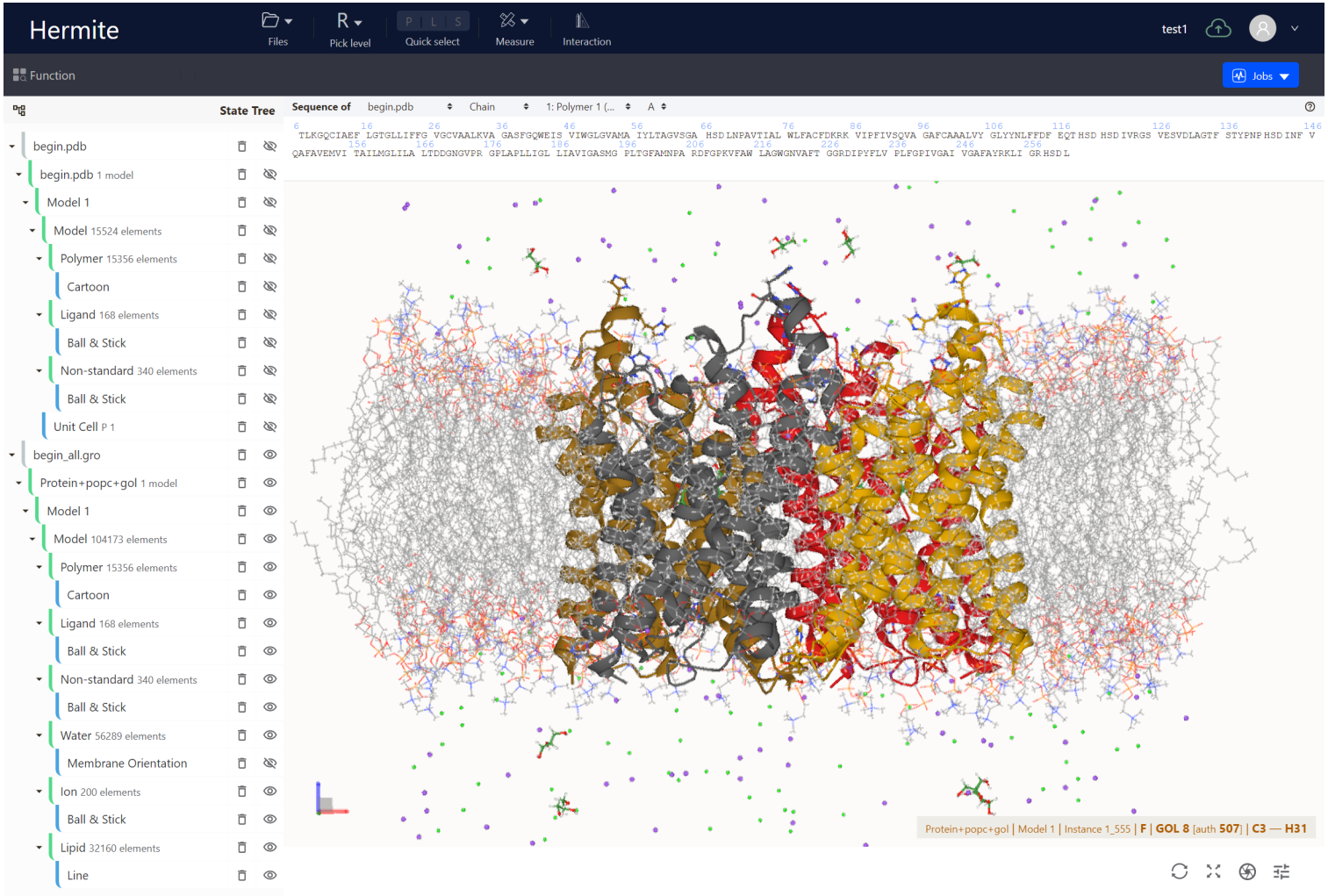
Hermite: a cloud-native and "AI+Science" solution for drug design



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Outline

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Conclusion and outlook

- **Learning assisted physical models:**
  - from CCSD(T) to DFT;
  - from DFT to MD;
  - from MD to CGMD.
- **Softwares and engineering efforts:**
  - DeePMD-kit, DP-GEN;
  - DP@HPC&Cloud, Hermite;
- **More challenges:**
  - QM: more efficient algorithm for strongly correlated systems;
  - MD: long-range electrostatics;
  - Dynamics at all scales.
  - etc.

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Welcome to DeepModeling!

The DeepModeling Manifesto

The integration of machine learning and physical modeling is changing the paradigm of scientific research. Those who hope to extend the frontier of science and solve challenging practical problems through computational modeling are coming together in new ways never seen before. This calls for a new infrastructure--new platforms for collaboration, new coding frameworks, new data processing schemes, and new ways of using the computing power. It also calls for a new culture—the culture of working together closely for the benefit of all, of free exchange and sharing of knowledge and tools, of respect and appreciation of each other's work, and of the pursuit of harmony among diversity.

The DeepModeling community is a community of such a group of people.

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- **Collaborators**: Jun Cheng, Mohan Chen, Tong Zhu, Marcos Andrade, Hsinyu Ko, Lin Lin, Weile Jia, Lei Wang, etc.
- ...

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