Image Credit:
NASA/JWST

AI-Accelereated Astrochemistry: NQE (Nuclear Quantum Effects) in Dust-catalyzed Molecular Hydrogen Formation

Main Manuscript: Yang, Wang, Li & Xu, 2025, arXiv:2509.25070

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When you know ANN-based AI generally comes as

high-dimensional functions,

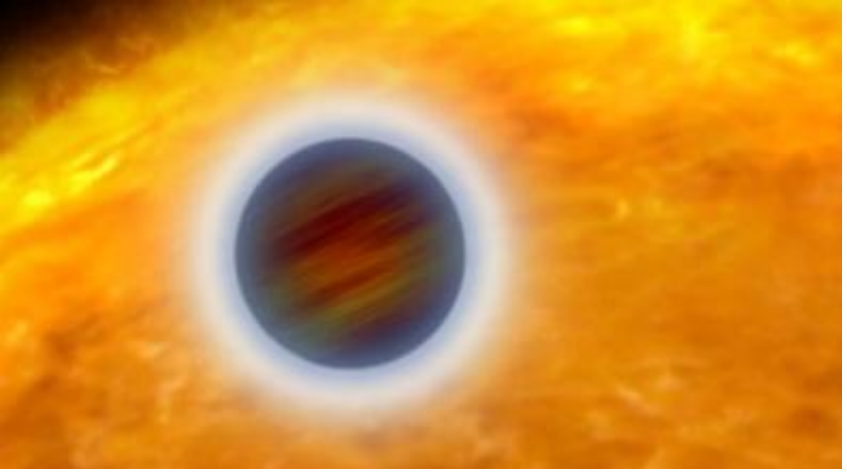
What can we simulation people do with AI?

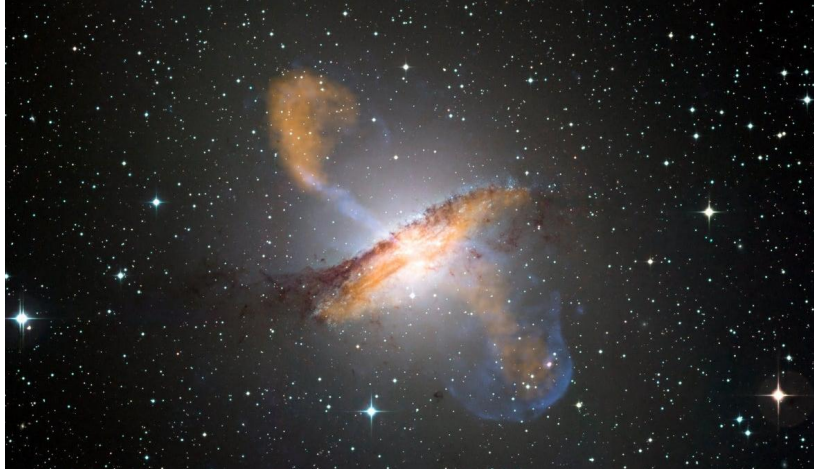
There is an classical Chinese joke:

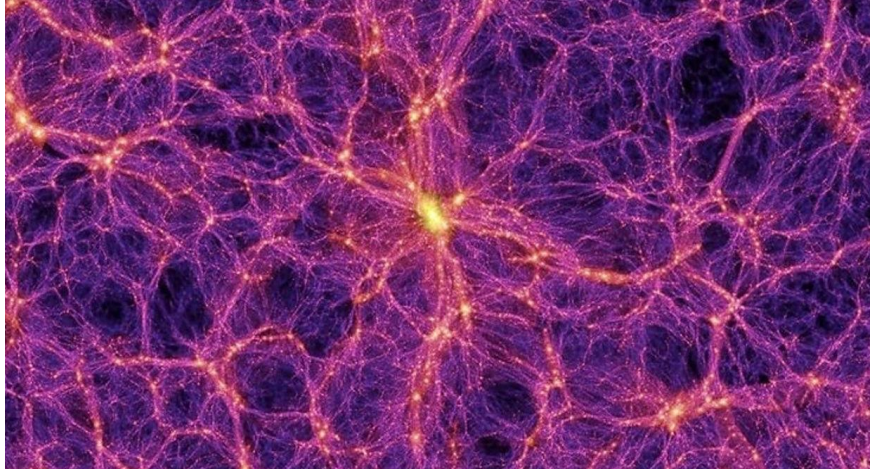
拿着一把锤子，看谁都是钉子

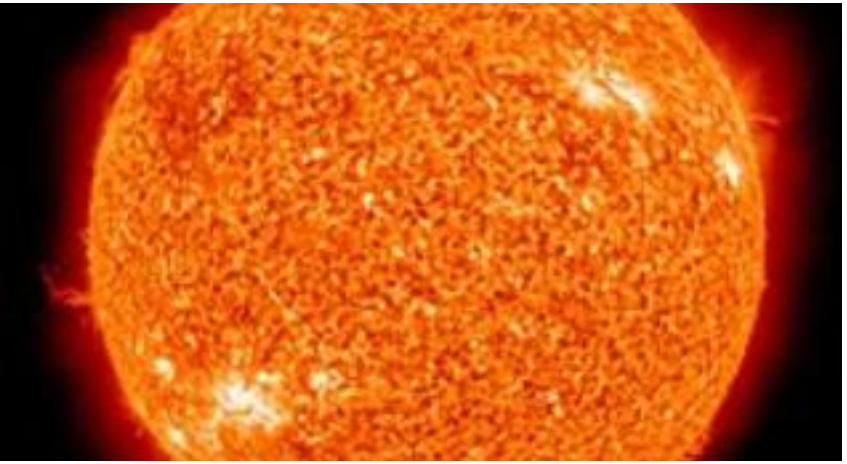
When your best tool is a hammer,

every job looks like a nail.









H_2 is Important in Multiple Aspects of Astrophysics

Molecular Clouds:
Formation, Evolution, and Star Formation

Star Formation and Supernova Feedback

Protoplanetary Disks and Planet Formation

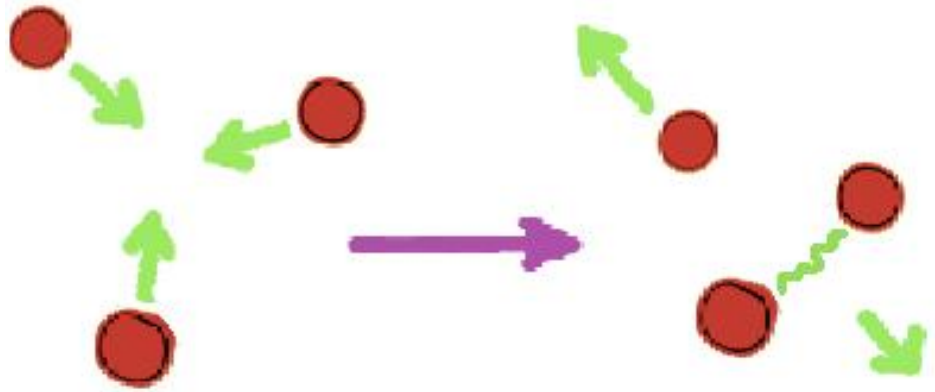
Galaxy Formation and Evolution

Intergalactic Physics and Structure Formation

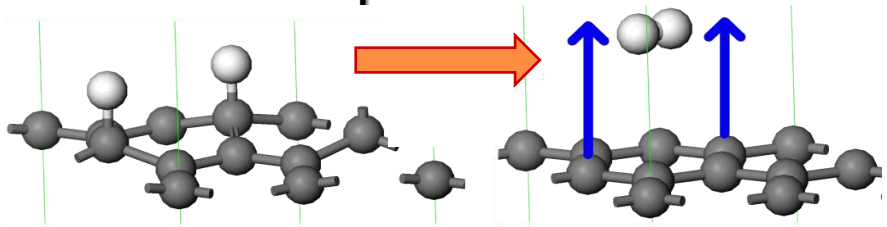
Gas Planets and Planetary Atmospheres

- Lack of lowest multipole moments: Efficient dispersal of momentum and energy
- Raw rate coefficient $\sim 10^{-29}\ \mathrm{cm}^3\ \mathrm{s}^{-1}$
- Common formation channels for H_2
  1. 3-Body reaction (requires $n(\mathrm{H}) > 10^6\ \mathrm{cm}^{-3}$)
  2. H^- reactions ejecting e^- (e.g. the Sun)
  3. **Dust-catalyzed reactions**

     Lattice vibrations (phonons…) for energy and momentum dispersal



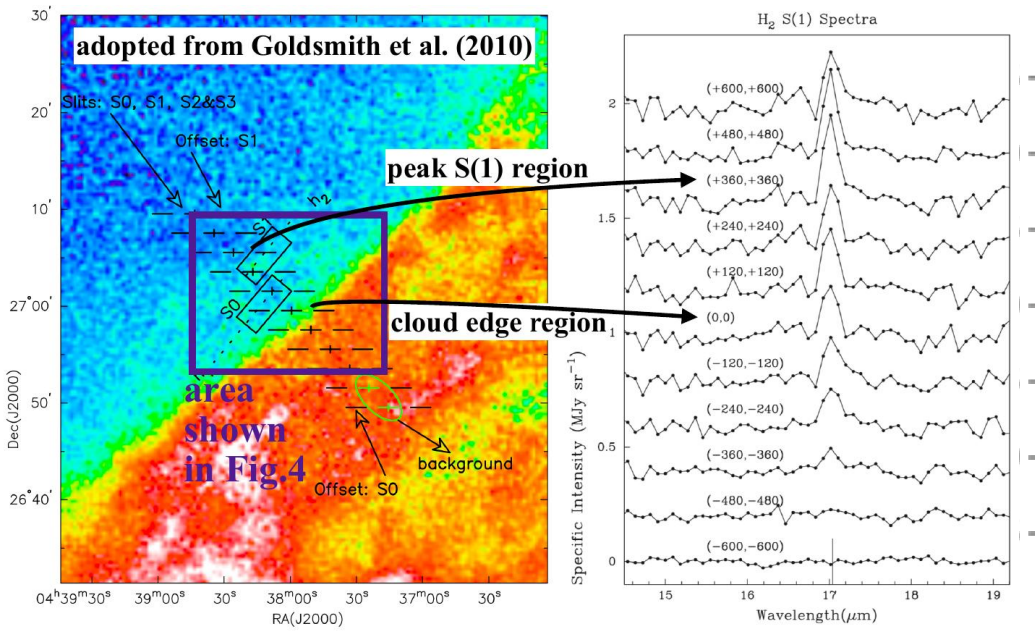
- In molecular gases, 1 or 3 are important
  - 1: turbulences; 2: ionization
  - 3: Godilocks temperature or some ad-hoc assumptions



Major Formation Channels of H_2

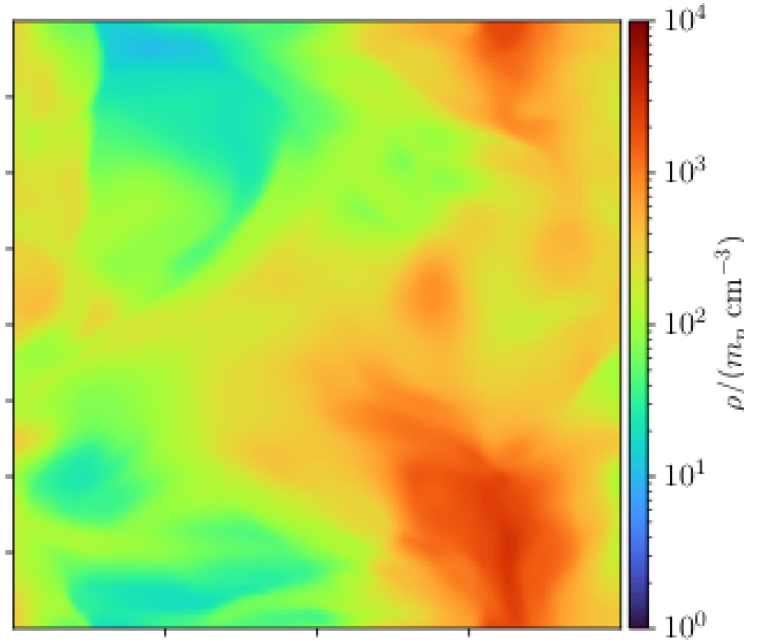
Hmmmmm...

Spitzer



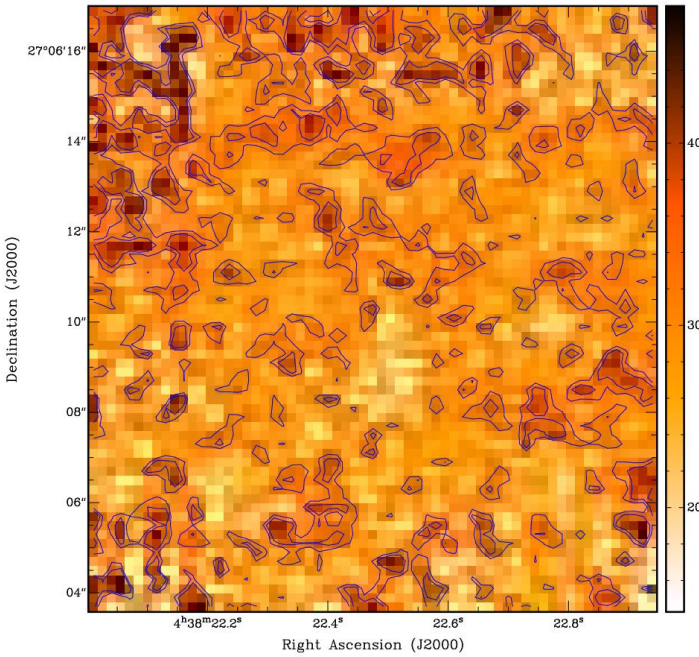
Goldsmith et al.
2010 ApJ, 715, 1370

GPU-based Simulations



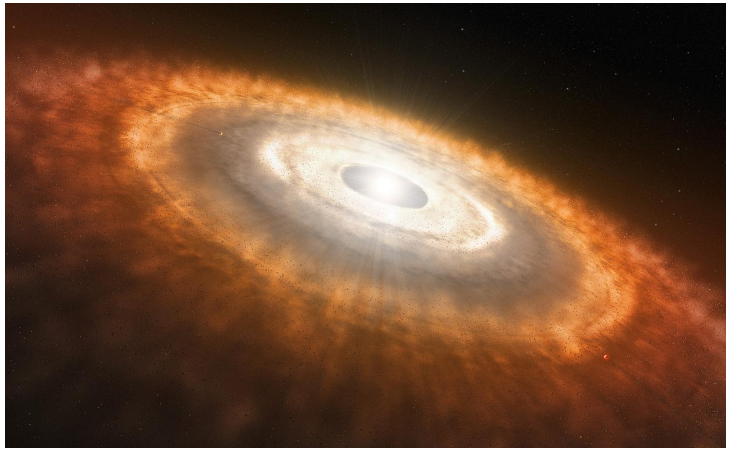
Yue, **Wang**, Bisbas, Quan, Li
2024 ApJ, 973, 37

JWST for S(1) of H_2

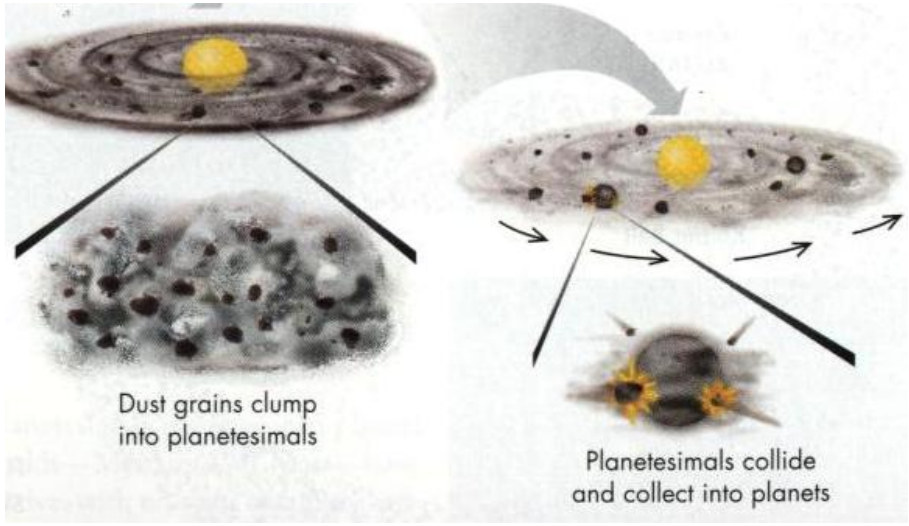


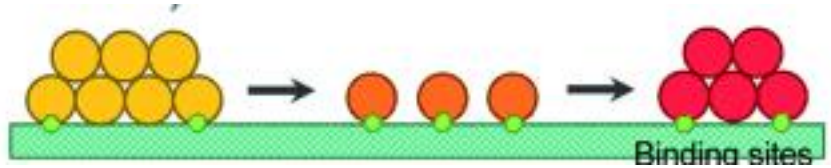
Goldsmith et al. (including L. Wang),
2025 ApJ, 985, 4

Turbulences? Not perfect morphological match



1.	X^+	+	gr^{2-}	$\longrightarrow$	gr^-	+	X
2.	X^+	+	gr^-	$\longrightarrow$	gr	+	X
3.	e^-	+	gr^-	$\longrightarrow$	gr^{2-}		
4.	e^-	+	gr	$\longrightarrow$	gr^-		
5.	e^-	+	gr^+	$\longrightarrow$	gr		
6.	e^-	+	gr^{2+}	$\longrightarrow$	gr^+		
7.	gr^+	+	gr^-	$\longrightarrow$	gr	+	gr
8.	gr^{2+}	+	gr^{2-}	$\longrightarrow$	gr	+	gr
9.	gr^+	+	gr^{2-}	$\longrightarrow$	gr^-	+	gr
10.	gr^-	+	gr^{2+}	$\longrightarrow$	gr^+	+	gr

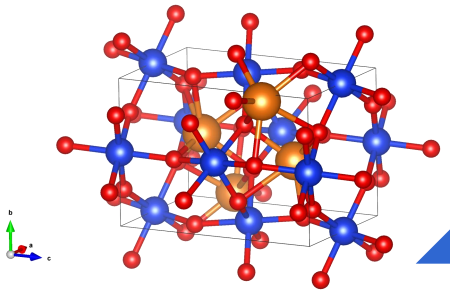




Dust Grains Have Multiple Roles...

Microscopic Dust Grain Processes

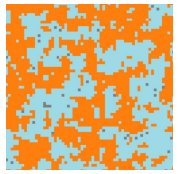
Macroscopic Astrophysical Observables



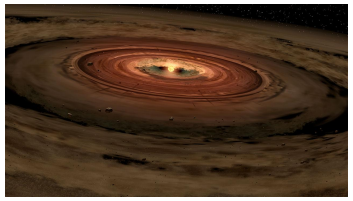
DPMD

for Atomic Interactions

KMC for "Medium" Scale Modeling

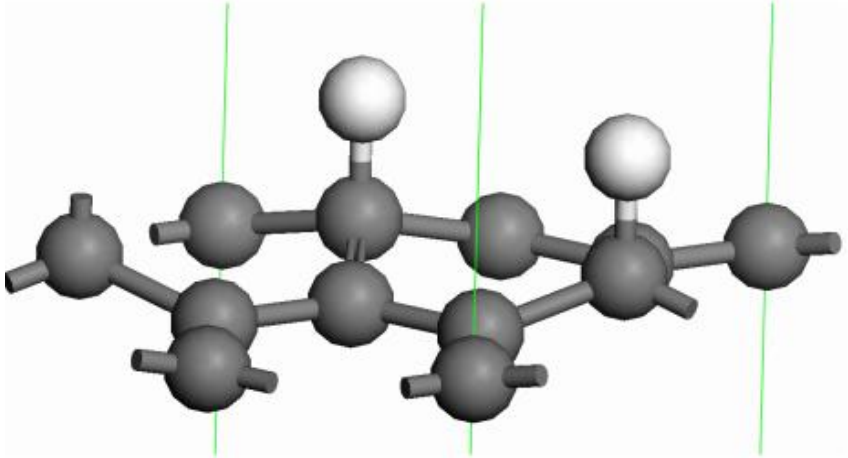


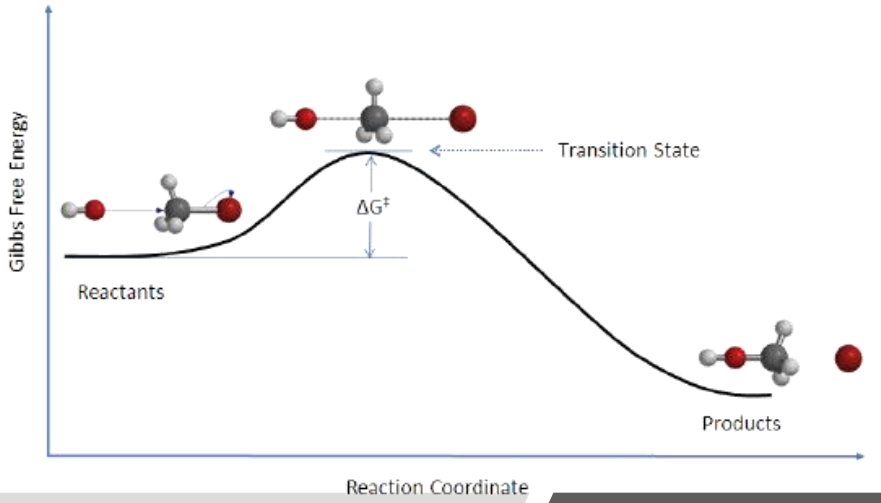
Astrophysical Simulations for Observables



… Consistently, with More Observables

- Typical side length of bonds:
  - C-C bond in graphene: 0.142 nm
  - H-H bond in H_2: 0.074 nm
- Typical Strength of bonds
  - H-H bond in H_2: $\sim 4.5\ \mathrm{eV}$
  - C-H bond on graphene (chemisorbed): $> 0.5\ \mathrm{eV}$
- $\exp(-0.5\ \mathrm{eV}/k_{\mathrm{B}}\ 20\ \mathrm{K}) \sim 10^{-108}$
- Previously thought to be physisorbed, Godilocks soup:
  - Not too hot to avoid instant desorption
  - Not too cold to inhibit motion on grain surfaces



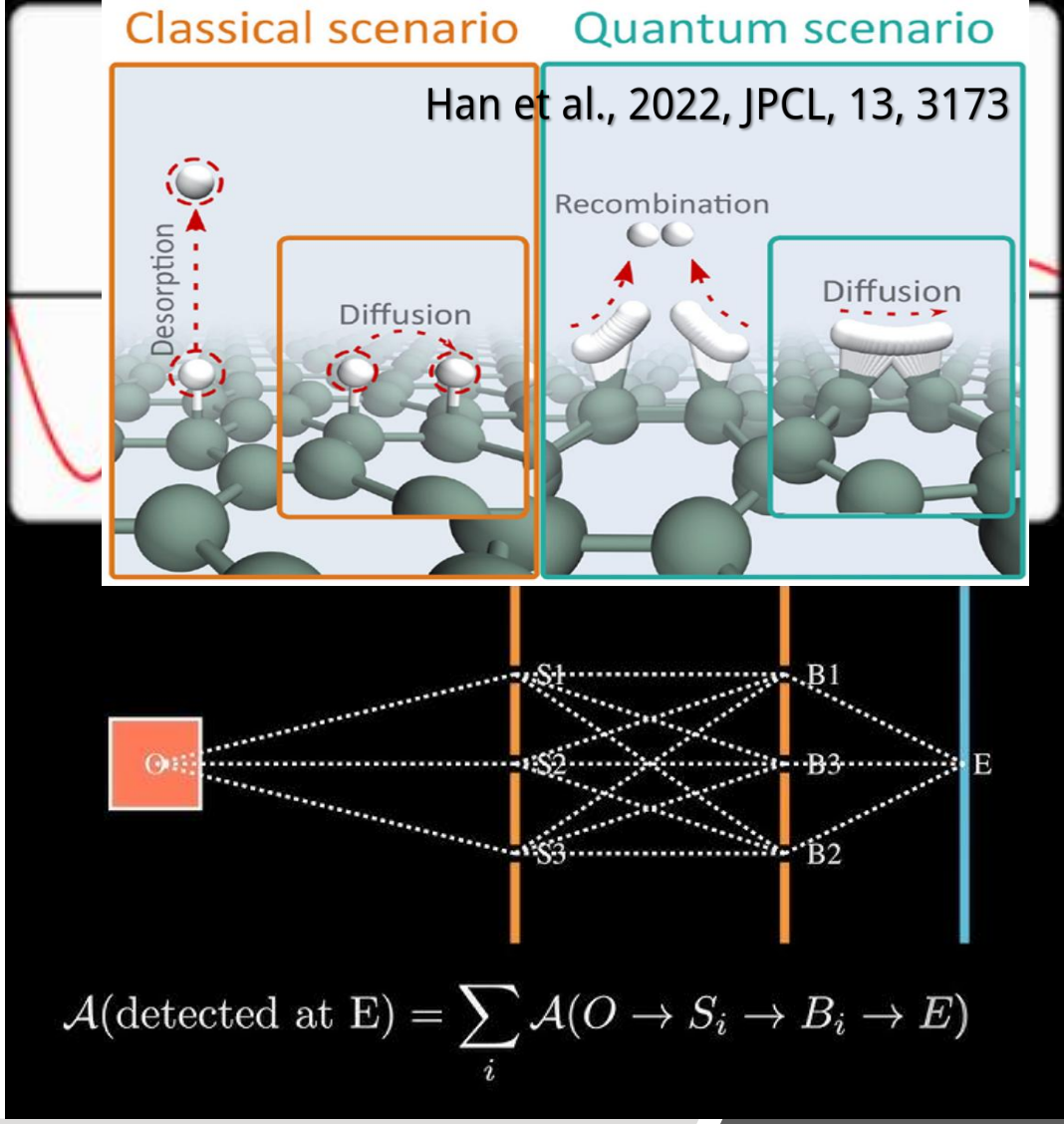


Grains Dominats H_2 Formation... But How?

How to Quantify Tunneling?

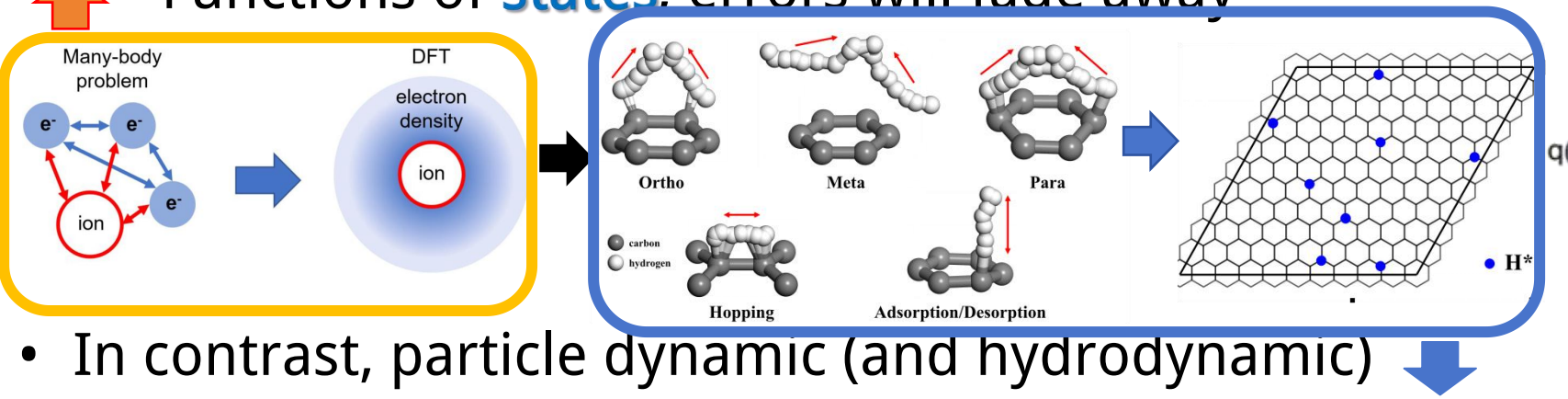
- Typical estimation: $P \sim \exp(-2l/\lambda)$,

  where $\lambda \sim h(2m_p \Delta E_A)^{-1/2} \sim 0.04\ \mathrm{nm}$
- However, "quantum chemistry" adopts Bohn-Oppenheimer approximation
  - Schroedinger or Kohn-Sham eq. for electrons
  - Classical mechanics for nuclei
- Feynman saves our day!
  - Classical: Minimum action principle
  - Quantum: Sum all paths, action as phase

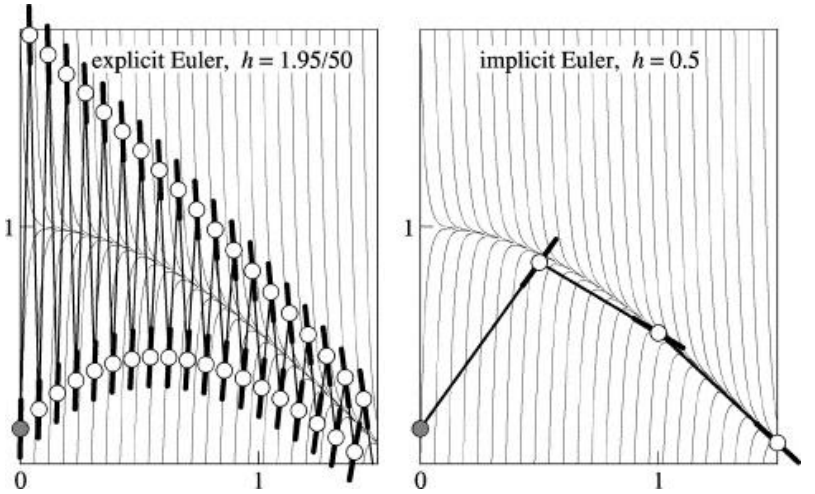


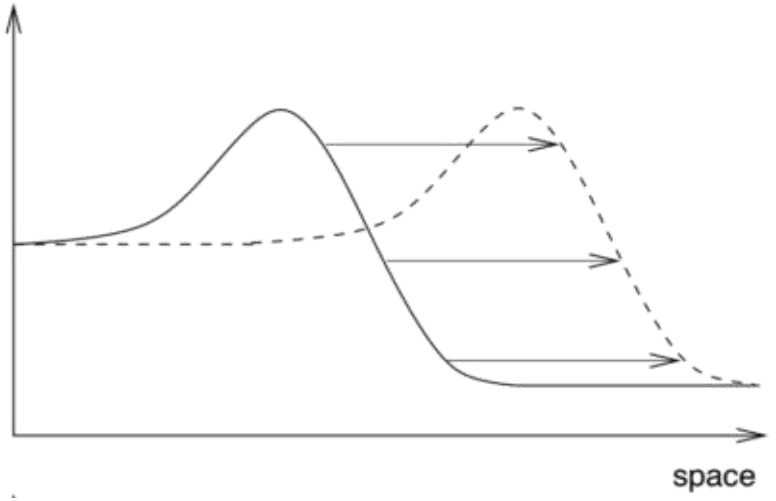
- Chinese joke (wisdom): 铁路警察，各管一段

  Railway securitymen only serve their own sectors
- Electronic structures are definite, eigensystem problems respond instantly to the atomic structures
  - Functions of **states**, errors will fade away



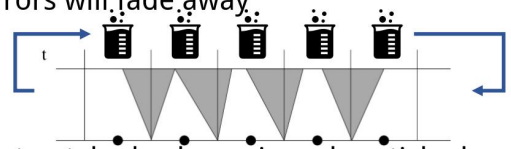
- In contrast, particle dynamic (and hydrodynamic) systems are basically hyperbolic
  - Functions of **paths**, errors will sustain and accumulate



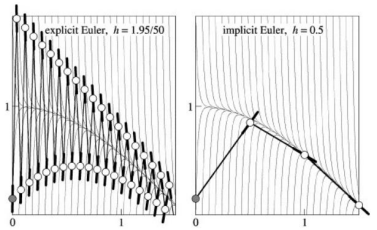


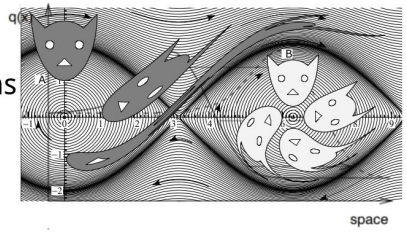
Which part shall we seek help from AI?

- Accelerate the reaction ODEs has higher priority
- Reaction systems obeying the mass-action law are generally parabolic
  - Errors will fade away

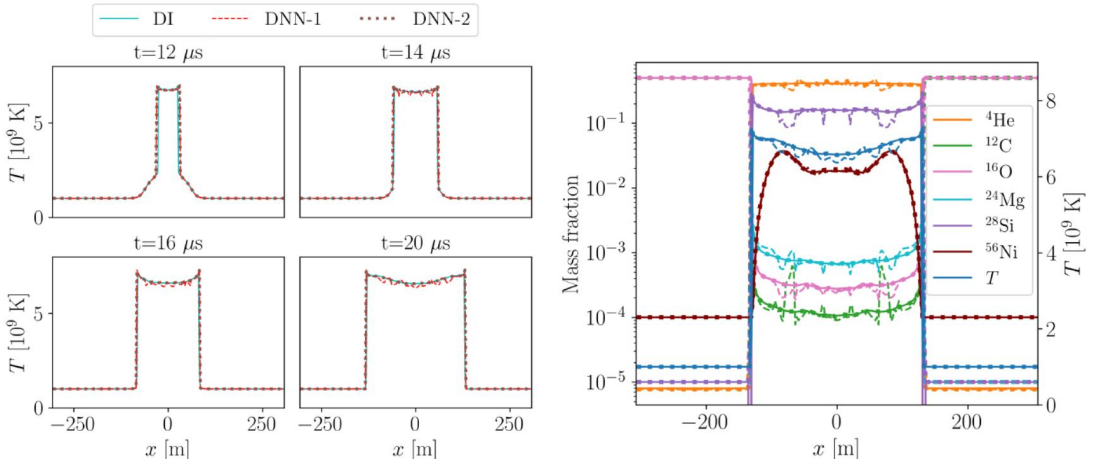


- In contrast, hydrodynamic and particle dynamic systems are basically hyperbolic
  - Errors will sustain and accumulate



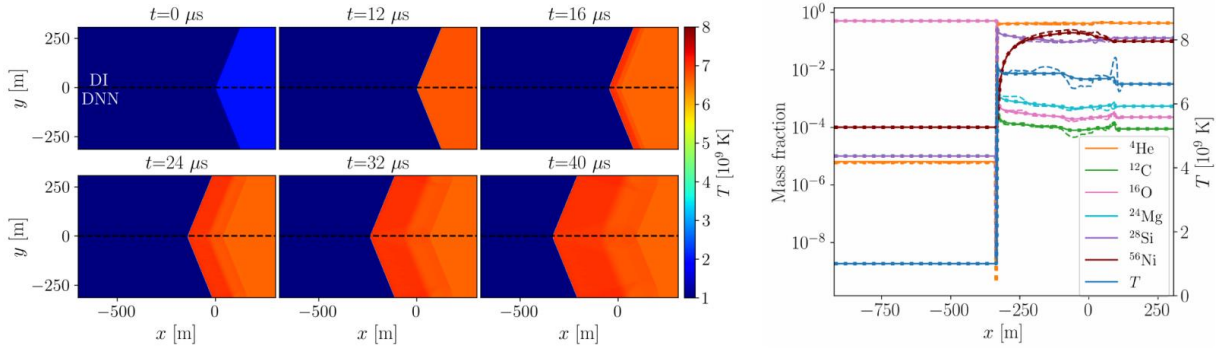


- DNN-2: Don't use DNN anymore for the "ashes" ($T > 6.5 \times 10^9$ K)



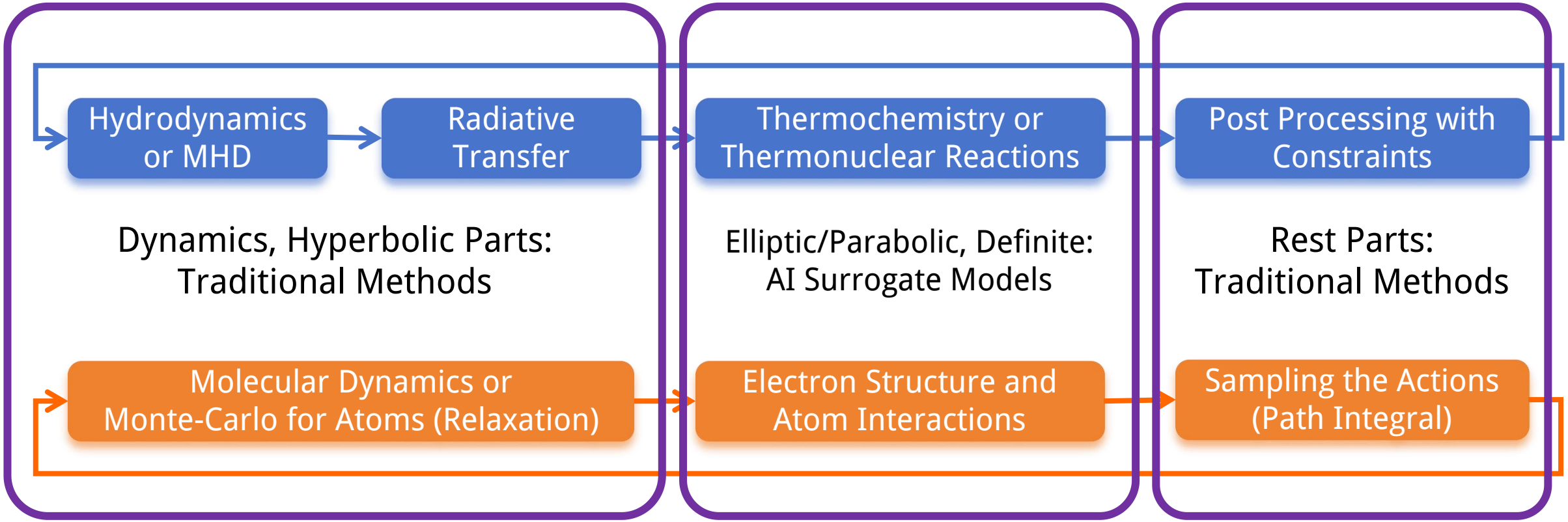
- Only do surrogate models for the elliptic, parabolic, or eigensystem problems
- Hyperbolic part is not slow whatsoever, but its secular evolution is mathematically prohibitive in theory and ML practices

- Detonation, inclined, 13 species (curves: $t = 40\ \mu s$)

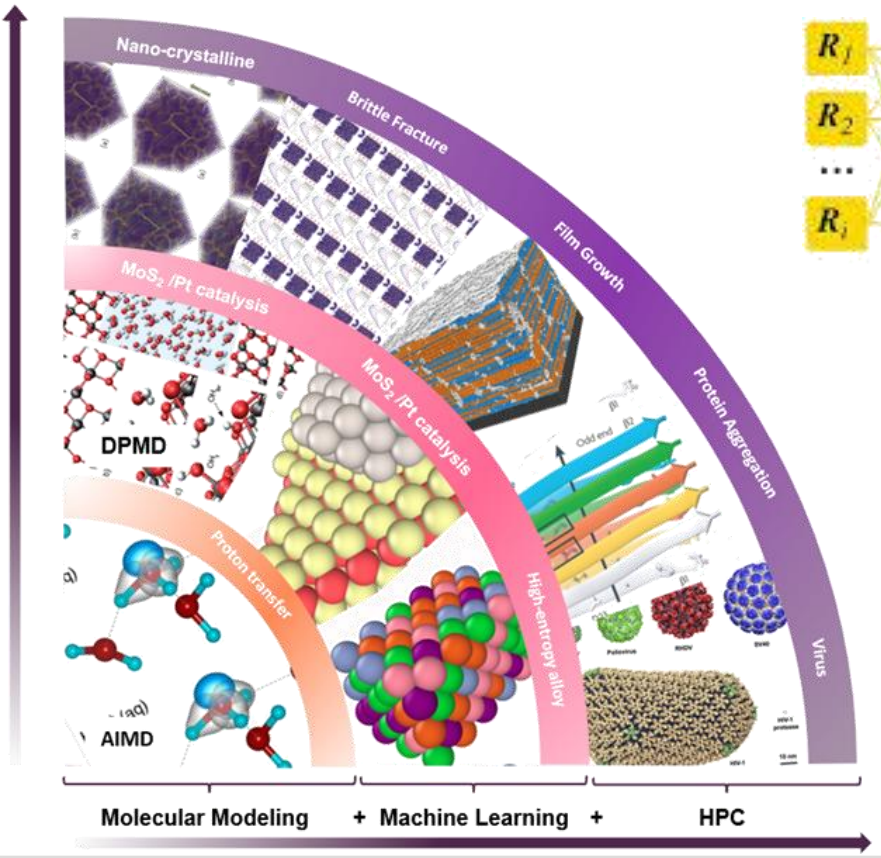


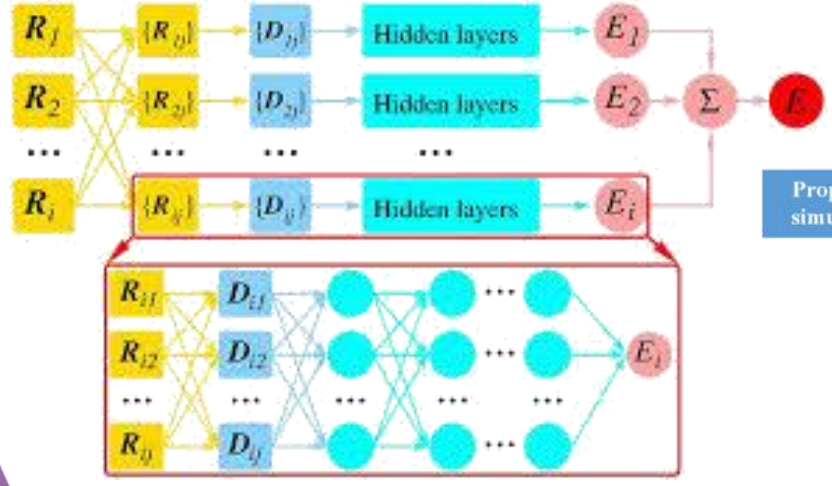
Also applicable in reaction flow surrogate models (from another talk 2 days ago…)

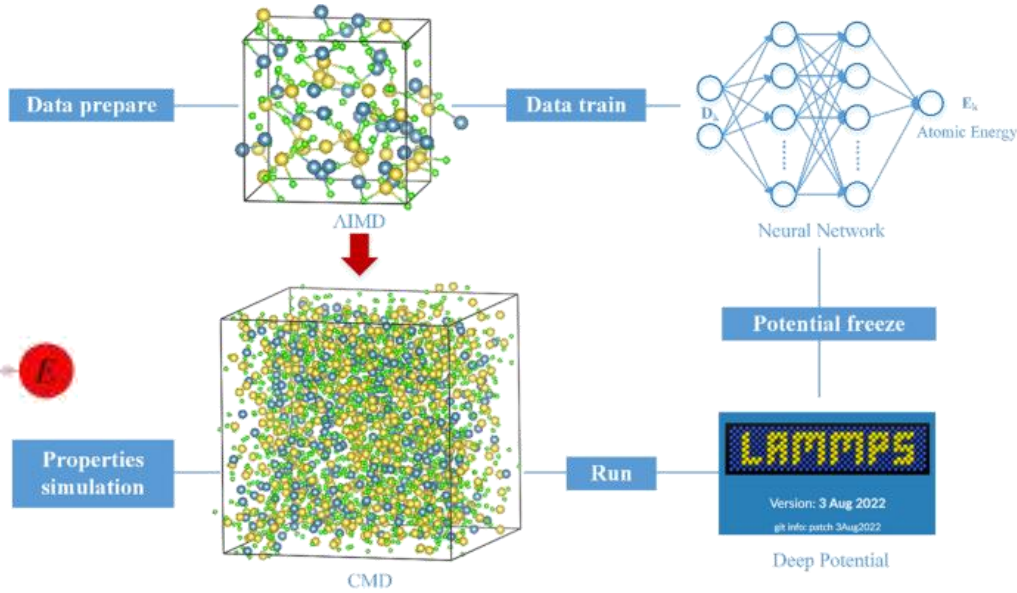
Zhang , Yi, **Wang** et al.
2025 ApJ, 990, 105
arXiv: 2504.14180



The same philosophy in the current stage of AI4S







Deep Potential Molecular Dynamics: A Scalable Model with the Accuracy of Quantum Mechanics
Linfeng Zhang, Jiequn Han, Han Wang,
Roberto Car, Weinan E
Phys. Rev. Lett., 2018, 120, 143001.

DeePMD-kit

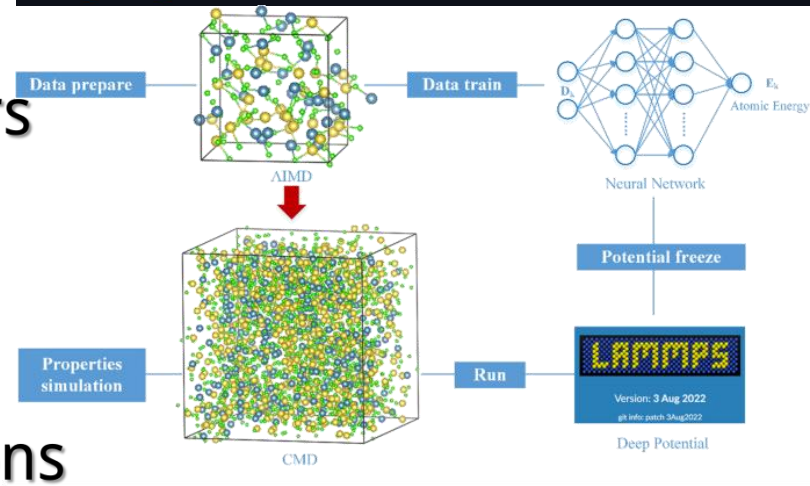
Wang, H., Zhang, L. F., Han, J. Q. & E, W. N. DeePMD-kit: A deep learning package for many-body potential energy representation and molecular dynamics. *Comput. Phys. Commun.* **228**, 178-184 (2018).

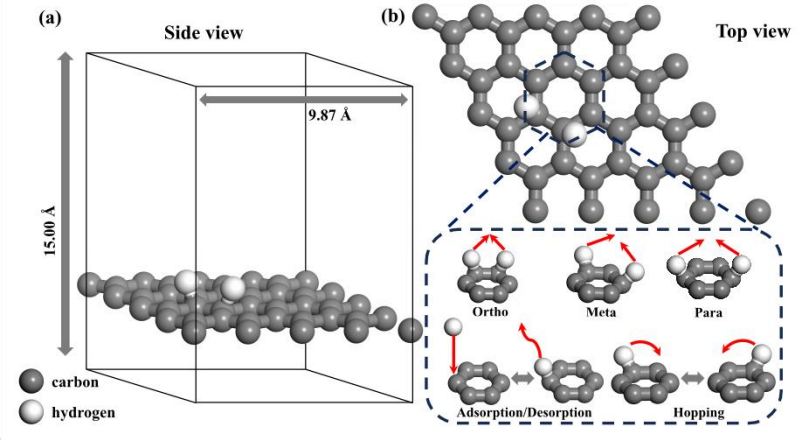
The Idea of DPMD

How to Quantify Tunneling? (cont.)

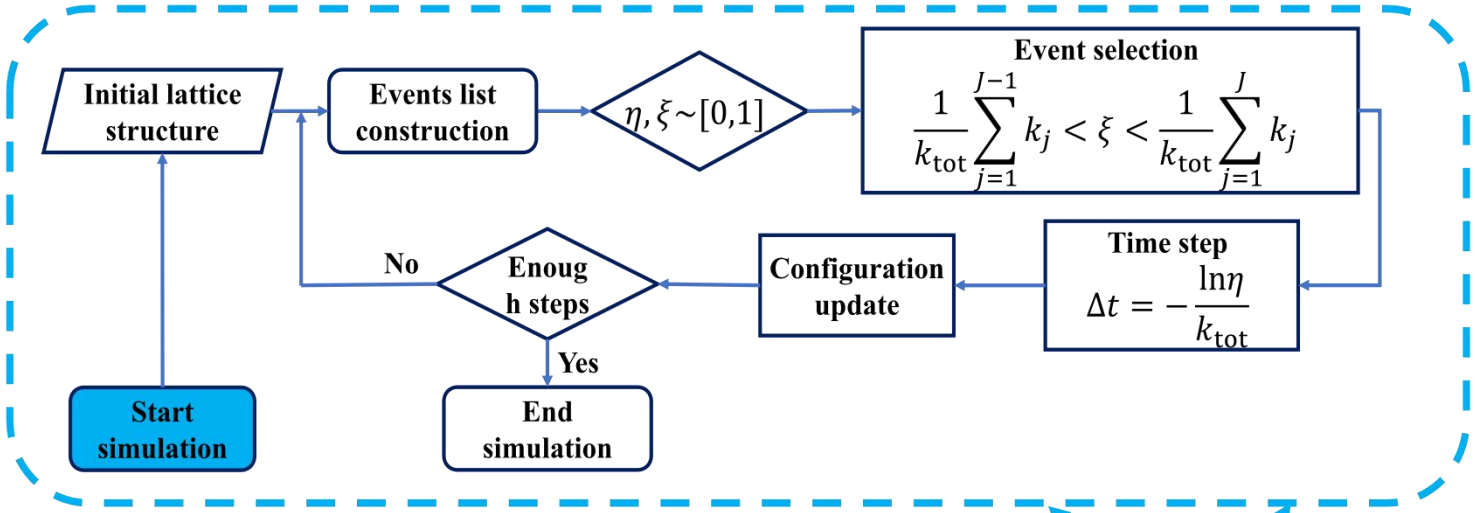
- DPMD (Deep-Potential Molecular Dynamics) basics:
  - DNN trained with DFT interatomic potentials
  - Atoms are affected by the closest and second neighbors
  - Use trained DNN in full MD
- Use DPMD as the fundation of NQE
  - Multiple possible paths with constaints to sample actions
  - Use actions as phases (as in $e^{-i\varphi}$) and sum all paths
  - Calculate an effective, reduced $\Delta E_{a,\mathrm{eff}}$
- Use KMC for overall efficiency of H_2 formation

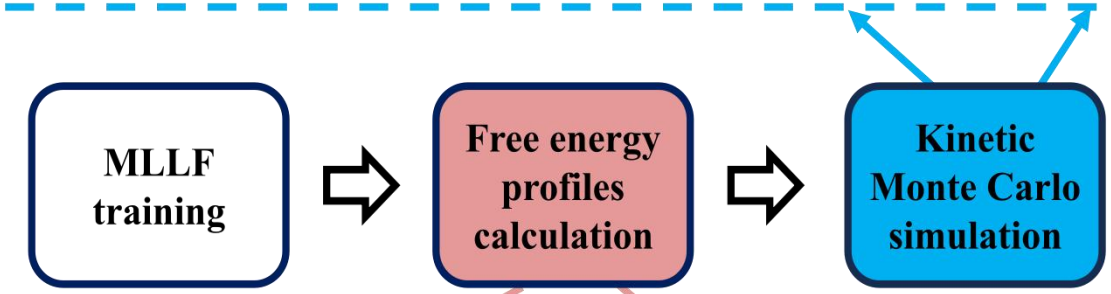
DeePMD-kit

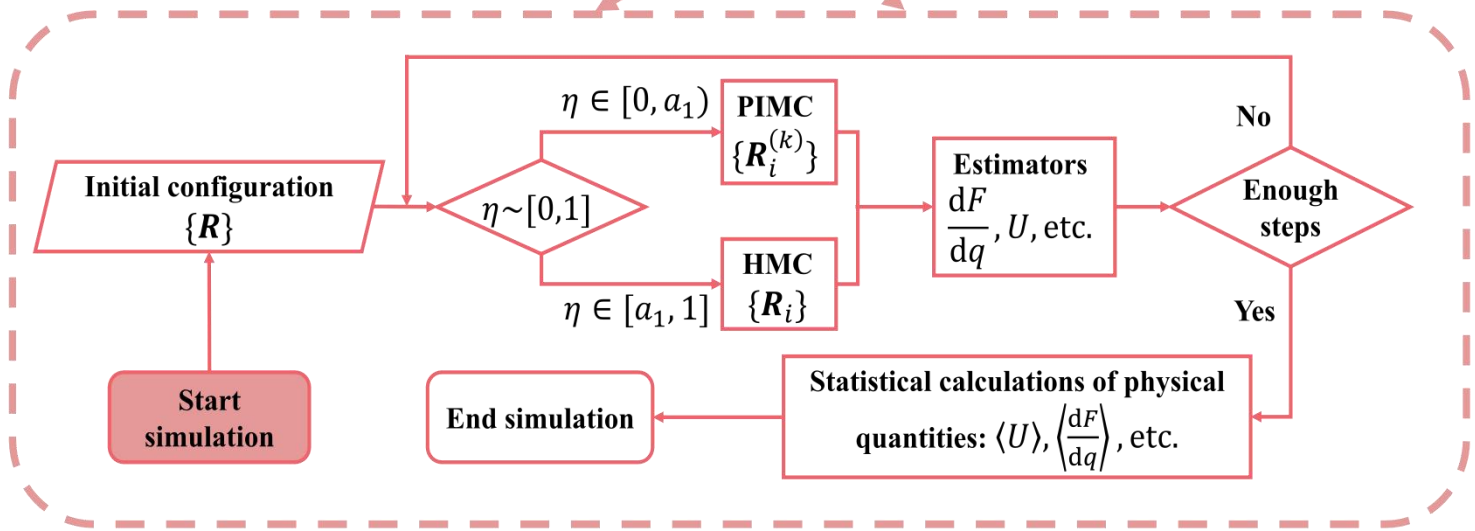


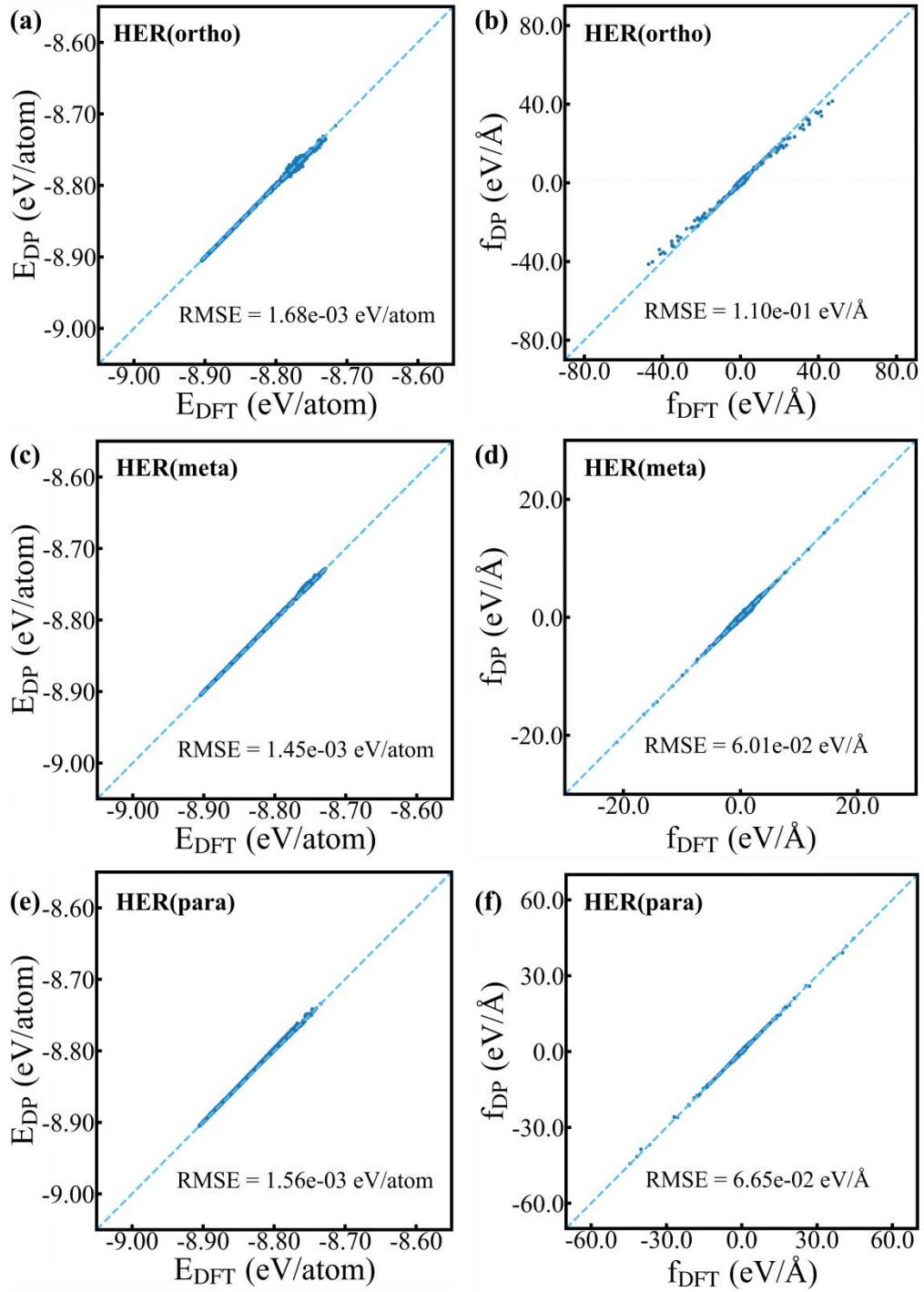


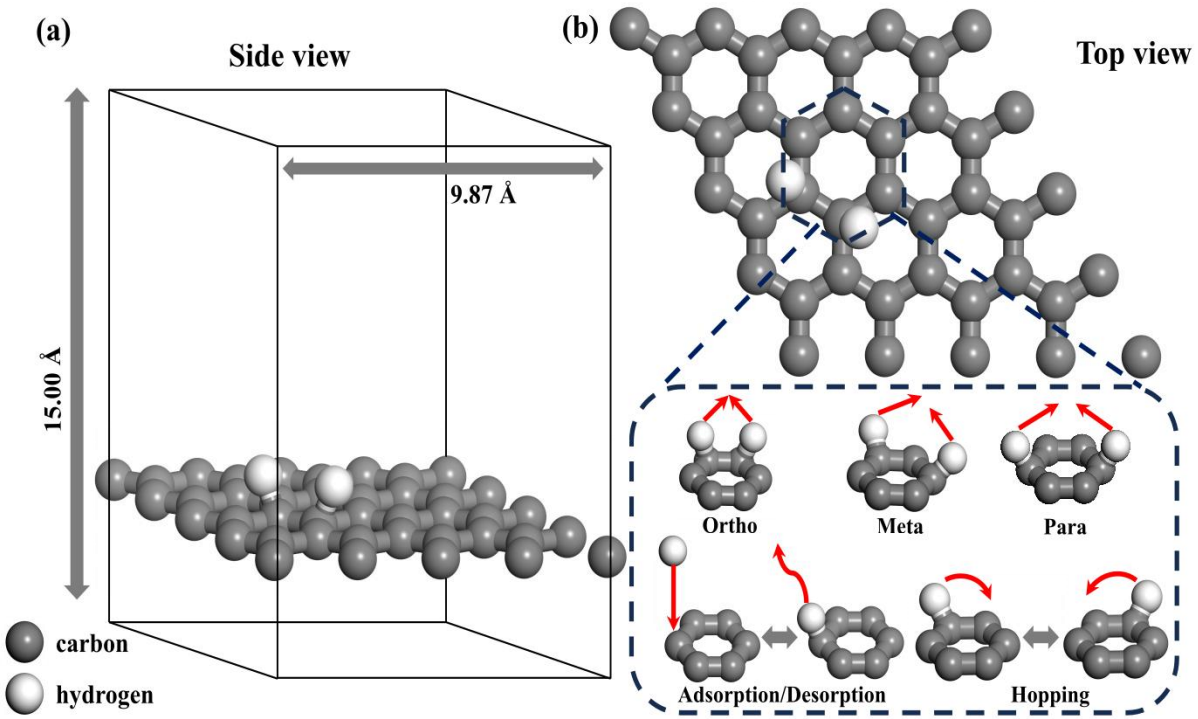
Yang, Wang, Li & Xu, 2025, arXiv:2509.25070

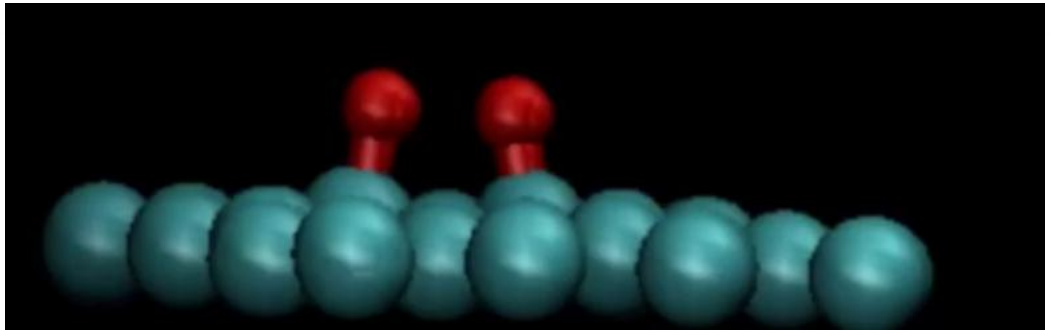

Initial lattice structure
Events list construction
$\eta, \xi \sim [0,1]$
Event selection
$\frac{1}{k_{\mathrm{tot}}}\sum_{j=1}^{J-1} k_j < \xi < \frac{1}{k_{\mathrm{tot}}}\sum_{j=1}^{J} k_j$
Time step
$\Delta t = -\frac{\ln\eta}{k_{\mathrm{tot}}}$
Configuration update
Enoug h steps
No
Yes
Start simulation
End simulation

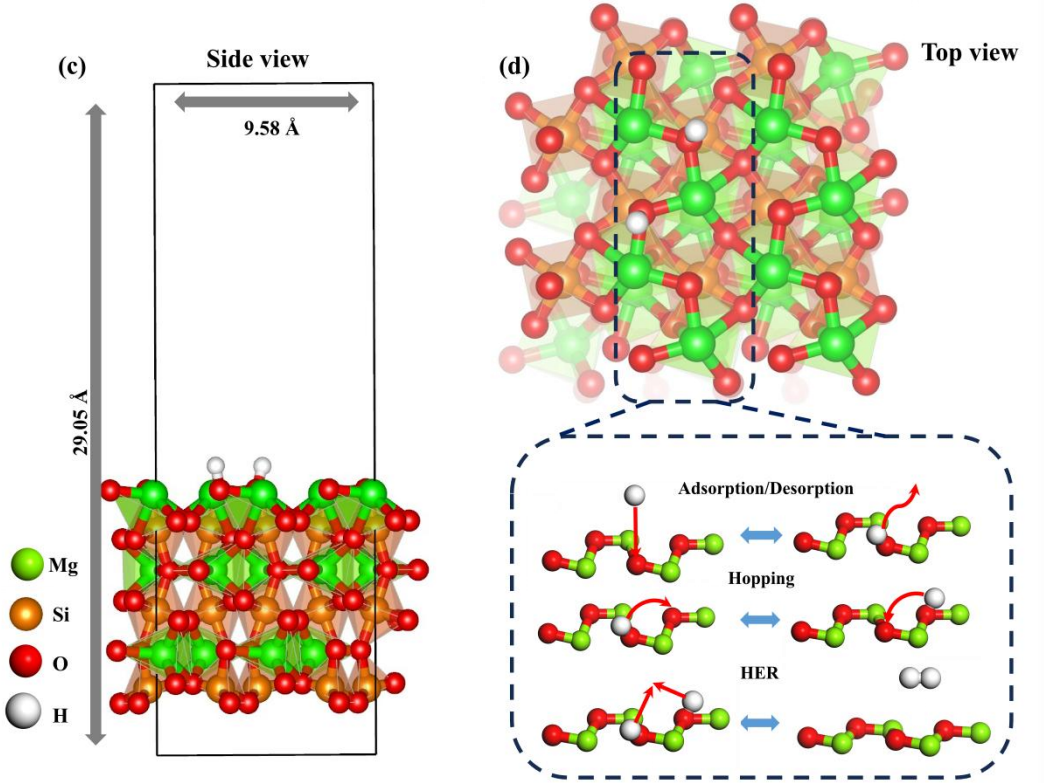

MLLF training
Free energy profiles calculation
Kinetic Monte Carlo simulation

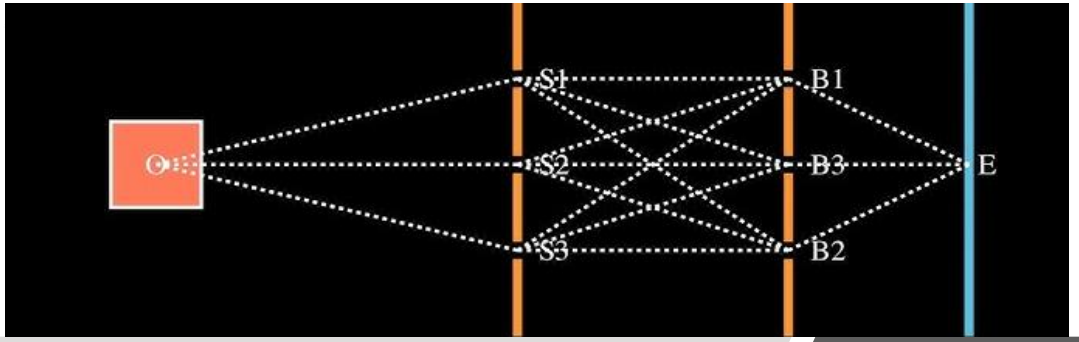

Initial configuration $\{\boldsymbol{R}\}$
$\eta \sim [0,1]$
$\eta \in [0, a_1)$
PIMC $\{\boldsymbol{R}_i^{(k)}\}$
$\eta \in [a_1, 1]$
HMC $\{\boldsymbol{R}_i\}$
Estimators $\frac{\mathrm{d}F}{\mathrm{d}q}, U$, etc.
Enough steps
No
Yes
Statistical calculations of physical quantities: $\langle U \rangle, \left\langle \frac{\mathrm{d}F}{\mathrm{d}q} \right\rangle$, etc.
End simulation
Start simulation


(a)
HER(ortho)
RMSE = 1.68e-03 eV/atom
E_{DP} (eV/atom)
E_{DFT} (eV/atom)
(b)
HER(ortho)
RMSE = 1.10e-01 eV/Å
f_{DP} (eV/Å)
f_{DFT} (eV/Å)
(c)
HER(meta)
RMSE = 1.45e-03 eV/atom
(d)
HER(meta)
RMSE = 6.01e-02 eV/Å
(e)
HER(para)
RMSE = 1.56e-03 eV/atom
(f)
HER(para)
RMSE = 6.65e-02 eV/Å



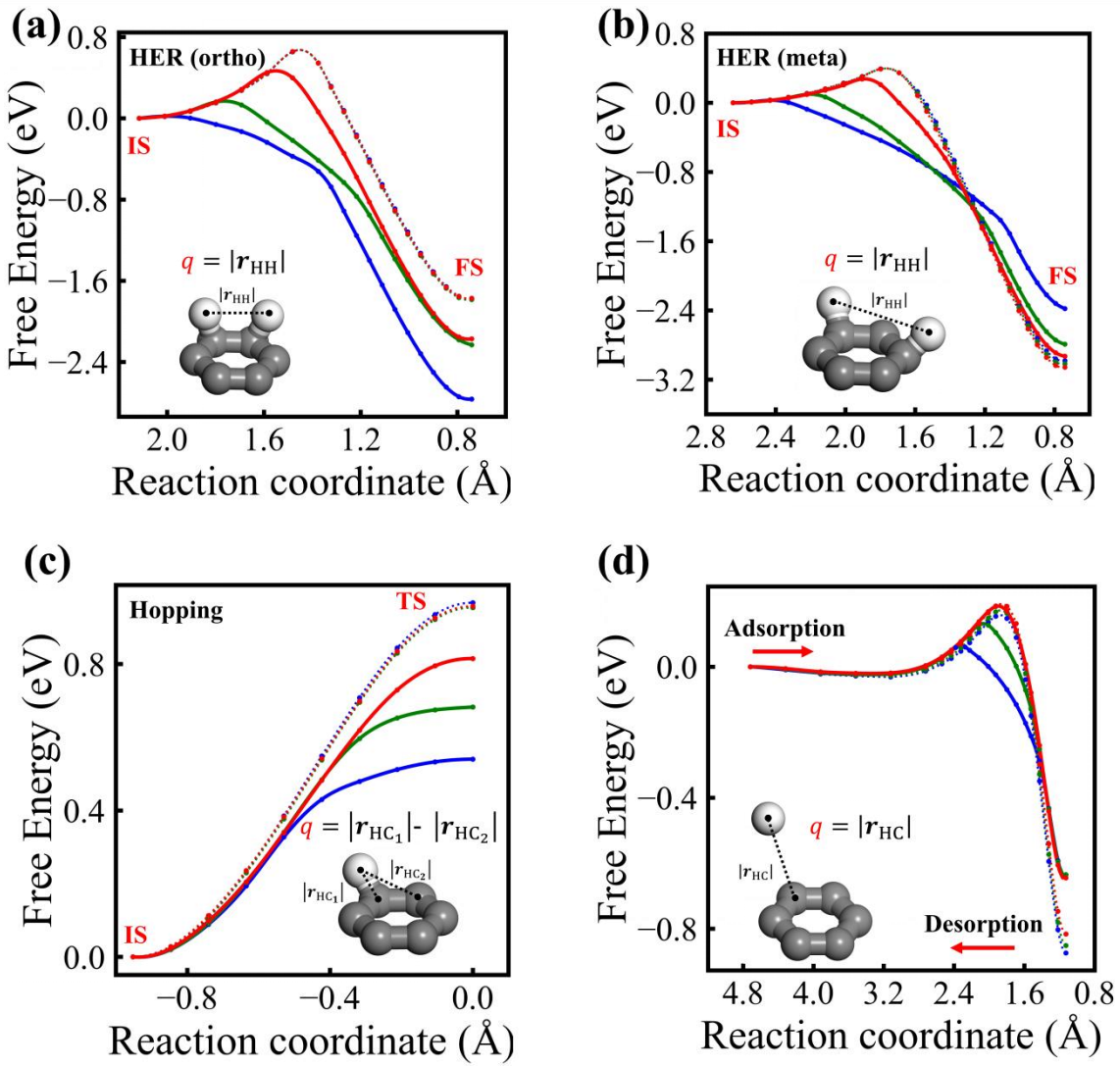






How to Quantify Tunneling? (cont.)

Yang, Wang, Li & Xu, 2025, arXiv:2509.25070

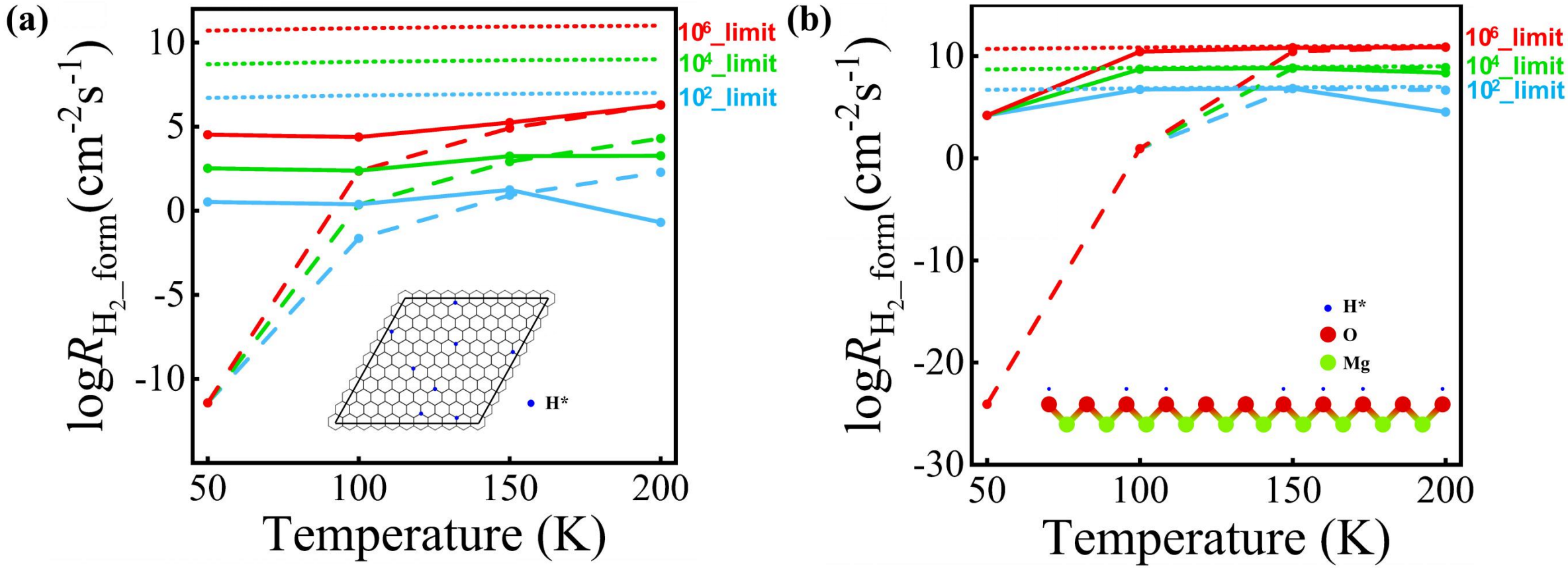


- NQE leads to significantly reduced $\Delta E_{\mathrm{a,eff}}$
  - Ortho: ~0.7 eV to ~0.03 eV
  - Meta: ~0.6 eV to ~0.02 eV
- Lower temperature, lower $\Delta E_{\mathrm{a,eff}}$
  - $\lambda_{\mathrm{th,H}} \sim 2.4\ \mathrm{nm} \times (T/20\ \mathrm{K})^{-1/2}$
  - Longer λ_{th}, more paths with high weights, possible to find paths with lower ΔE_{a}
- Physisorption barrier is indeed too shallow
- Chemisorption barrier: NQE needed

Results of NQE: Significantly Lower Barriers

Yang, Wang, Li & Xu, 2025, arXiv:2509.25070

- KMC rates of H_2 formation: "Lower-limit" at $T < 50$ K $\quad R = \frac{1}{2} n_H v_H n_d \sigma_d \eta S_H$
- Higher temperature ($T > 150$ K) drops: Desorption important



Results of NQE: More Accurate Coefficients

Yang, Wang, Li & Xu, 2025, arXiv:2509.25070

- Beyond the simplest model of dust-catalyzed H2 formation

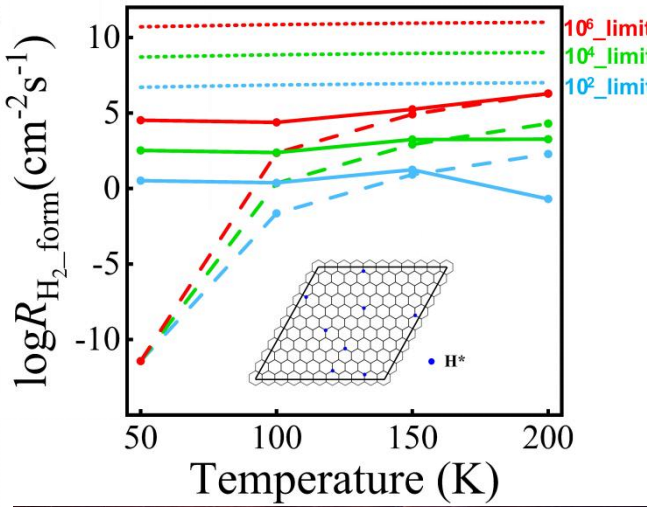
$$R = \frac{1}{2} n_H v_H n_d \sigma_d \eta S_H$$

  - Efficiency does not go to zero outside the Godilocks soup
  - NQE no longer require local defects to trap atomic hydrogen
- Combined with other constraints (e.g. HINSA for HI...):

  More accurate constraints on ISRF and dust properties
- Relation between SFR and dusts revisited with consistency

  (No need to manipulate for $z > 1$, even $z > 6$ galaxies)
- Silicate are more efficient, while graphite may also be useful

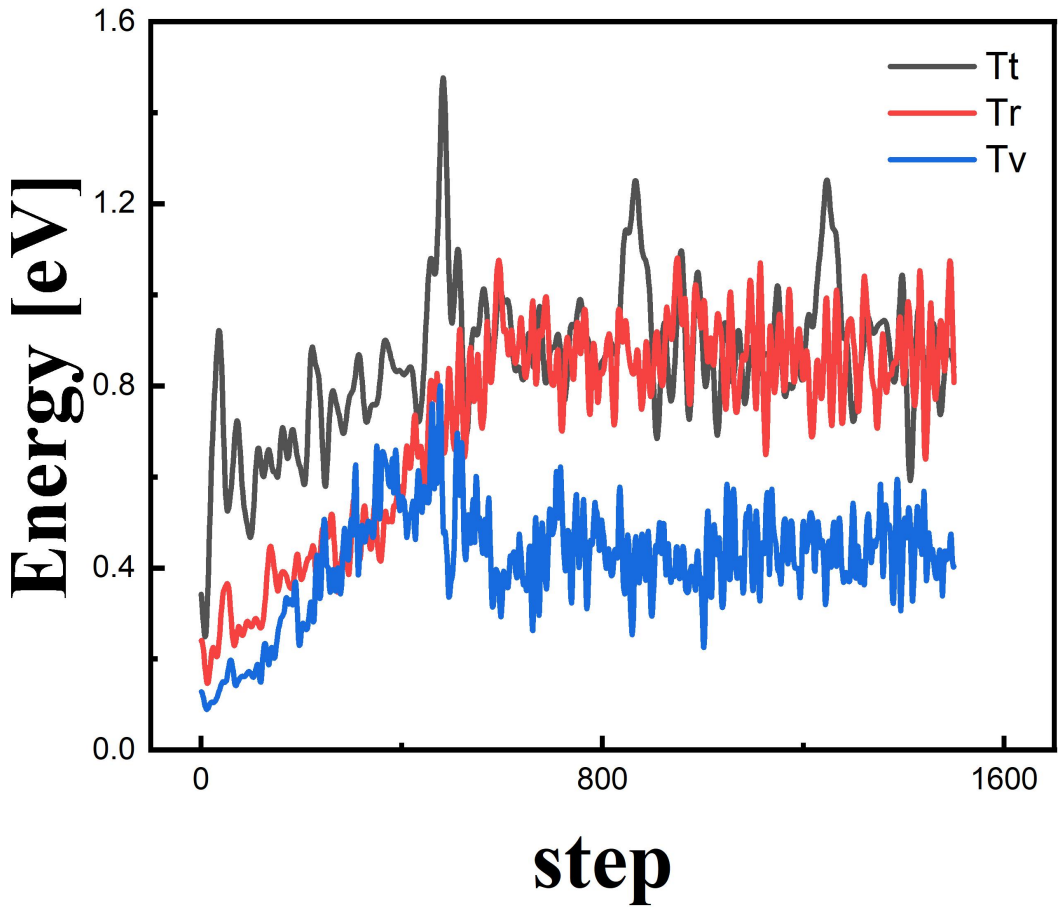
  in turbulences and esp. shocks

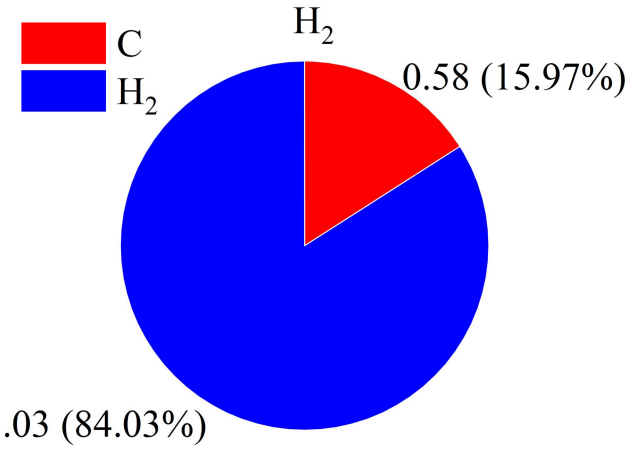


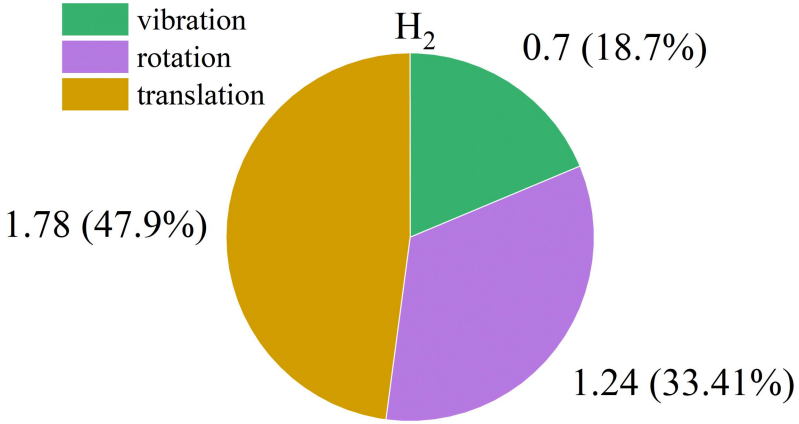
Astrophysical Implications

Yang, Wang, Li & Xu, 2025, arXiv:2509.25070

50 K, 26 trajectories, 1500 steps, 0.2 fs, P=64.







Astrophysical Implications: Partition of Energy

WORK IN PROGRESS

When you know ANNs are high-dimensional functions in general,

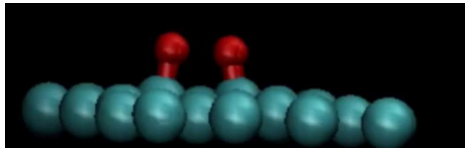
What can we simulation people do with AI?

A better applicable nail

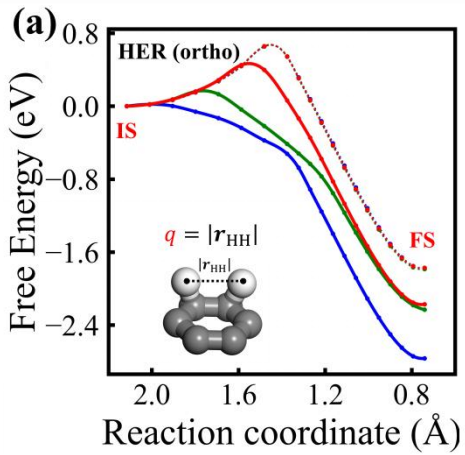
when you get a hammer, is probably the **definite** part of the system that are **functions of states**.

Take-homes and Future Works

- **Surrogate models may better avoid the hyperbolic (causalistic) part of the problem**



- Equipped with DPMD, NQE can be simulated with consistent path integral
- NQE is the key for H_2 formation on dusts
  - Effective barrier from 0.5 eV to 0.02 eV
  - Formation efficiency issue resolved quantitatively



- Follow-up works: more consistent computational astrochemical dust modeling
  - Insert into co-evolved thermochem-MHD
  - Energy partition of products, constrain the formation/sublimation rates against thermal excitation (semi-finished)