Generative AI for Science

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https://wangleiphy.github.io

Discriminative learning

$$y = f(\boldsymbol{x})$$

or $p(y \mid \boldsymbol{x})$

Generative learning

$$p(\boldsymbol{x}, y)$$

Generative AI: a new buzz word in silicon valley

A Coming-Out Party for Generative A.I., Silicon Valley's New Craze

A celebration for Stability AI, the start-up behind the controversial Stable Diffusion image generator, represents the arrival of a new A.I. boom.

New York Times

Kevin Roose

Oct. 21, 2022

Sequoia's Sonya Huang: The generative AI hype is 'absolutely justified'

She's bullish on generative AI given the "superpowers" it gives humans who work with it.

Protocol

Biz Carson

October 21, 2022

https://www.sequoiacap.com/article/generative-ai-a-creative-new-world/

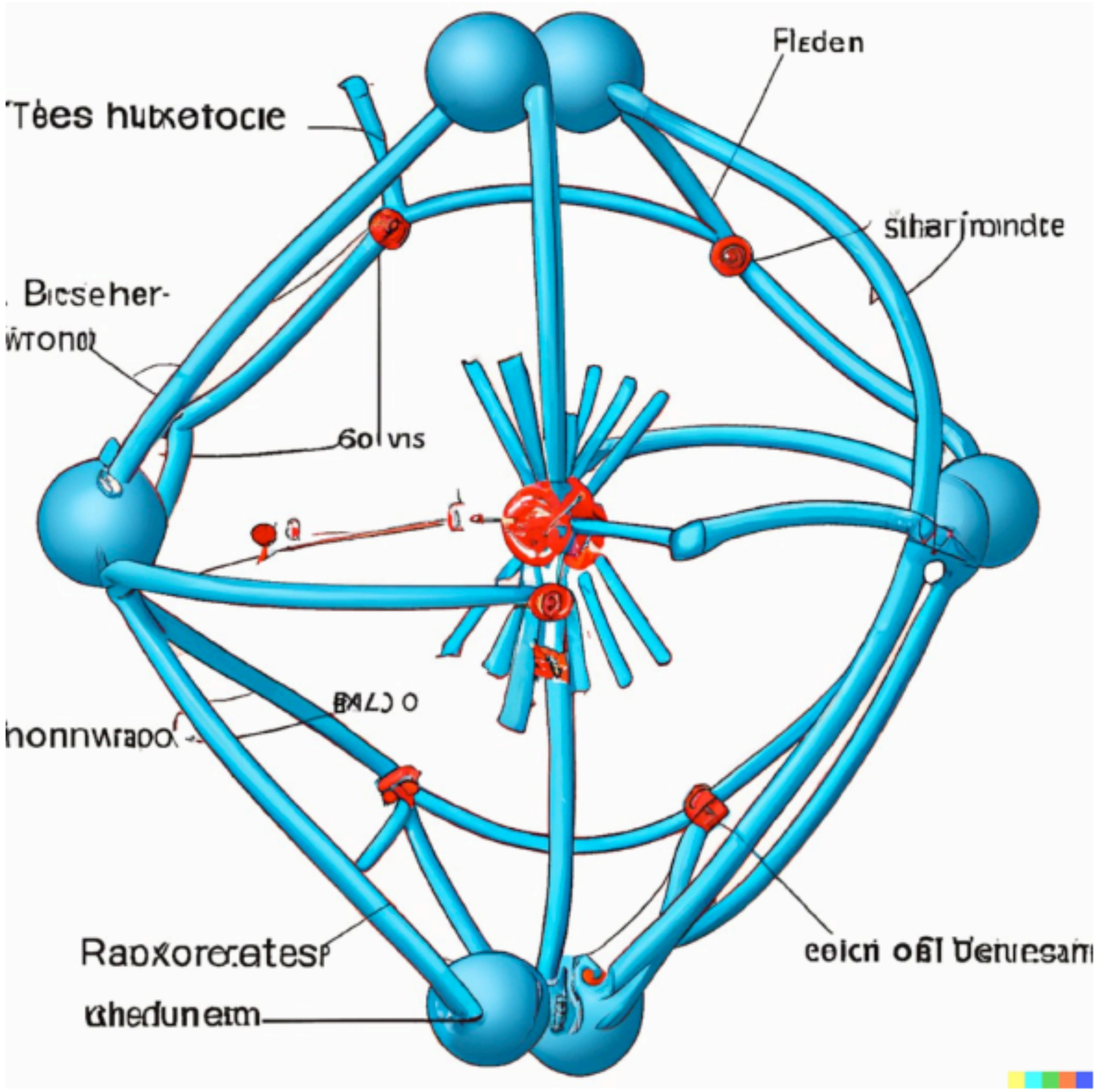
by Sonya Huang, Pat Grady and GPT-3

	PRE-2020	2020	2022	2023?	2025?	2030?
TEXT	Spam detection Translation Basic Q&A	Basic copy writing First drafts	Longer form Second drafts	Vertical fine tuning gets good (scientific papers, etc)	Final drafts better than the human average	Final drafts better than professional writers
CODE	1-line auto-complete	Multi-line generation	Longer form Better accuracy	More languages More verticals	Text to product (draft)	Text to product (final), better than full-time developers
IMAGES			Art Logos Photography	Mock-ups (product design, architecture, etc.)	Final drafts (product design, architecture, etc.)	Final drafts better than professional artists, designers, photographers)
VIDEO / 3D / GAMING			First attempts at 3D/video models	Basic / first draft videos and 3D files	Second drafts	AI Roblox Video games and movies are personalized dreams

Large model availability: First attempts · Almost there · Ready for prime time https://huggingface.co/spaces/stabilityai/stable-diffusion

the inner structure of an electron

Generate image



https://future.com/how-to-build-gpt-3-for-science/

How to Build a GPT-3 for Science (scientific literature and data)

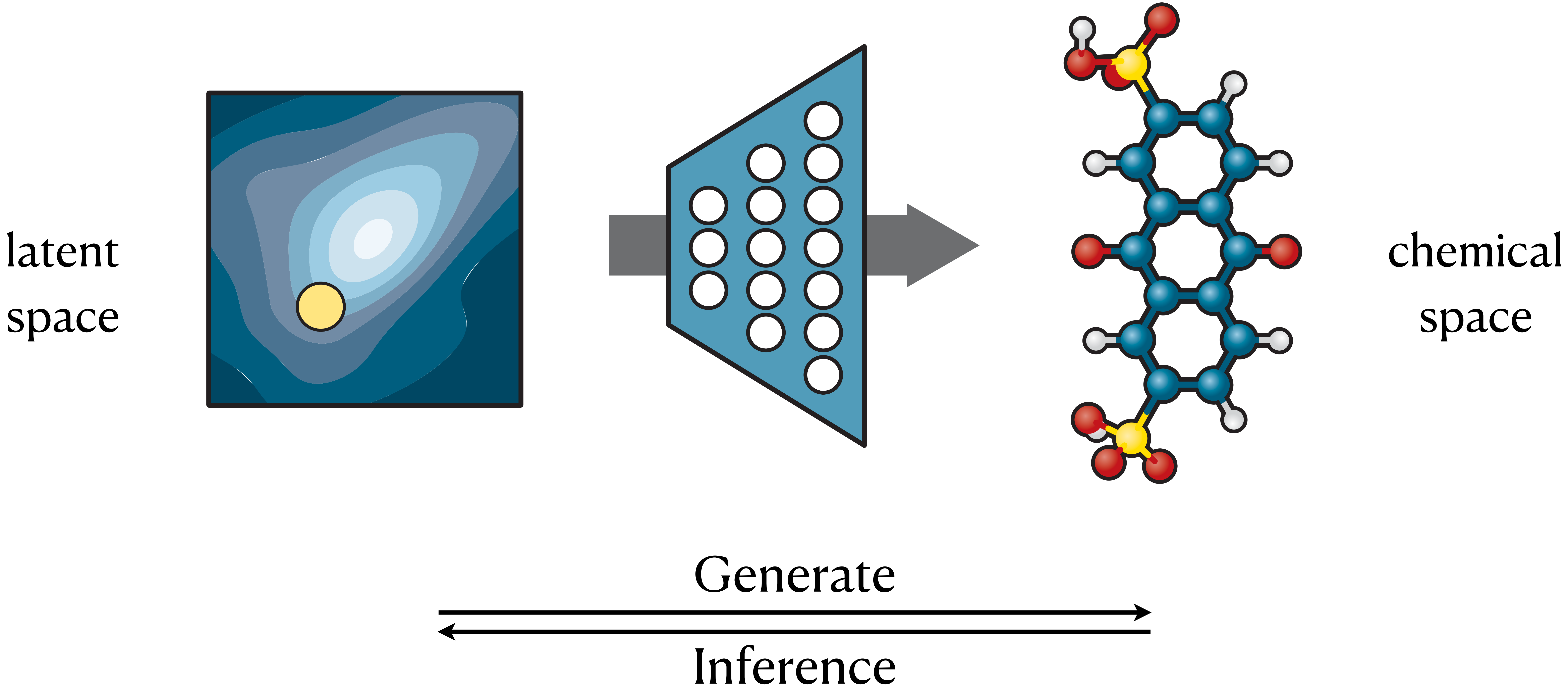
Josh Nicholson

Posted August 18, 2022

Some examples of complex potential prompts are:

"Tell me why this hypothesis is wrong"
"Tell me why my treatment idea won't work"
"Generate a new treatment idea"
"What evidence is there to support social policy X?"
"Who has published the most reliable research in this field?"
"Write me a scientific paper based on my data"

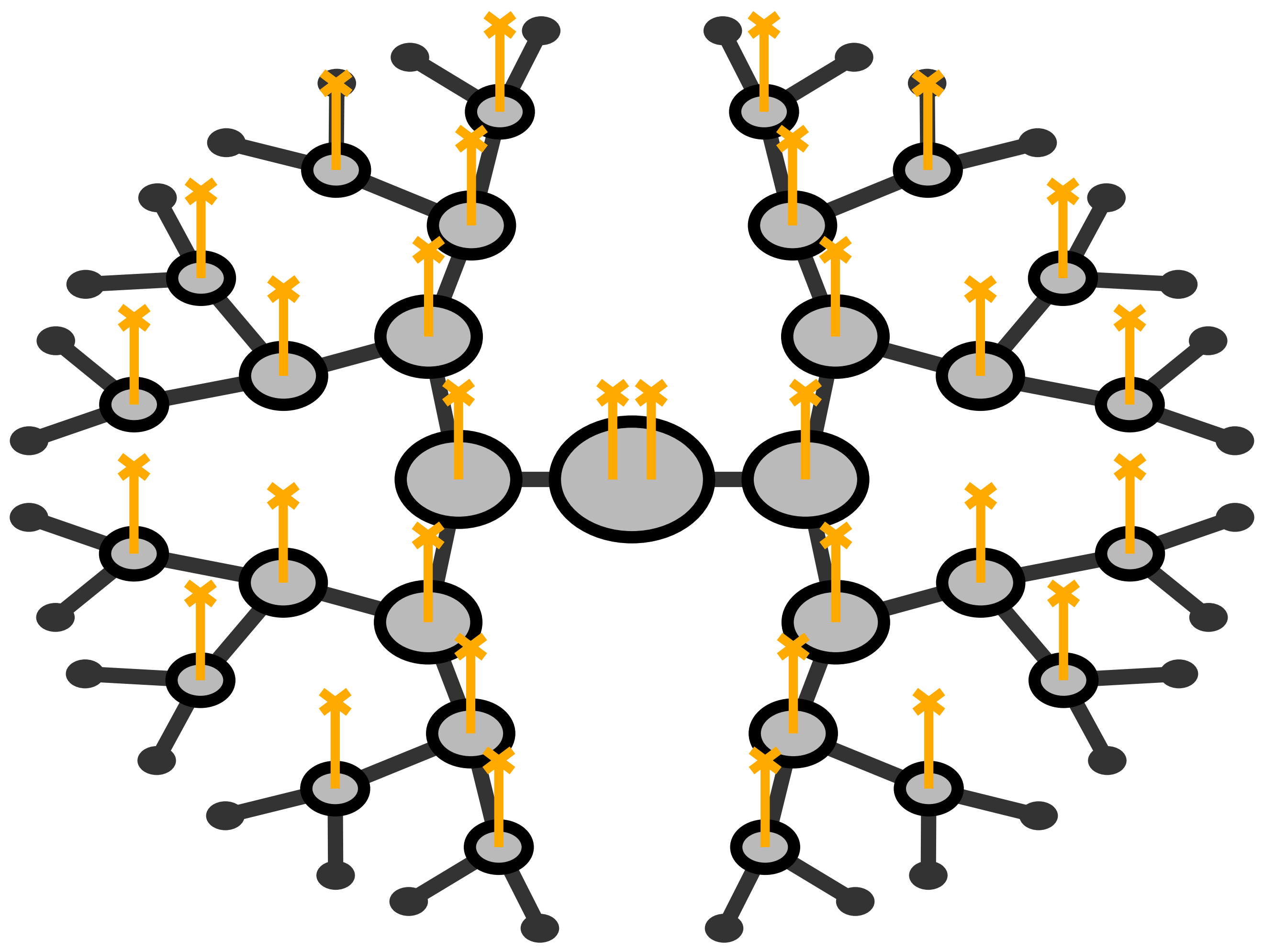
Generative AI for matter engineering



Review: “Inverse molecular design using machine learning”, Sanchez-Lengeling & Aspuru-Guzik, Science ’18

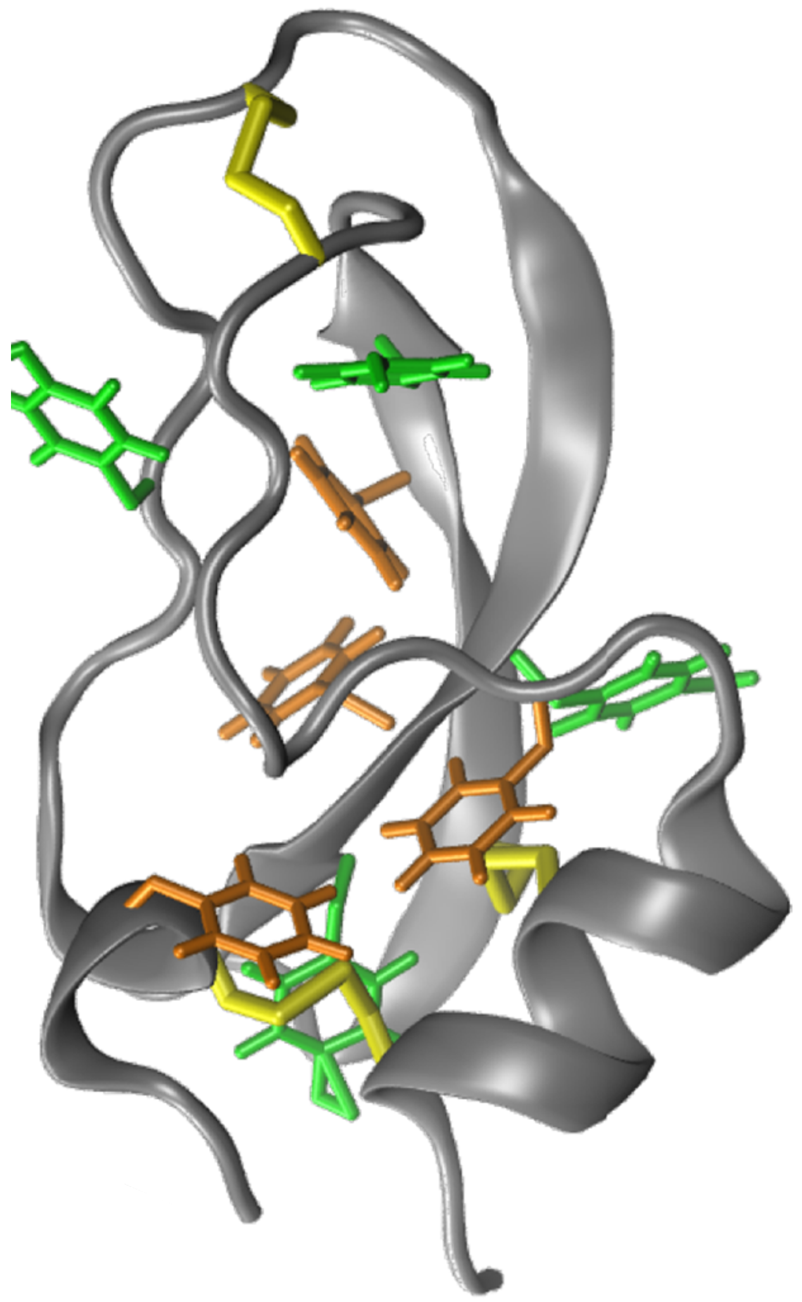
Generative AI for statistical physics

Renormalization group



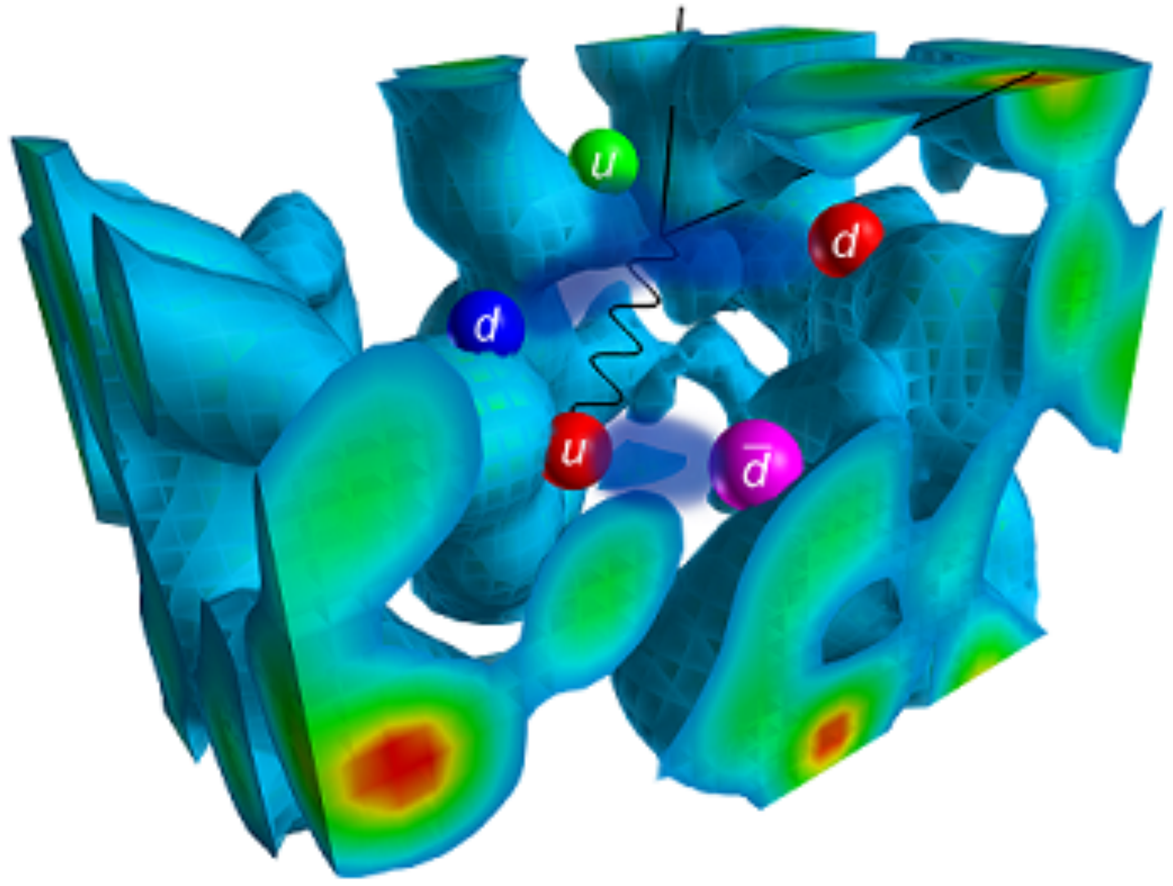
Li and LW, PRL '18
Li, Dong, Zhang, LW, PRX '20

Molecular simulation



Noe et al, Science '19
Wirnsberger et al, JCP '20

Lattice field theory



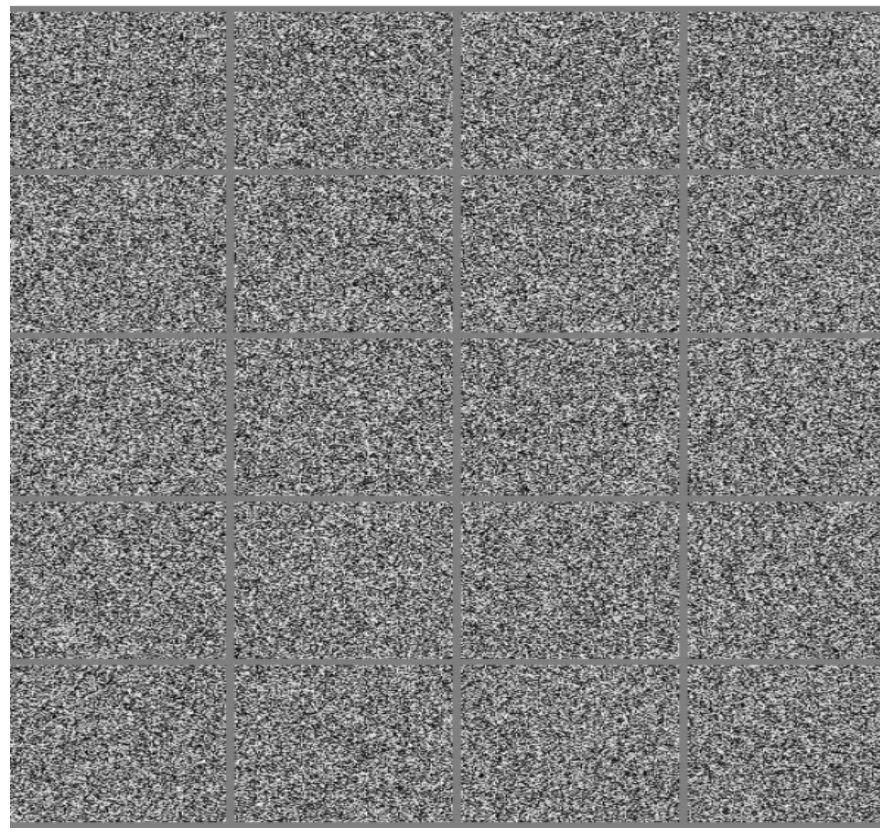
Albergo et al, PRD '19
Kanwar et al, PRL '20

These are principled computation: quantitatively accurate, interpretable, reliable, and generalizable even without data

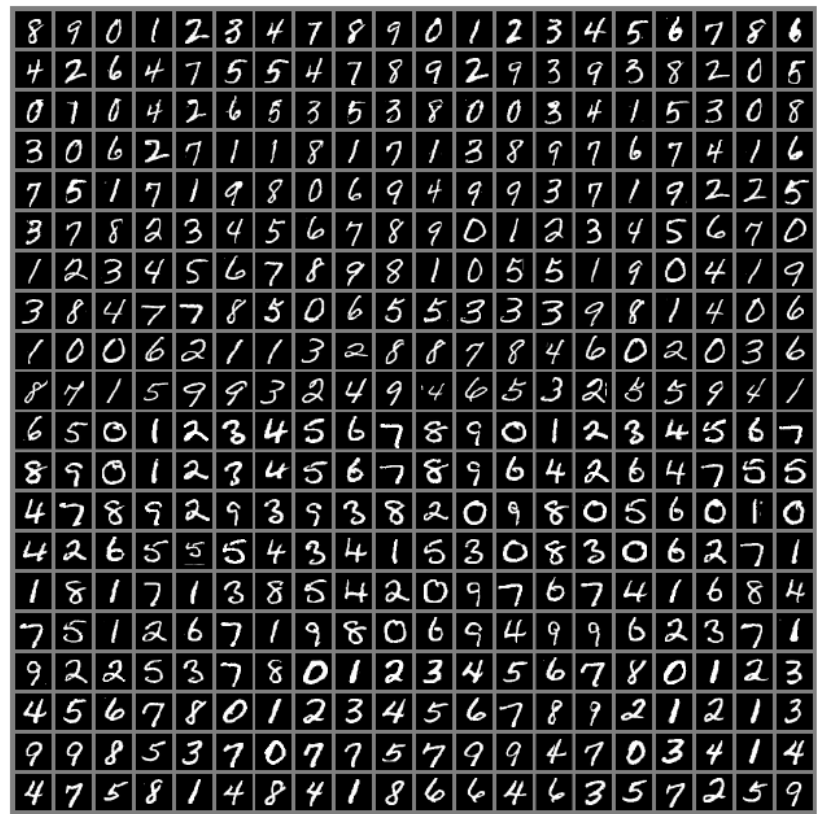
Probabilistic Generative Modeling

$$p(\boldsymbol{x})$$

How to express, learn, and sample from a high-dimensional probability distribution ?



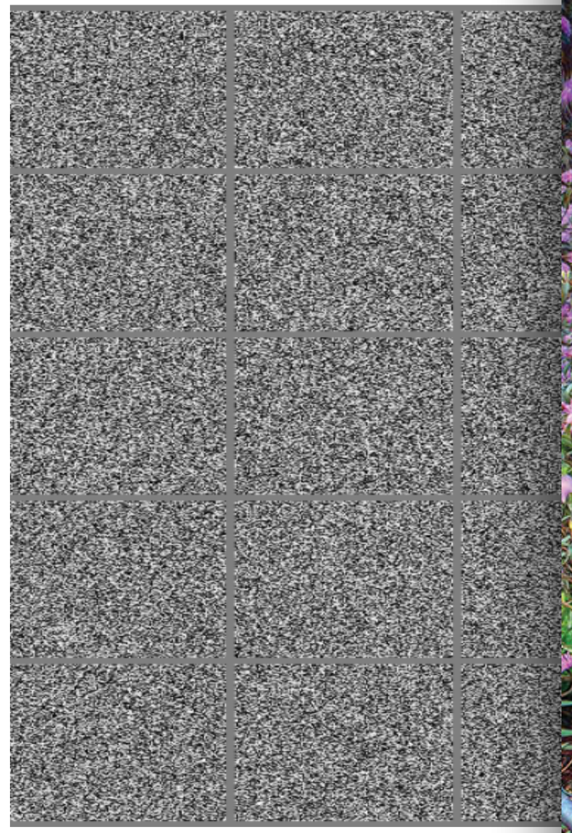
“random” images



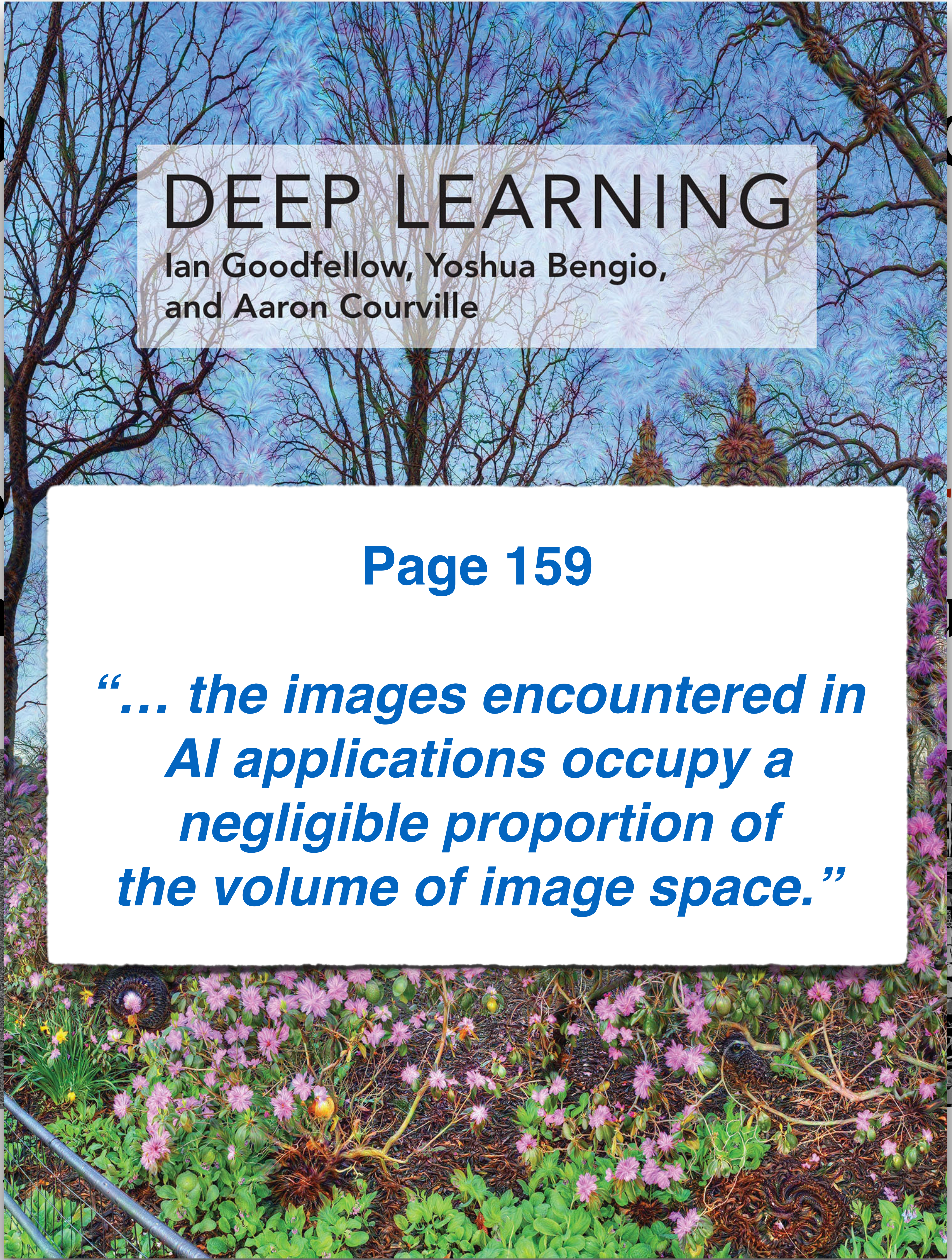
“natural” images

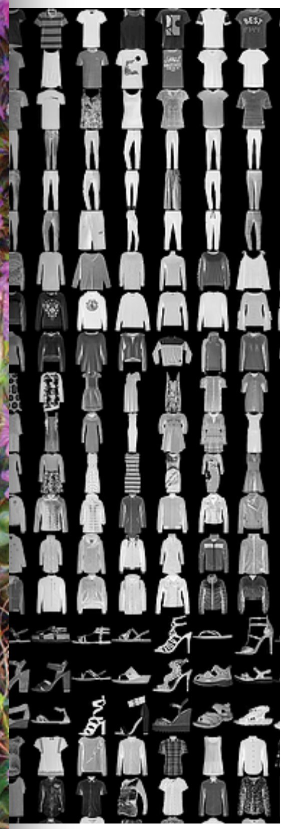
Probab deling

How to om a
high-din tion ?



“random”





Probabilistic Generative Modeling

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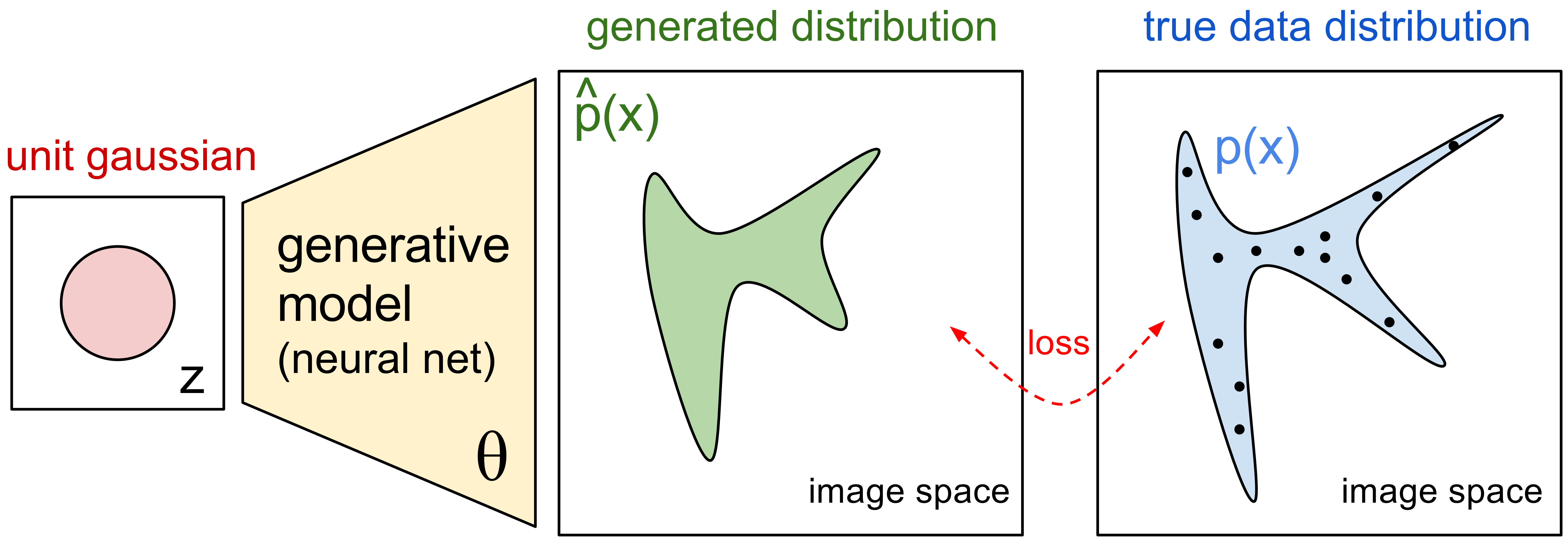


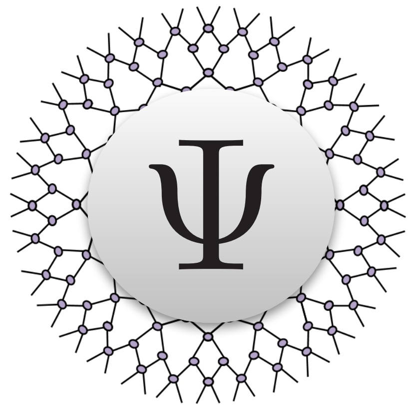
https://blog.openai.com/generative-models/

Generative models and their physics genes

Goodfellow, NIPS tutorial, 1701.00160

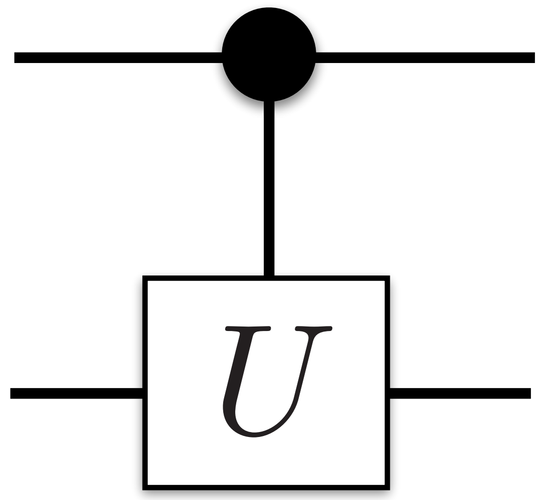
$p(\boldsymbol{x})$

- Explicit density
  - Tractable density
    - -Fully visible belief nets
      - -NADE
      - -MADE
      - -PixelRNN
    - -Change of variables models (nonlinear ICA)
  - Approximate density
    - Variational
      - Variational autoencoder
    - Markov Chain
      - Boltzmann machine
- Implicit density
  - Direct
    - GAN
  - Markov Chain
    - GSN



Tensor Networks

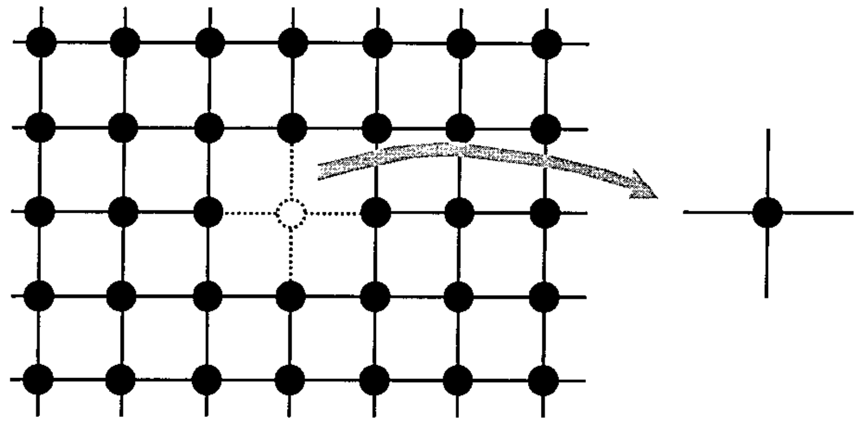
Han, Wang, Fan,LW,Zhang PRX '18

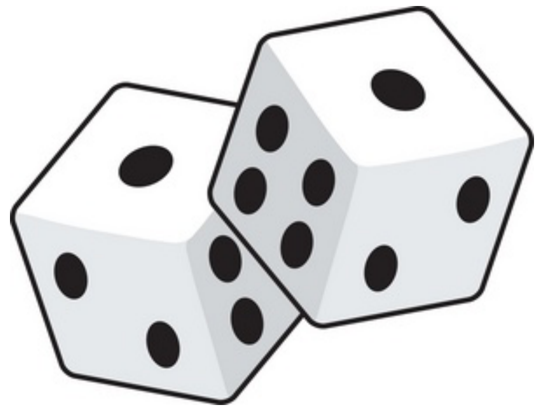


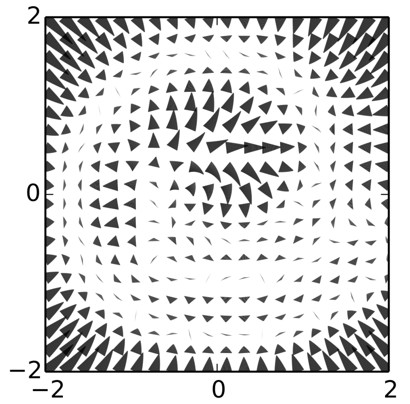
Quantum Circuits

Liu, LW, PRA '18

+Diffusion models







Generative modeling	**Statistical physics**
Negative log-likelihood	Energy function
Score function	Force
Latent variables	Collective variables/coarse graining/renormalization group
Partition function	Free energy calculation
Sample diversity	Enhanced sampling

Two sides of the same coin

Generative modeling

Known: samples

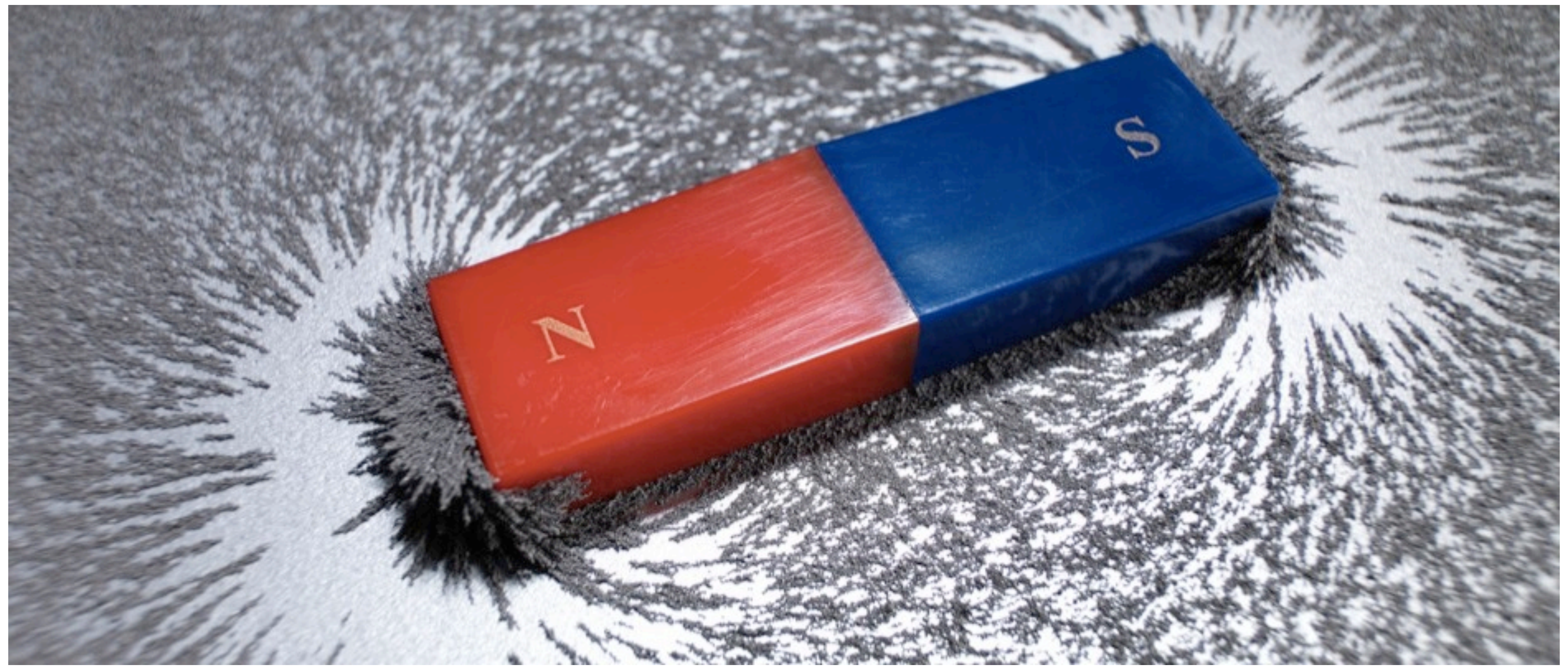
Unknown: generating distribution

Maximum likelihood estimation

"learn from data"

$$\mathscr{L} = -\mathbb{E}_{\boldsymbol{x}\sim\text{dataset}}\left[\ln p(\boldsymbol{x})\right]$$

Statistical physics



Known: energy function

Unknown: samples, partition function

Variational free energy

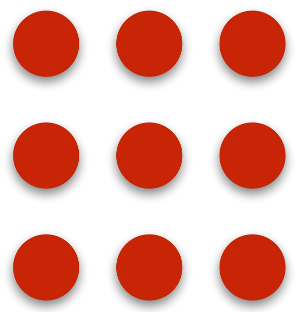
"learn from Hamiltonian"

$$F = \mathop{\mathbb{E}}_{\boldsymbol{x}\sim p(\boldsymbol{x})}\left[H(\boldsymbol{x}) + k_B T \ln p(\boldsymbol{x})\right]$$

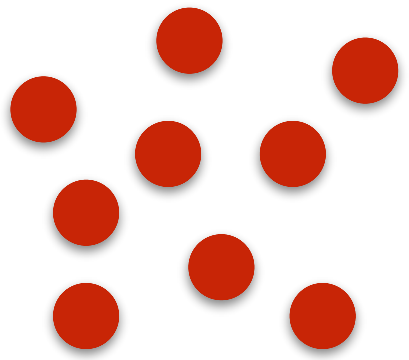
Nature tries to minimize free energy

$$F = E - TS$$

energy



entropy



F is the generating function of all other thermodynamic quantities

Unfortunately, it is "intractable" to compute

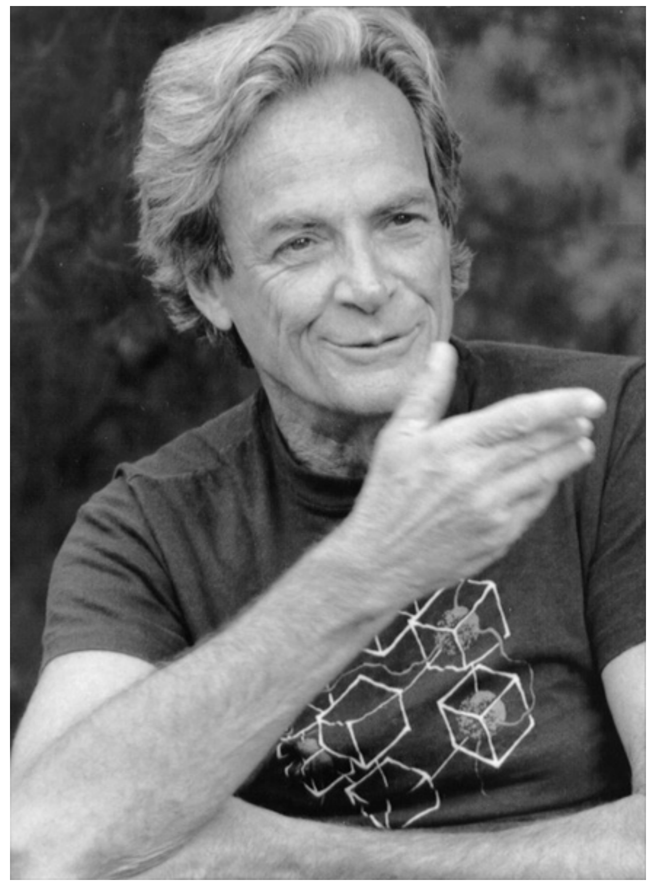
The variational free-energy principle

$$F[p] = \int dx\, p(\boldsymbol{x}) \left[H(\boldsymbol{x}) + k_B T \ln p(\boldsymbol{x}) \right] \geq F$$

$\downarrow$ variational density

$\downarrow$ energy

$\downarrow$ entropy 😱



Difficulties in Applying the Variational Principle to Quantum Field Theories[1]

Richard P. Feynman

[1]transcript of his talk in 1987

Generative models!

Deep variational free-energy approach

Use deep generative models as the variational density

$$F[p] = \mathop{\mathbb{E}}_{\boldsymbol{x}\sim p(\boldsymbol{x})} \Big[\underbrace{H(\boldsymbol{x})}_{\text{energy}} + \underbrace{k_B T \ln p(\boldsymbol{x})}_{\text{entropy}} \Big]$$

😁

Li and LW, PRL ‘18
Wu, LW, Zhang, PRL ‘19

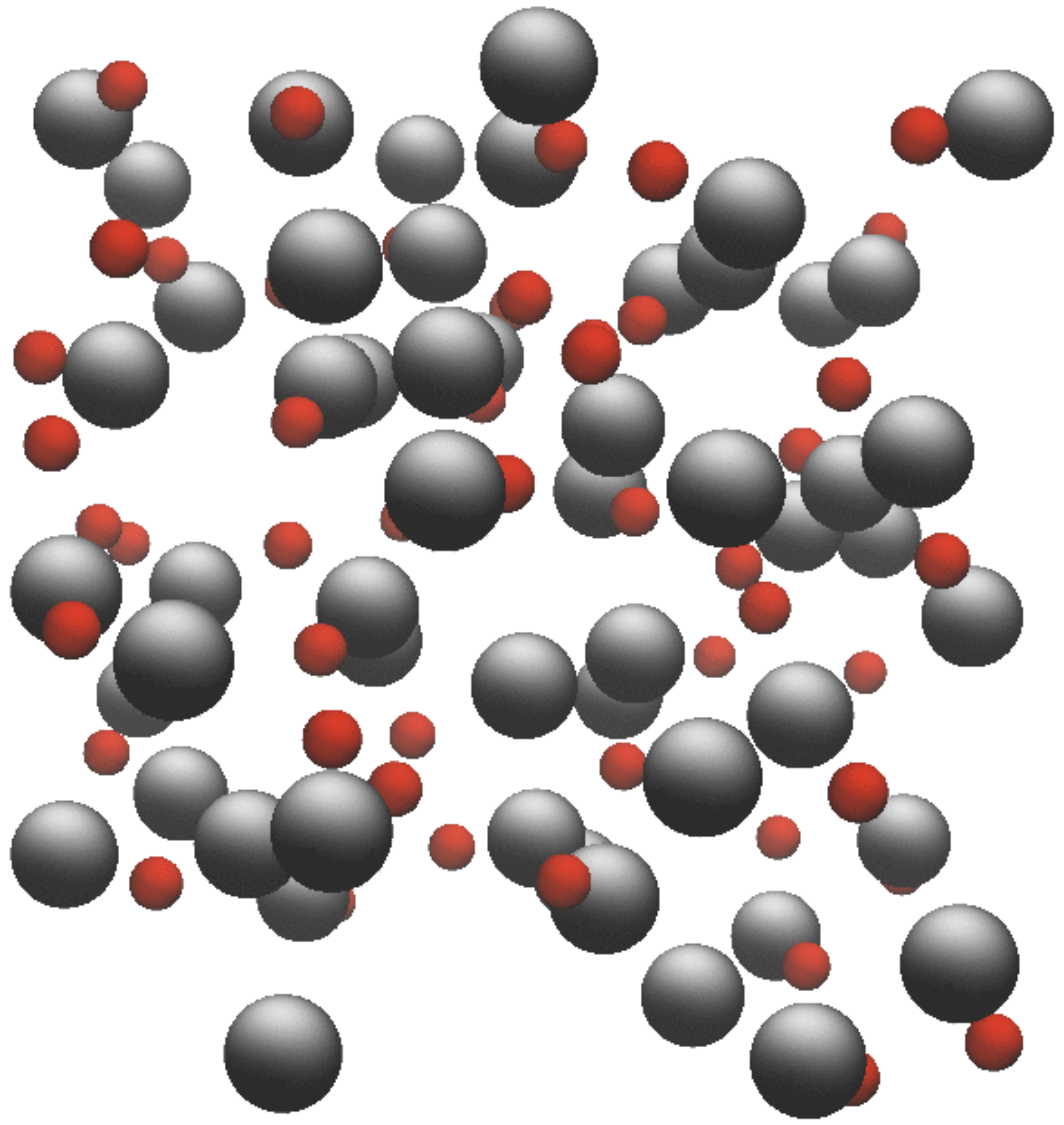
with normalizing flow & autoregressive models

✓ Tractable entropy ✓ Direct sampling

✓ Turning a sampling problem to an optimization problem better leverages the deep learning engine: 

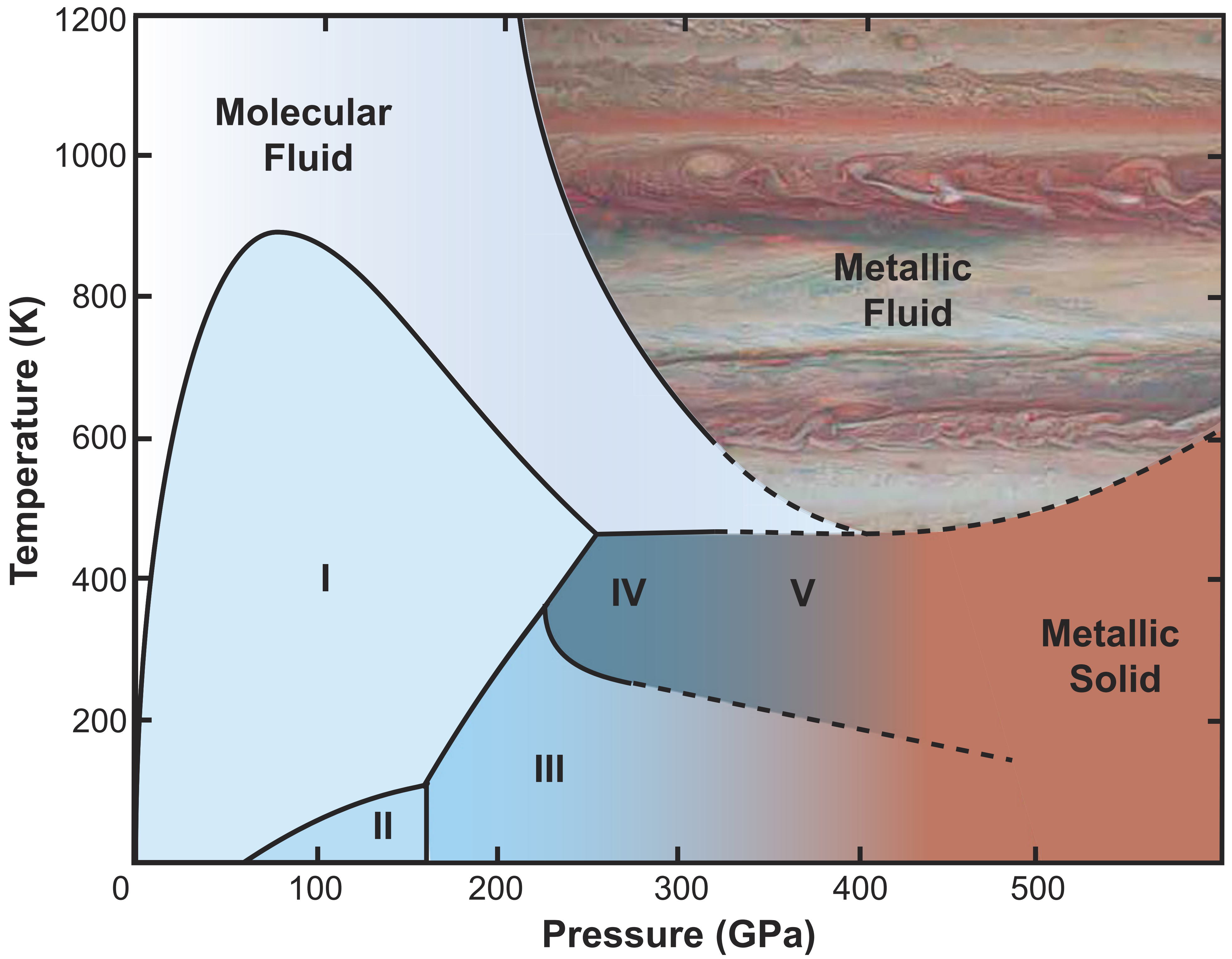
The dense hydrogen problem

Xie, Li, Wang, Zhang, LW, 2209.06095



N protons + N electrons in a box

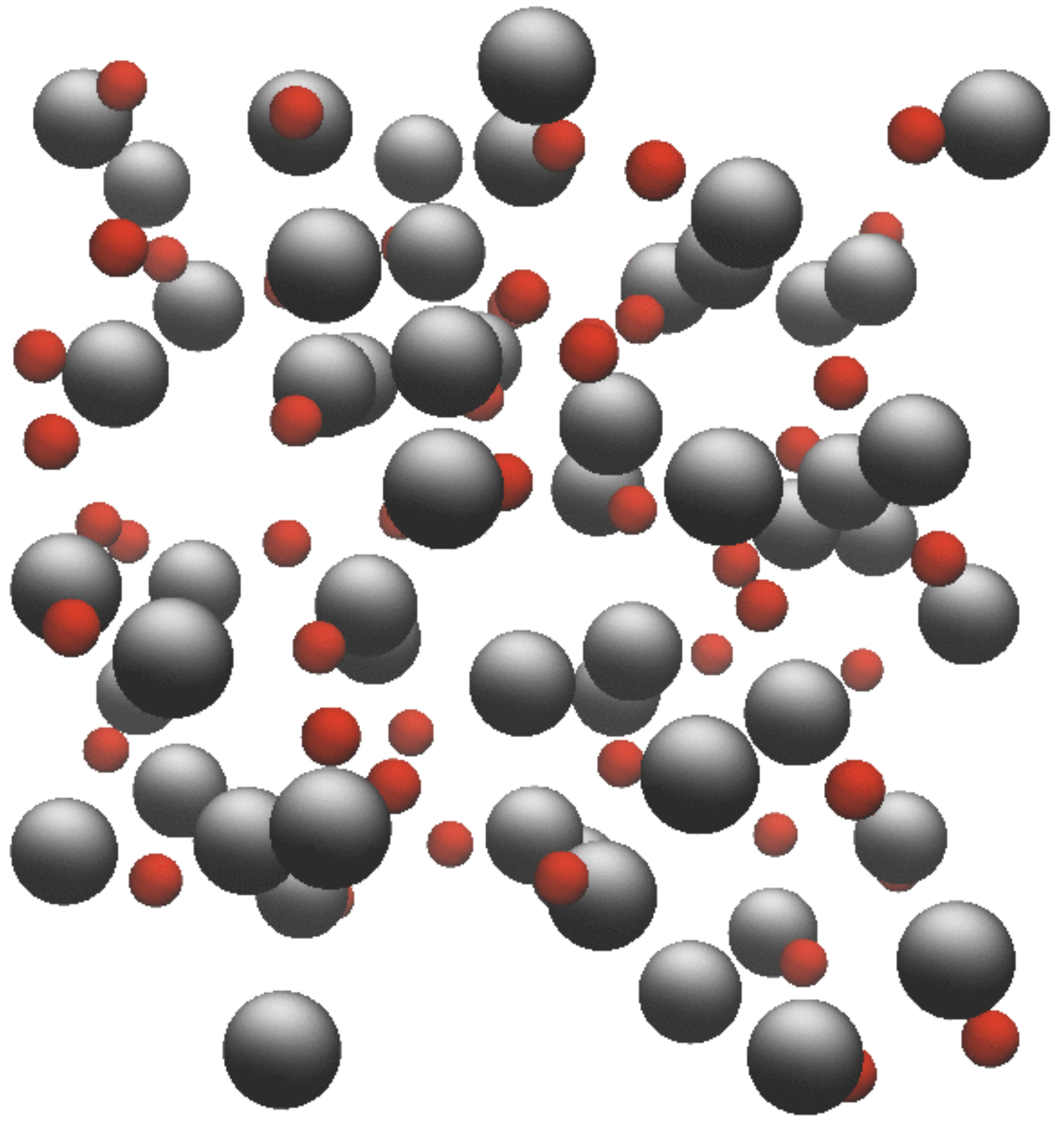
Radiat et al, Extremes, 2020



Generative model for proton probability density distribution
+ Deep neural network (Ferminet) for electron wavefunction

The dense hydrogen problem

Xie, Li, Wang, Zhang, LW, 2209.06095



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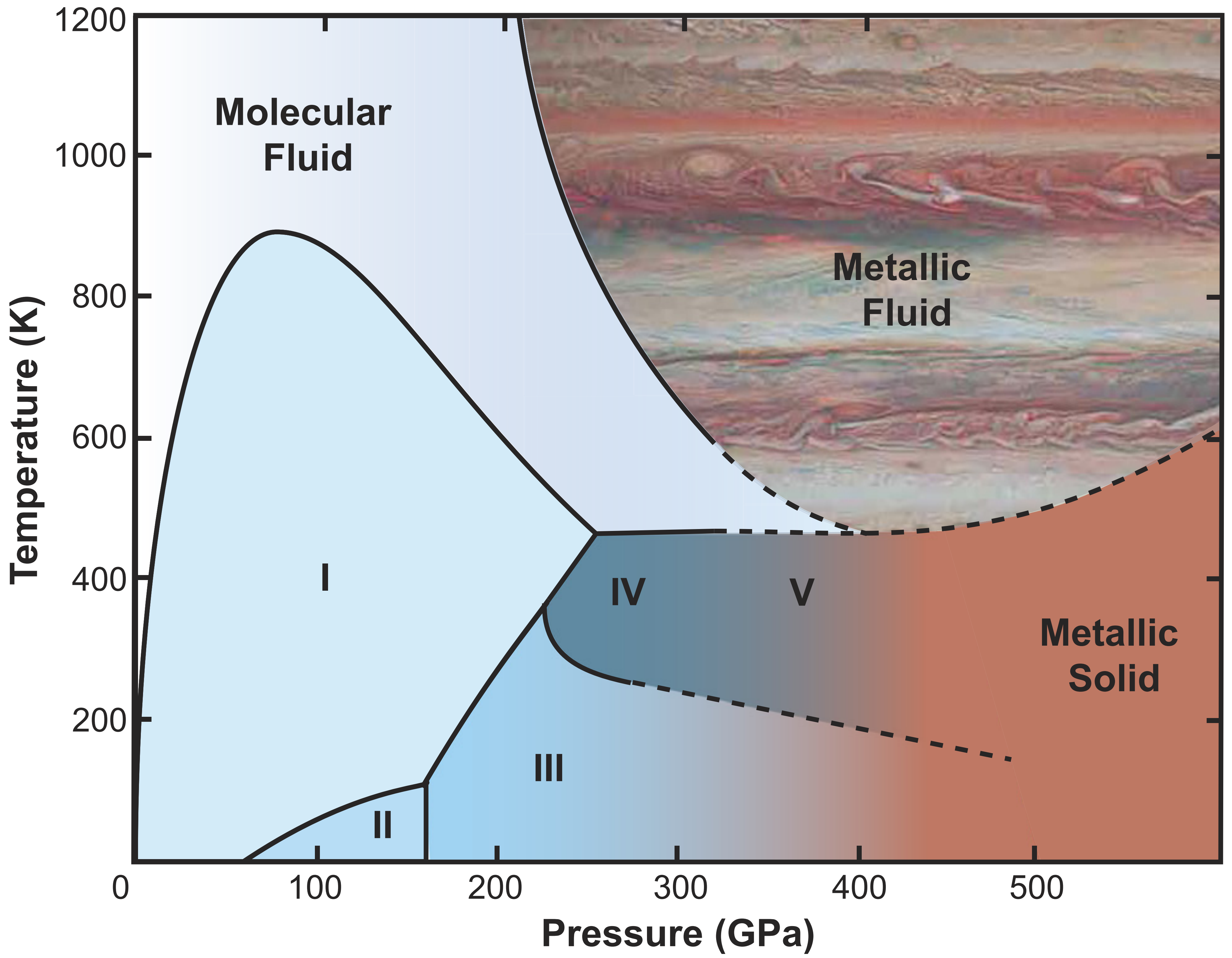

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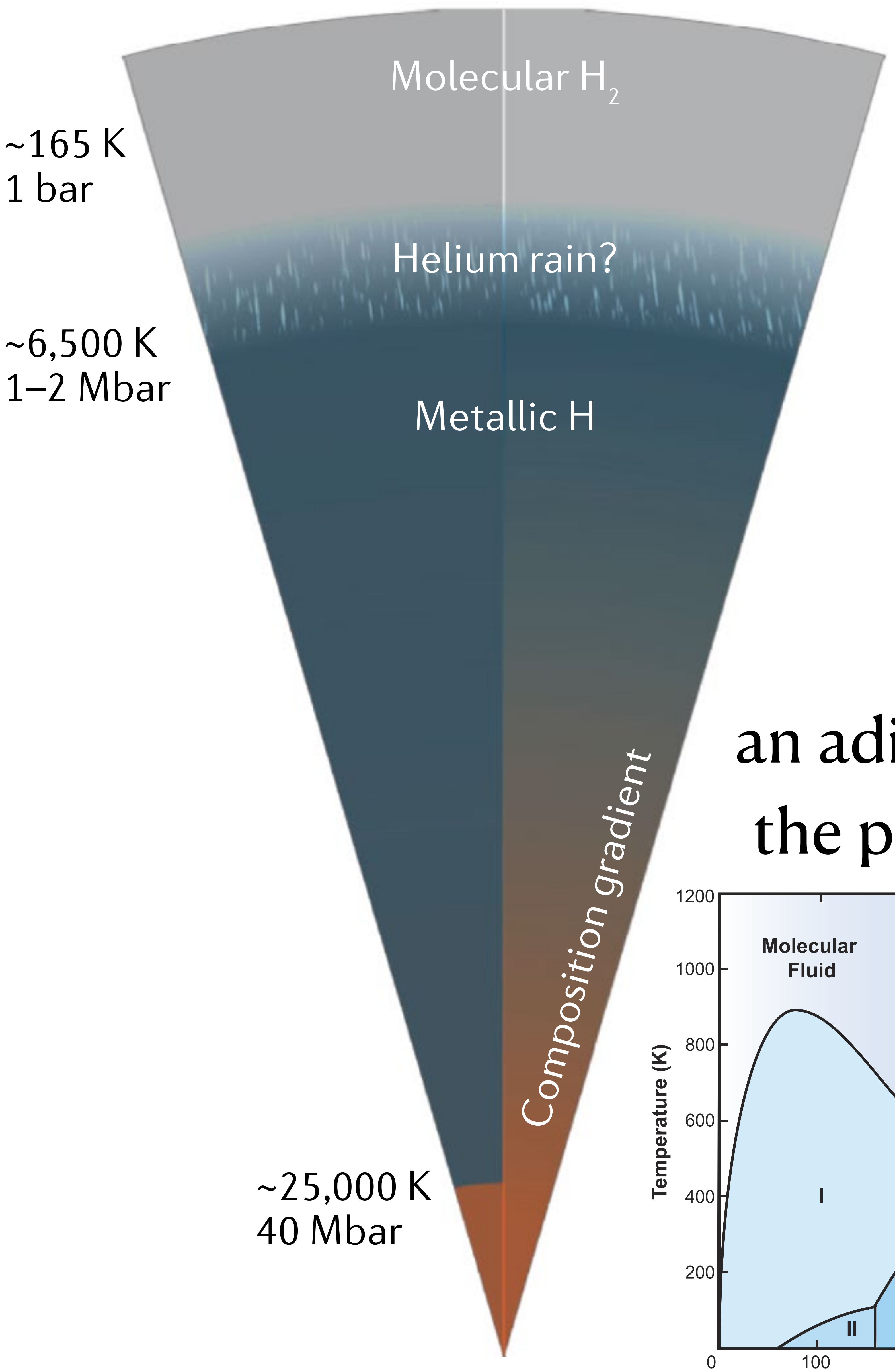
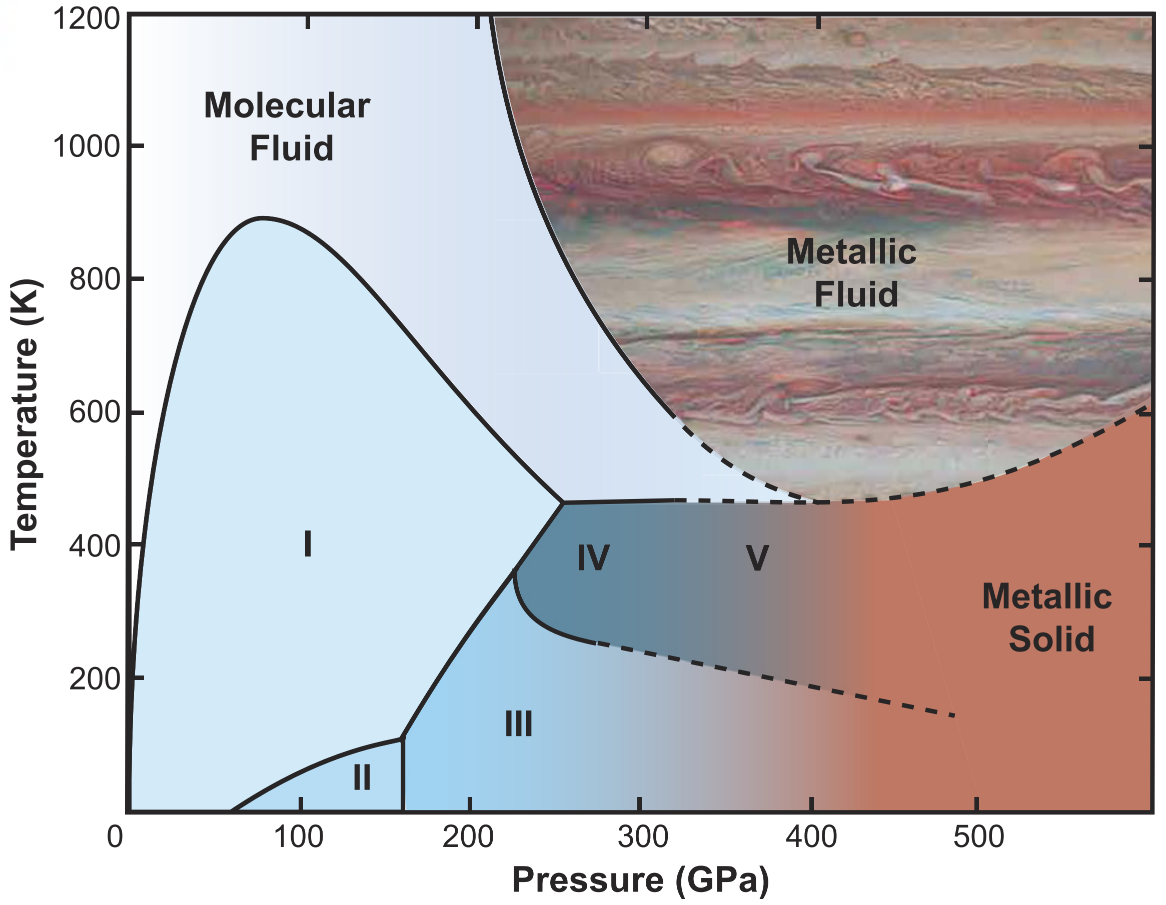
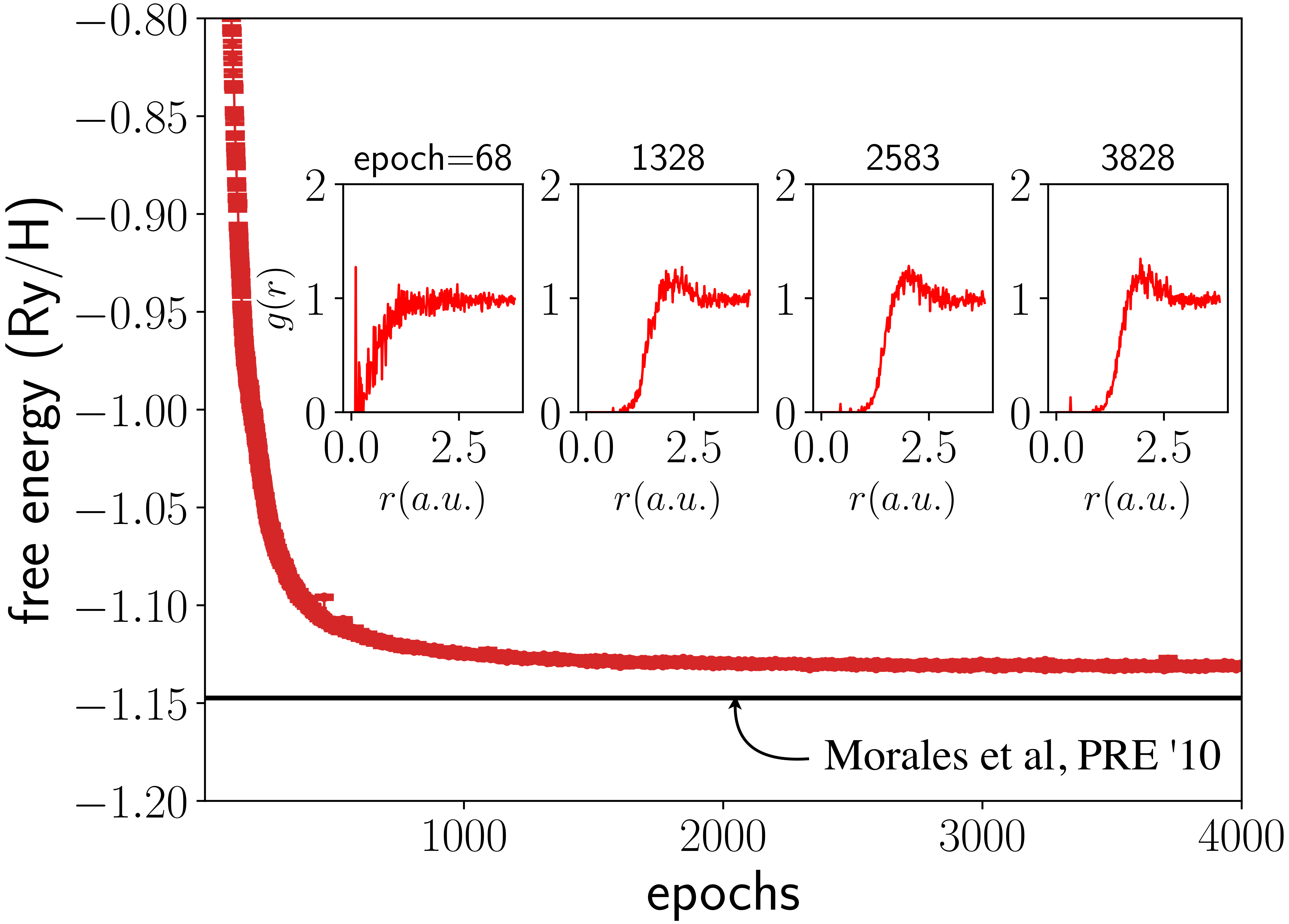
Dense hydrogen equation of state



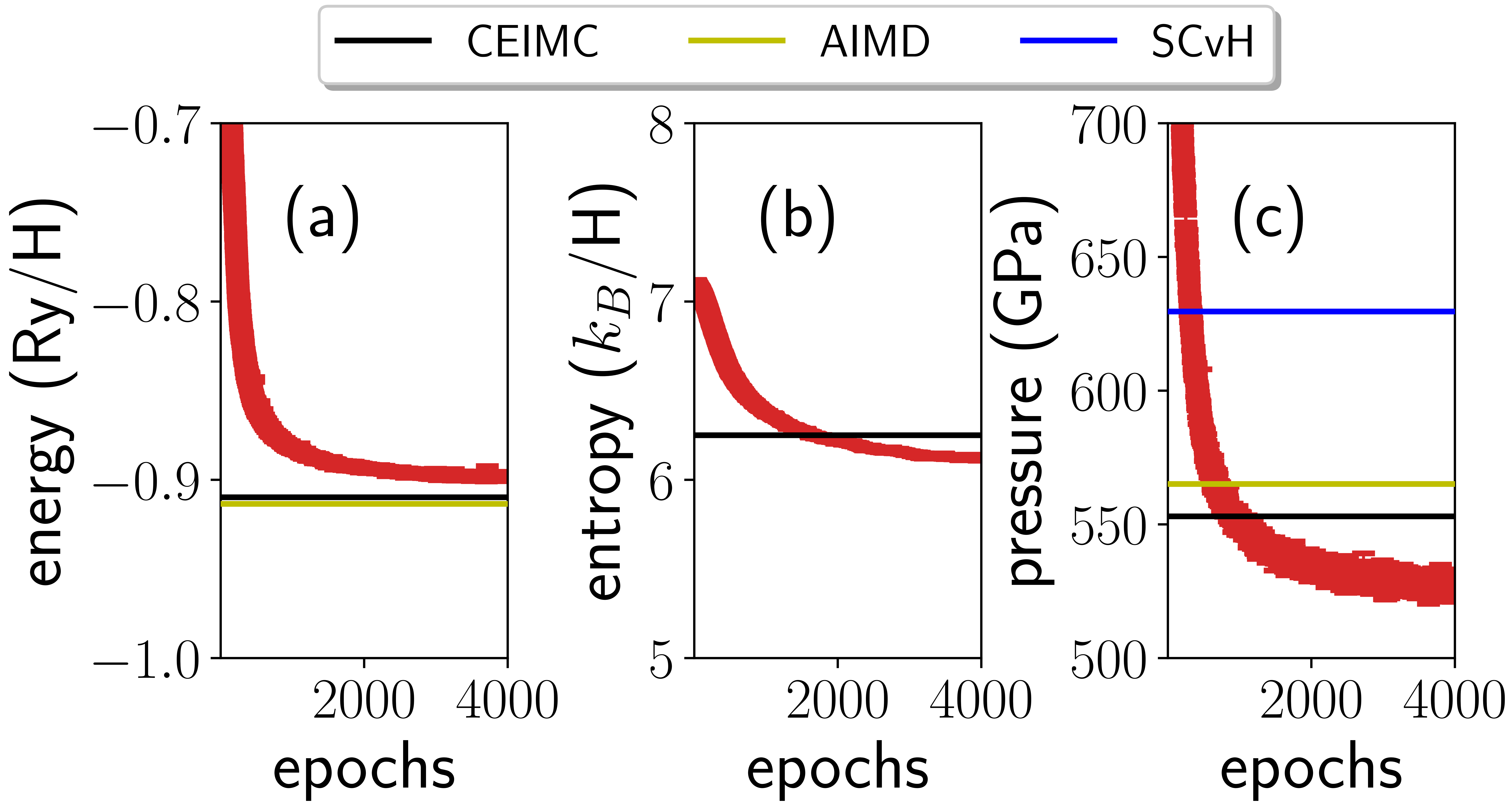
an adiabatic path in the phase diagram



$r_s = 1.25 \quad T = 6000\text{K}$



Xie, Li, Wang, Zhang, LW, 2209.06095



CEIMC
AIMD
SCvH
(a)
(b)
(c)
energy (Ry/H)
entropy (k_B/H)
pressure (GPa)
−0.7
−0.8
−0.9
−1.0
8
7
6
5
700
650
600
550
500
2000
4000
epochs
epochs
epochs

The Universe as a generative model

$$\mathcal{L} = \int d^4x \sqrt{-g} \Big[\frac{m_p^2}{2} R - \frac{1}{4} F^a_{\mu\nu} F_a^{\mu\nu} + i \bar{\psi}^i \gamma^\mu D_\mu \psi^i + \left(\bar{\psi}_L^i V_{ij} \Phi \psi_R^j + h.c. \right) - |D_\mu \Phi|^2 - V(\Phi) \Big]$$

Thank you!

Discovering physical laws: learning the action

Solving physical problems: optimizing the action