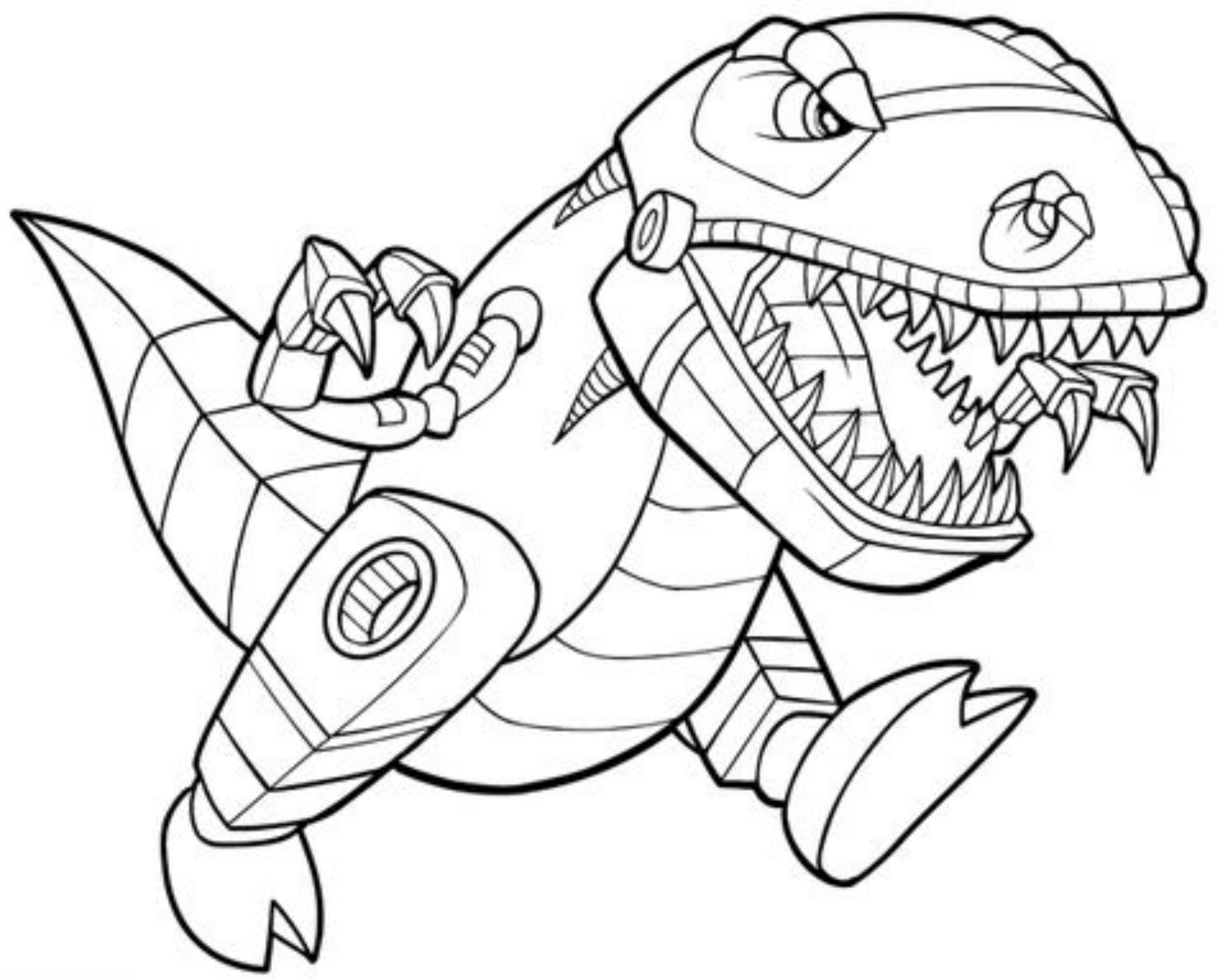
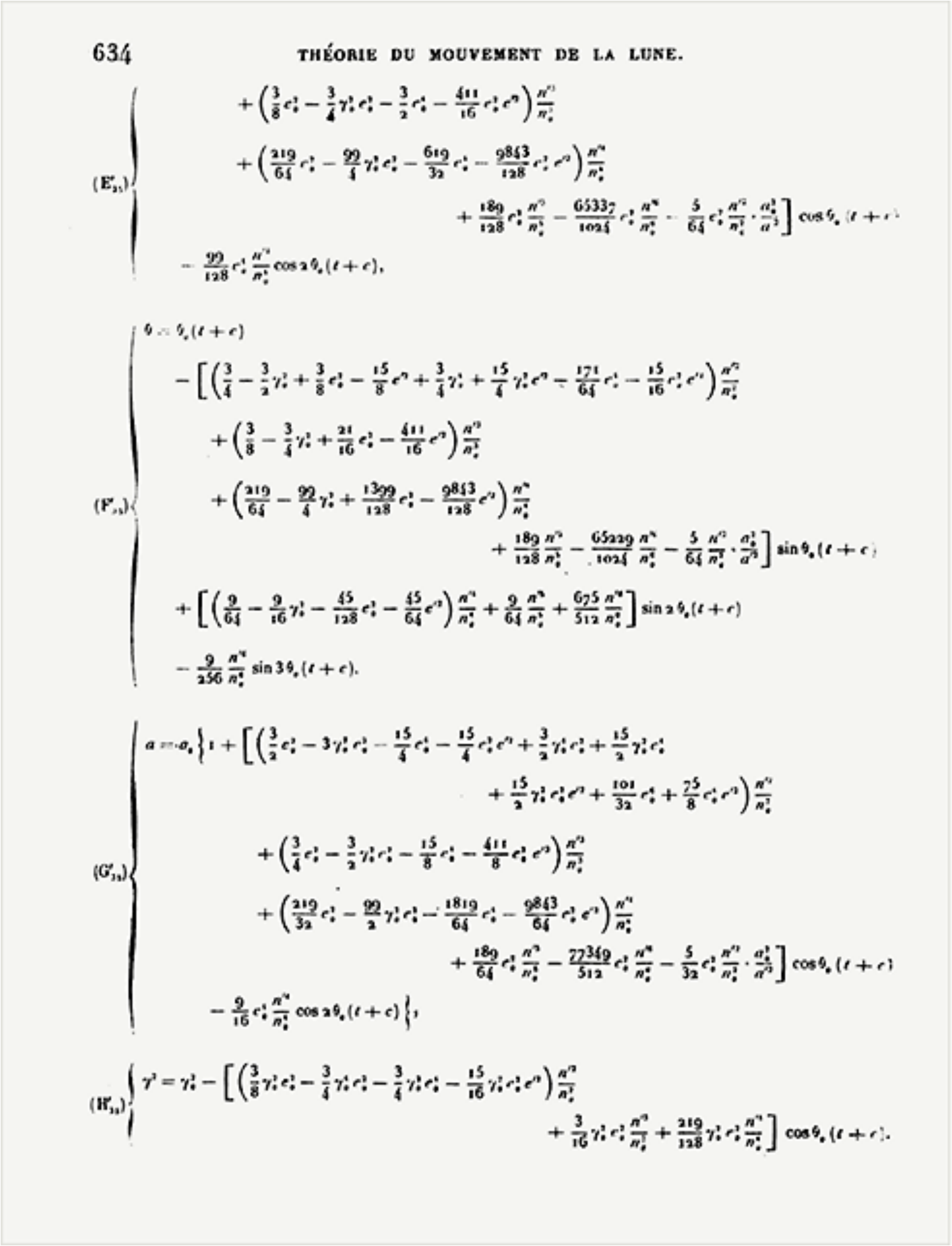
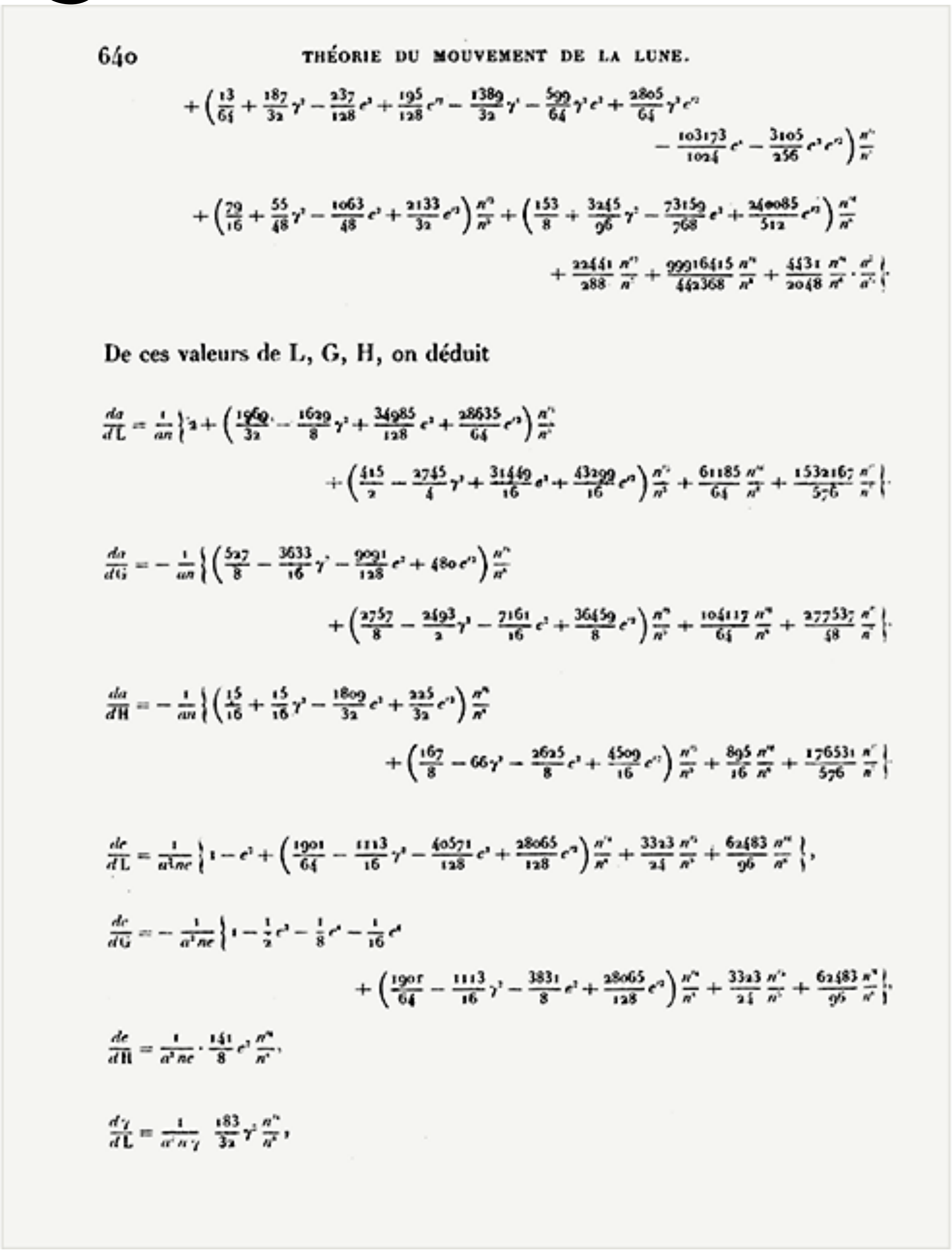


Neural Canonical Transformations

Lei Wang (王磊)
https://wangleiphy.github.io
Institute of Physics, CAS

Canonical transformation for Moon-Earth-Sun 3-body problem


634 THÉORIE DU MOUVEMENT DE LA LUNE.


640 THÉORIE DU MOUVEMENT DE LA LUNE.

De ces valeurs de L, G, H, on déduit

Charles Delaunay

↑

More than 1800 pages of this, ~20 years of efforts (1846-1867)

How to find useful canonical transformations for more complex systems?

Canonical transformations and deep learning

symplectic change of variables

$$\boldsymbol{X} = (p, q) \longleftrightarrow \boldsymbol{Z} = (P, Q)$$

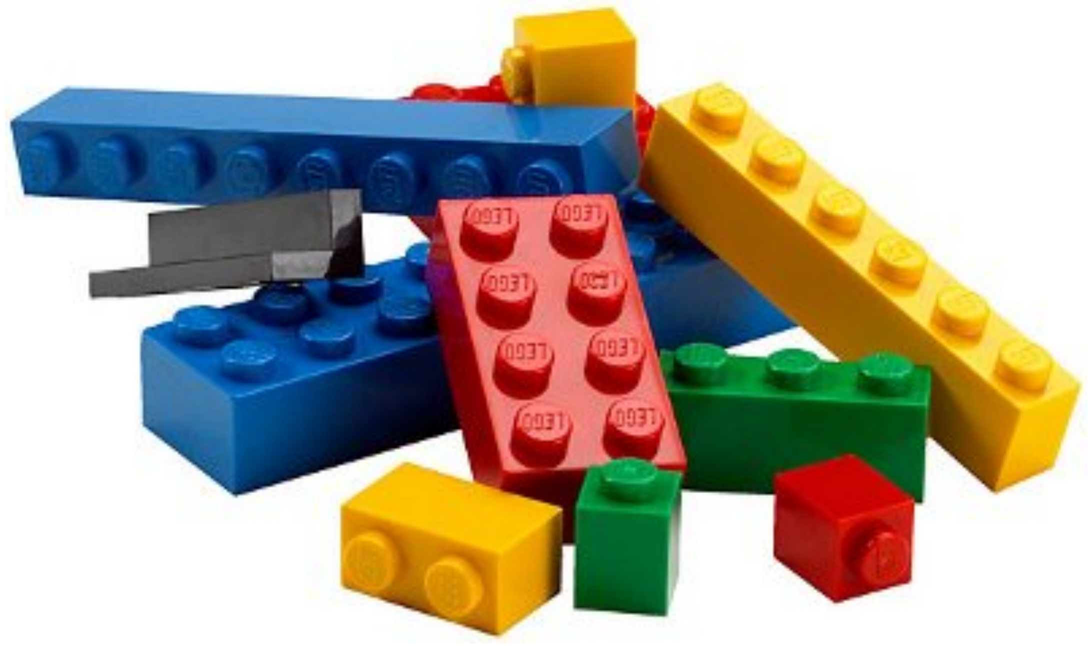
physical varaibles

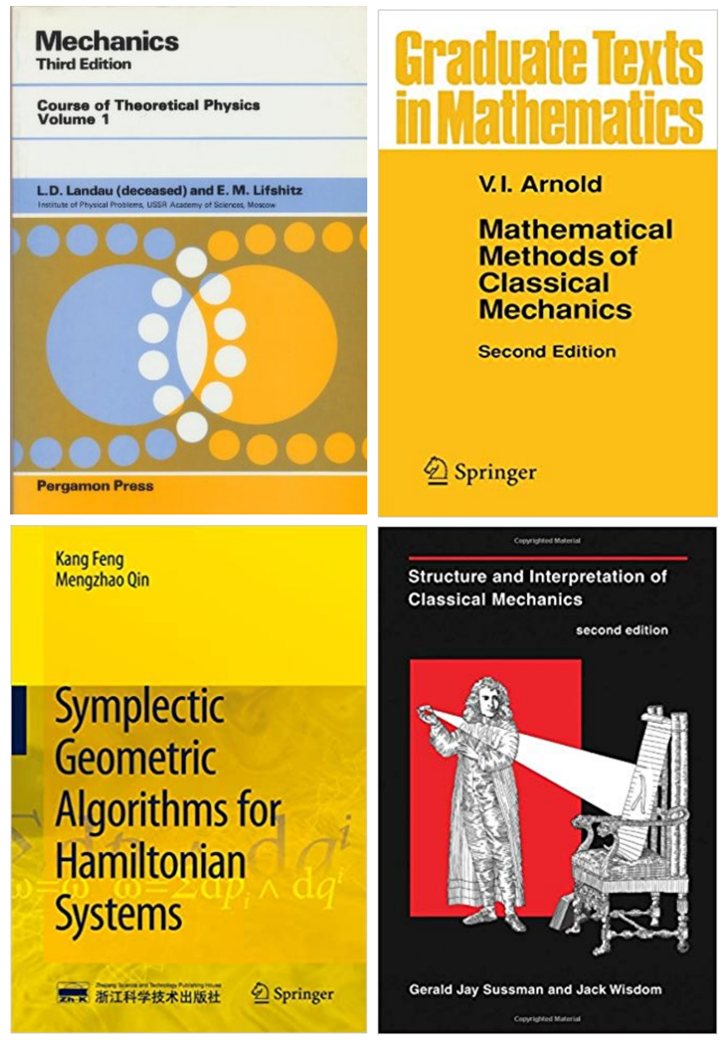
$$(\nabla_{\boldsymbol{X}} \boldsymbol{Z}) \begin{pmatrix} & I \\ -I & \end{pmatrix} (\nabla_{\boldsymbol{X}} \boldsymbol{Z})^T = \begin{pmatrix} & I \\ -I & \end{pmatrix}$$

latent varaibles

$$\boldsymbol{Z} = \mathcal{T}(\boldsymbol{X})$$

$$\mathcal{T} = \mathcal{T}_1 \circ \mathcal{T}_2 \circ \mathcal{T}_3 \circ \cdots$$

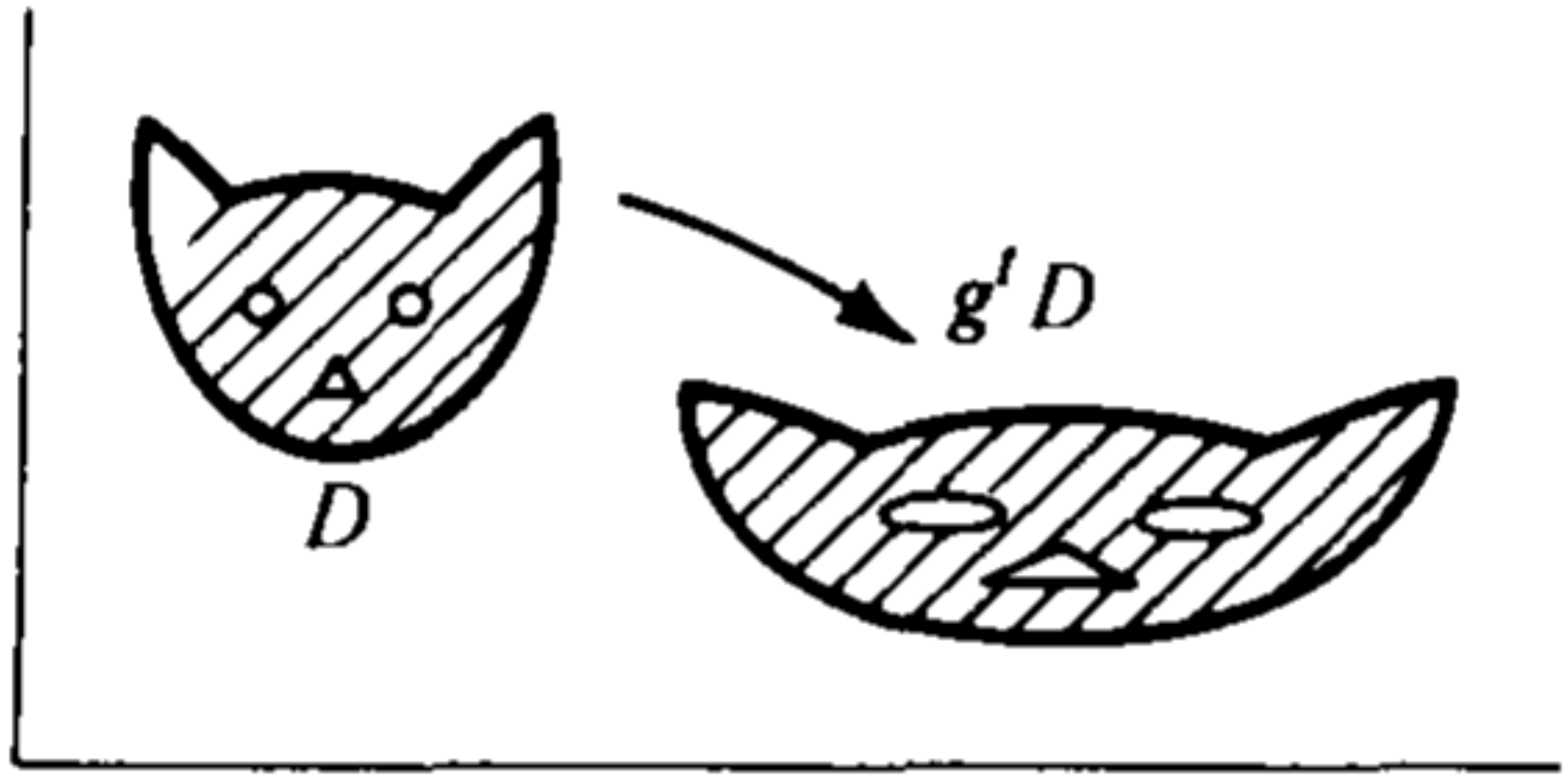




Compose symplectic blocks to form a deep neural network and learn them either from data or variationally

Canonical transformations and generative models

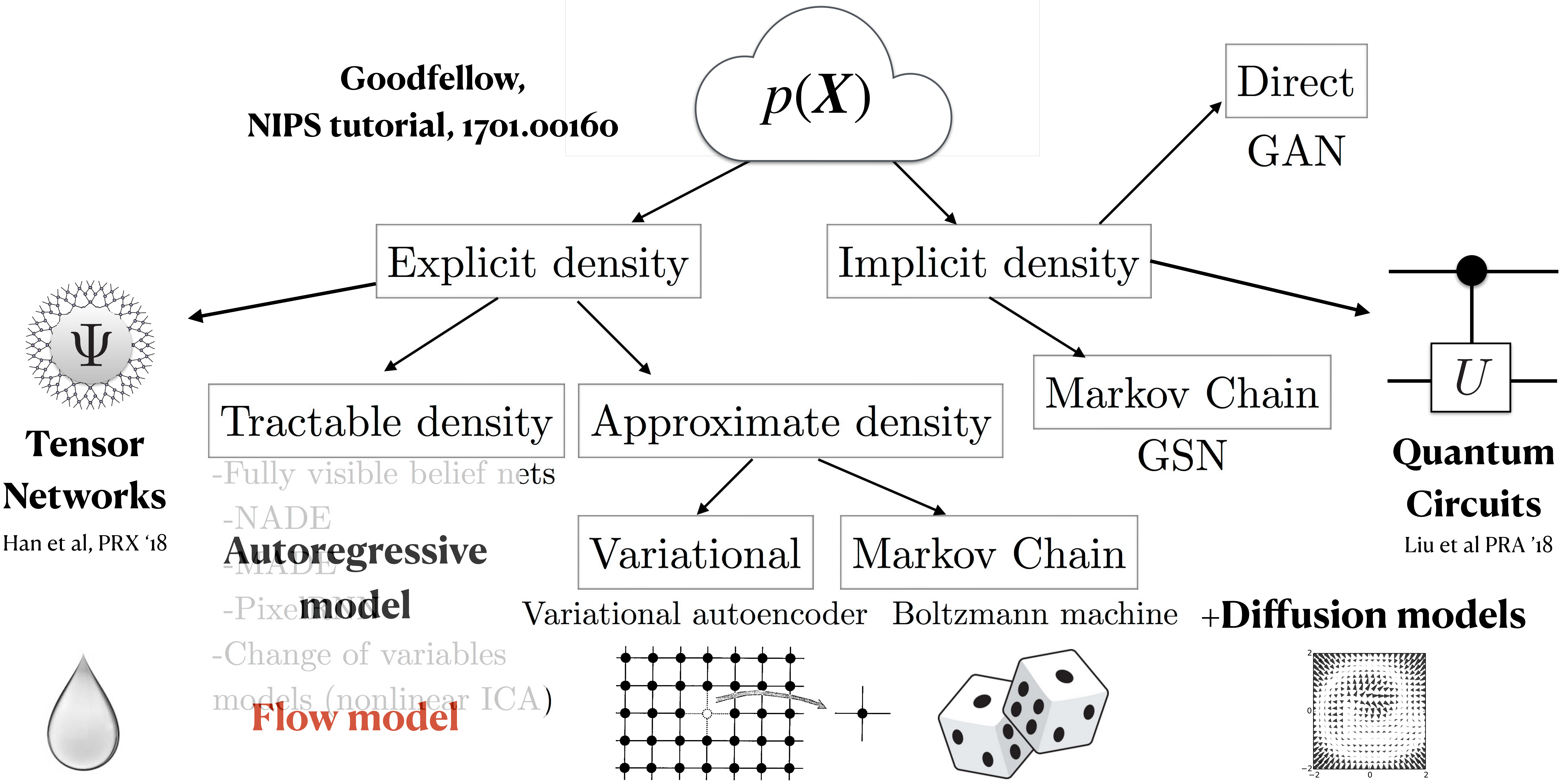
Canonical transformation deforms phase space density $p(\boldsymbol{X}) = e^{-\beta H(\boldsymbol{X})}$



Arnold, Mathematical Methods of Classical Mechanics '78

Modern generative models are good at transforming probability densities

Generative models and their physics genes



Flow-based generative models

Parallel WaveNet 1711.10433

https://deepmind.com/blog/high-fidelity-speech-synthesis-wavenet/

Glow 1807.03039

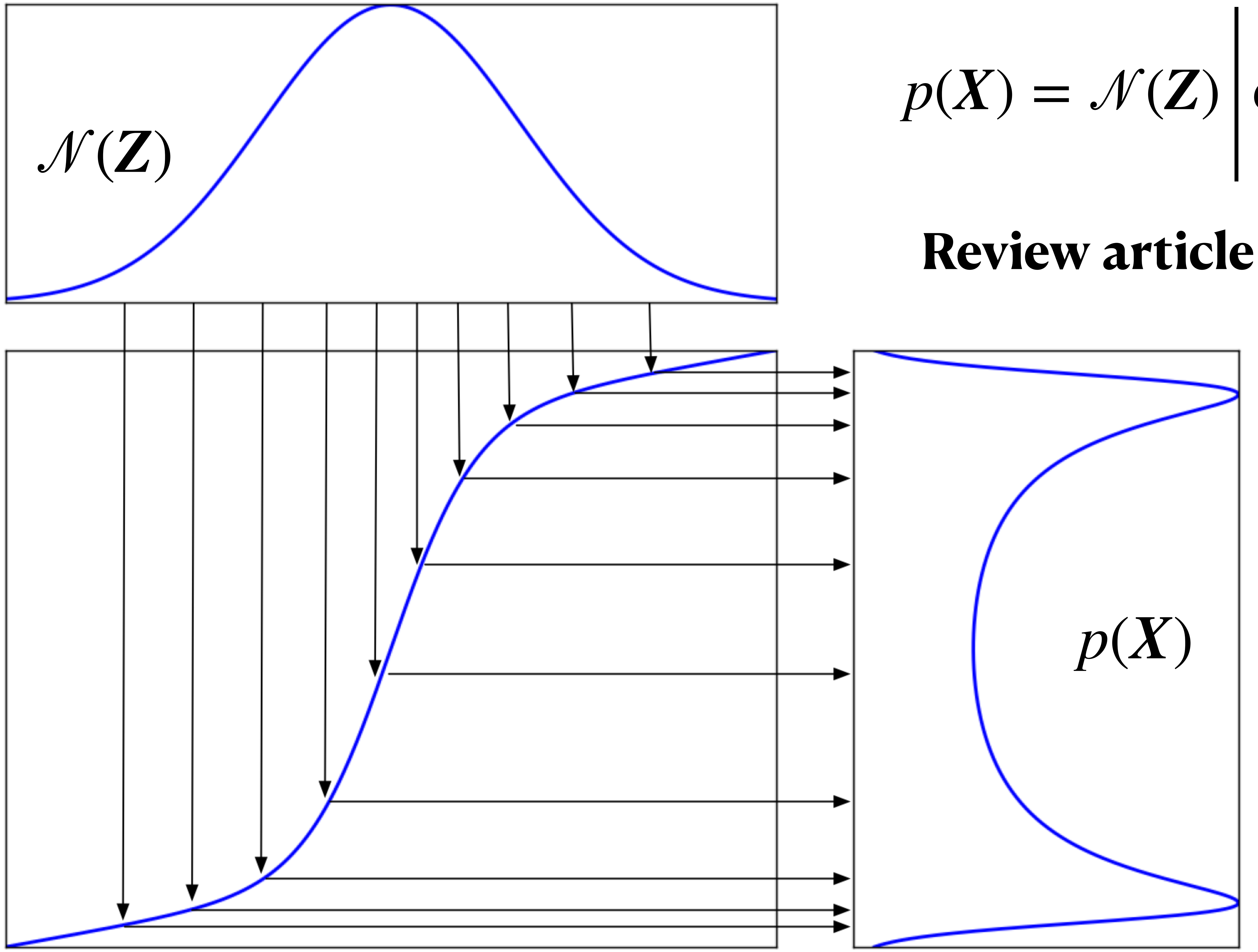
https://blog.openai.com/glow/

Flow model in a nutshell

Base density

$$p(\boldsymbol{X}) = \mathcal{N}(\boldsymbol{Z}) \left| \det\left(\frac{\partial \boldsymbol{Z}}{\partial \boldsymbol{X}}\right) \right|$$

Review article 1912.02762



"neural net" with 1 neuron

Target density

Physics intuition of flow models

Li and LW, PRL '18

THURSDAY, 28 JUNE 2018 https://www.pks.mpg.de/machine-learning-for-quantum-many-body-physics

09:00 - 10:00

Lei Wang (Chinese Academy of Sciences)
overview talk

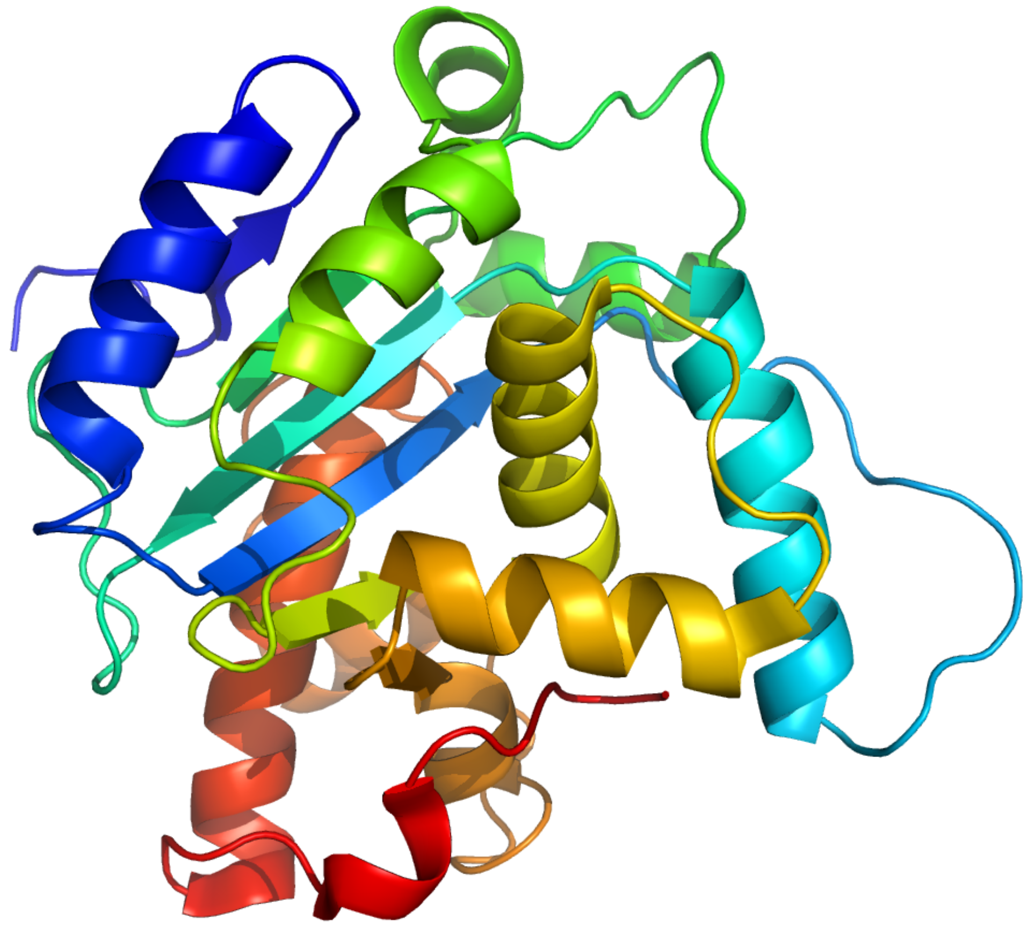
Neural Network Renormalization Group

High-dimensional, nonlinear, learnable, composable diffeomorphism

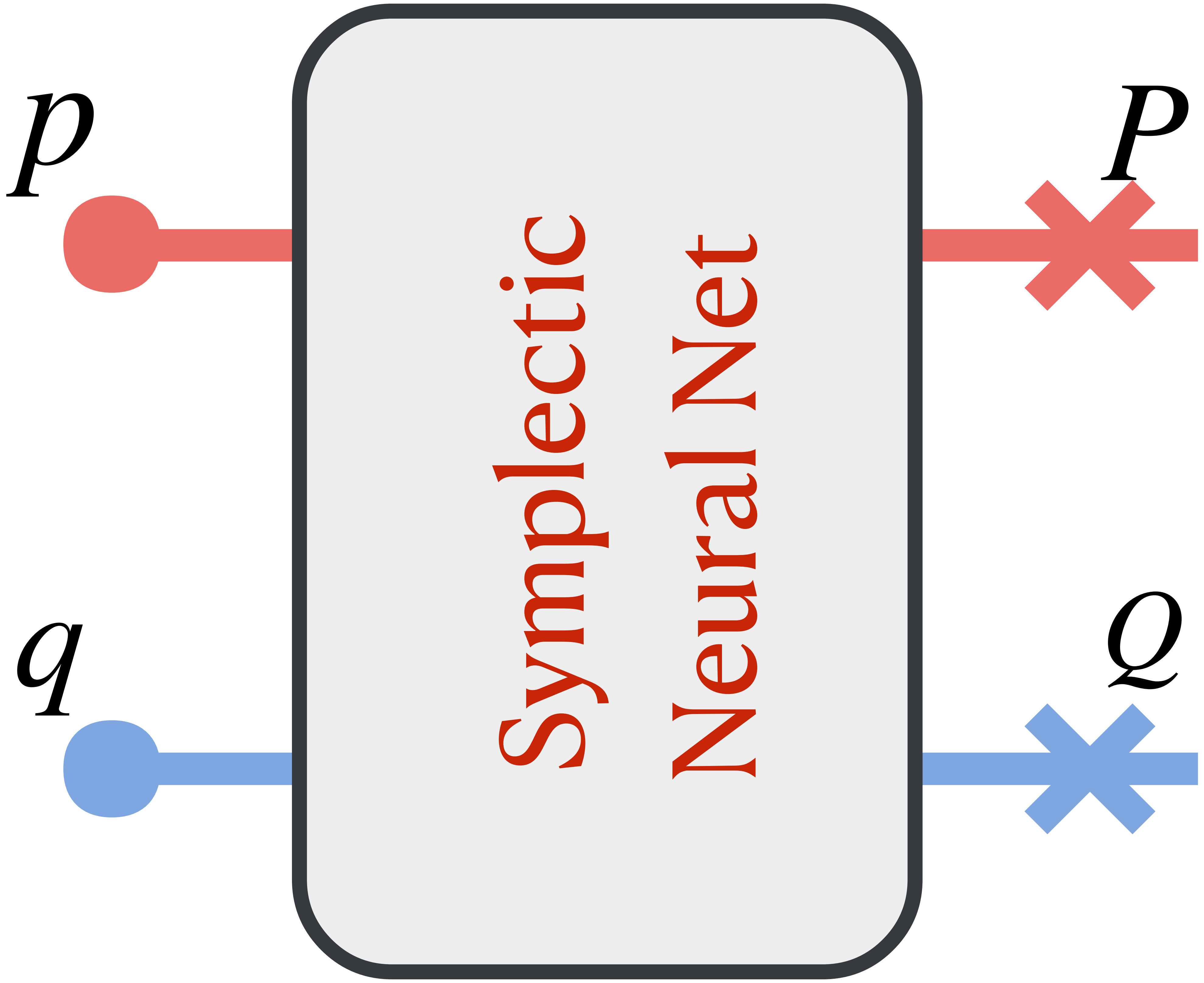
Neural canonical transformations

Li, Dong, Zhang, LW, PRX ‘20

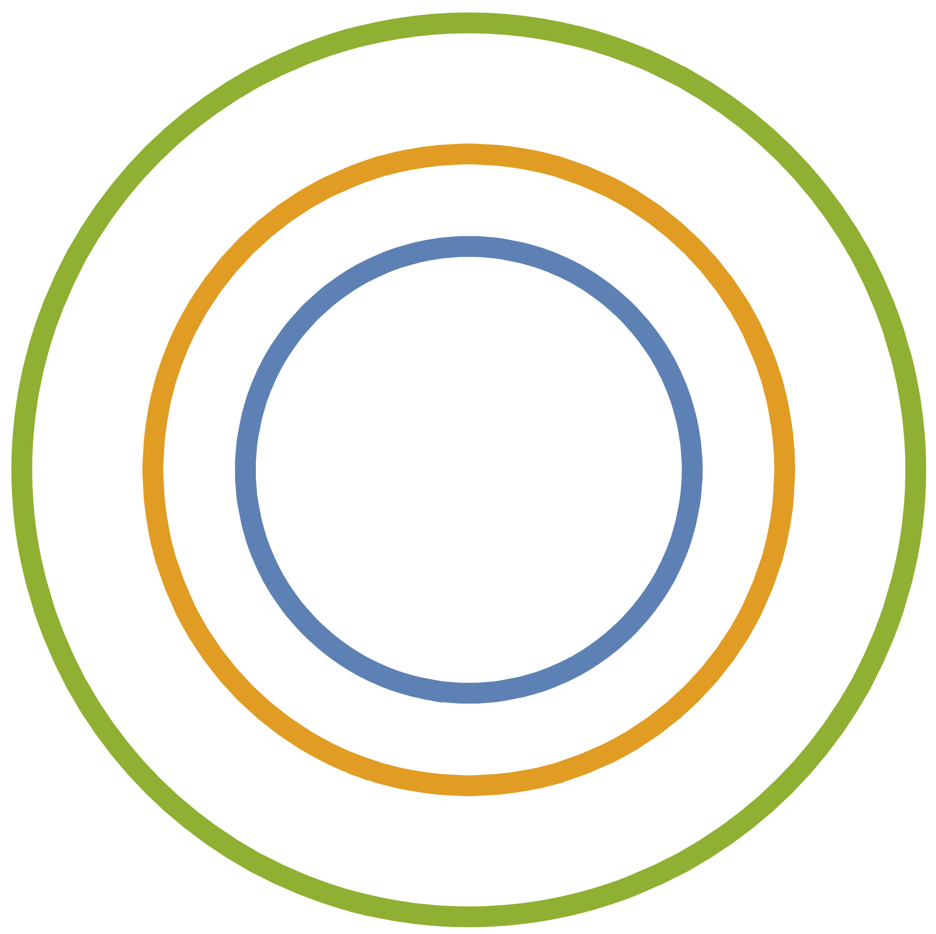
$H(p, q)$



physical phase space



$$K(P, Q) = \sum_k \frac{P_k^2 + \omega_k^2 Q_k^2}{2}$$

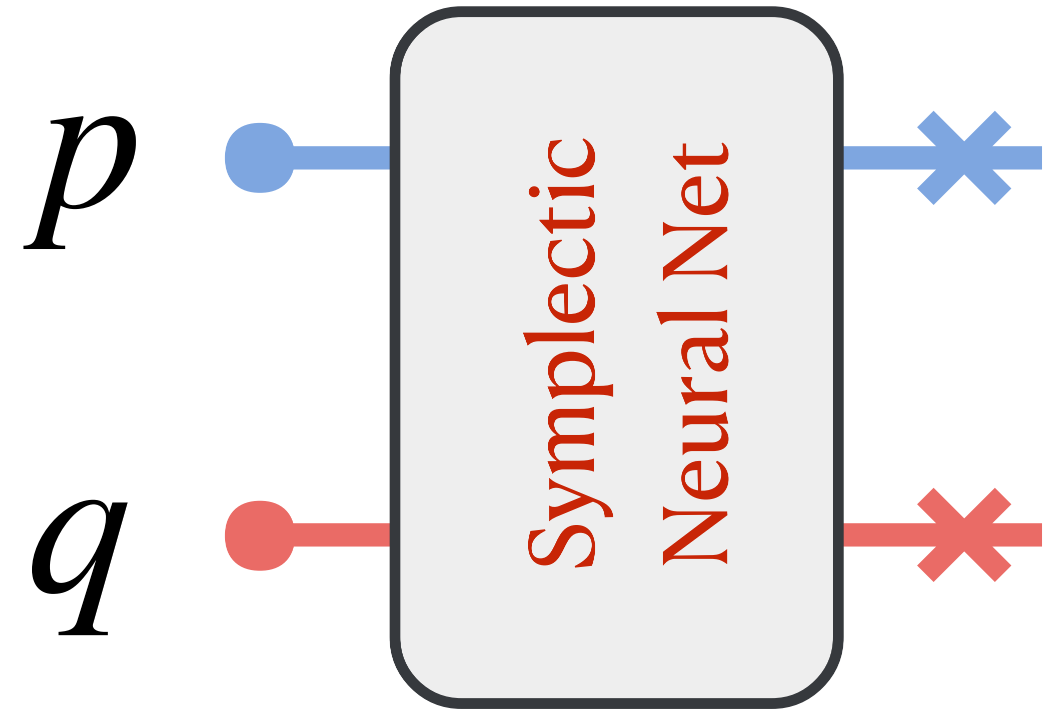


latent phase space

Learn the transformation and the latent harmonic frequencies

Symplectic blocks

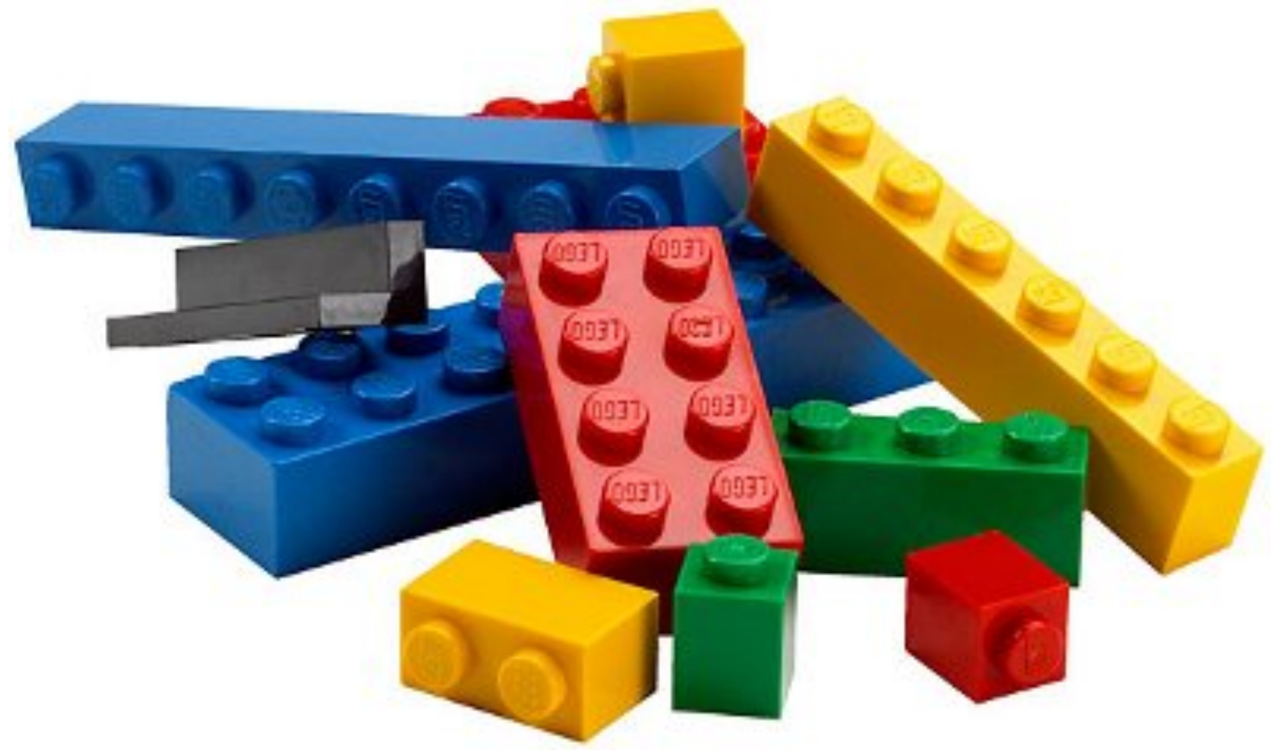
- **Neural point transformations** Li, Dong, Zhang, LW, PRX '20



$$P = p\left(\nabla_Q q\right)$$

$$Q = f(q)$$

arbitrary invertible neural net

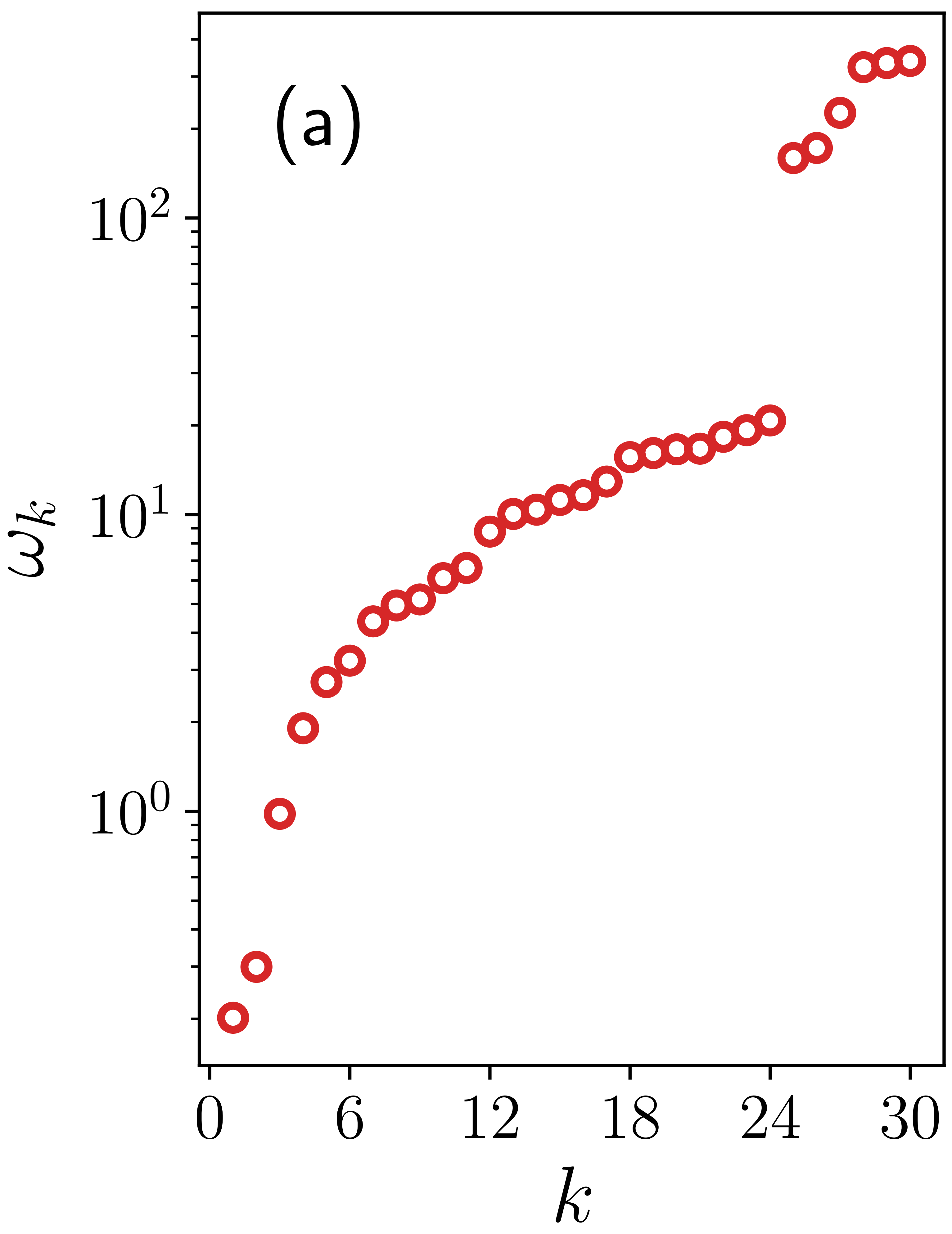


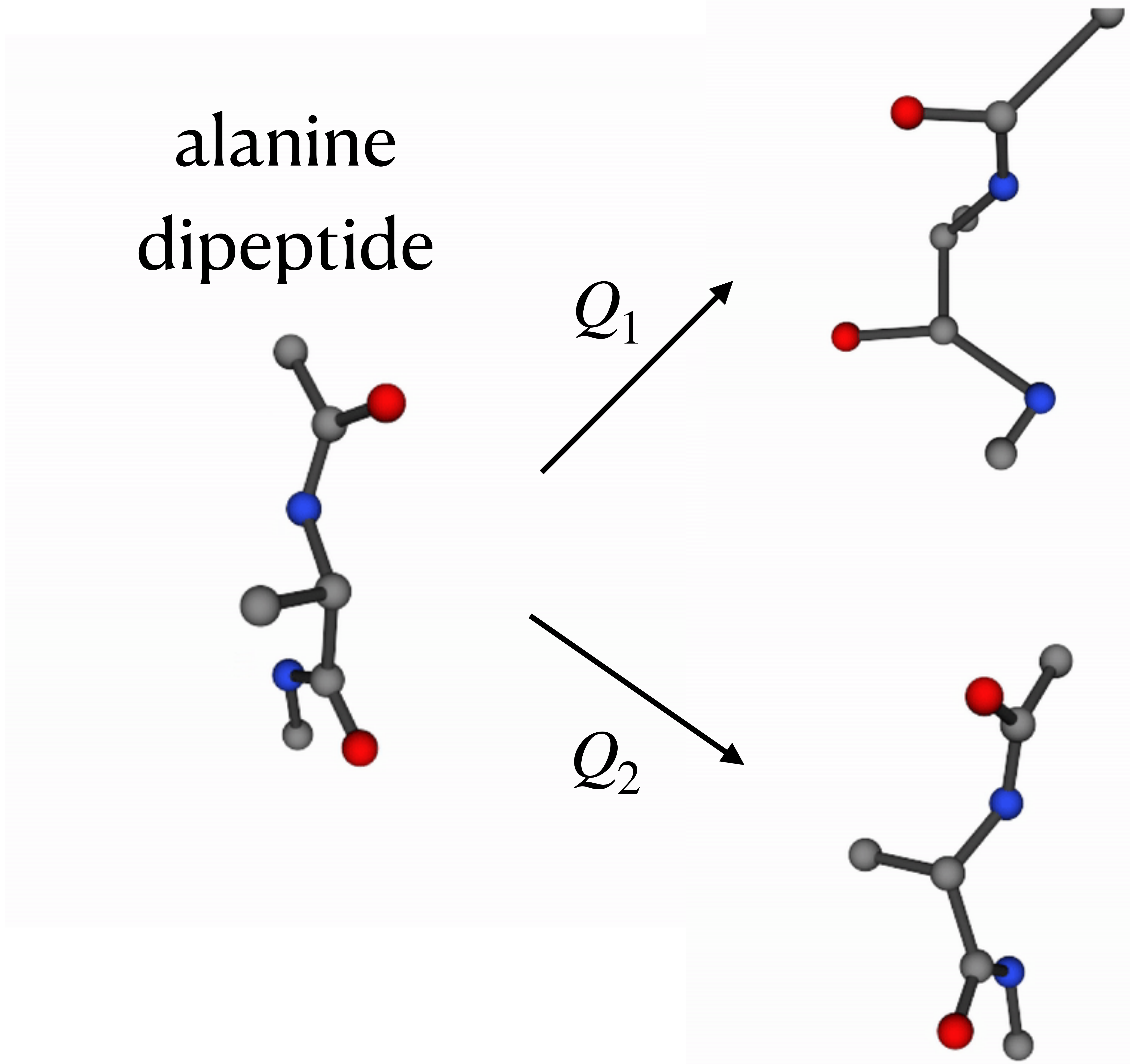
- Linear transformation: Symplectic Lie group Sp($2n$)

- Continuous-time flow: Symplectic generating functions via Hamiltonian dynaics See also Bondesan, Lamacraft, 1906.04645

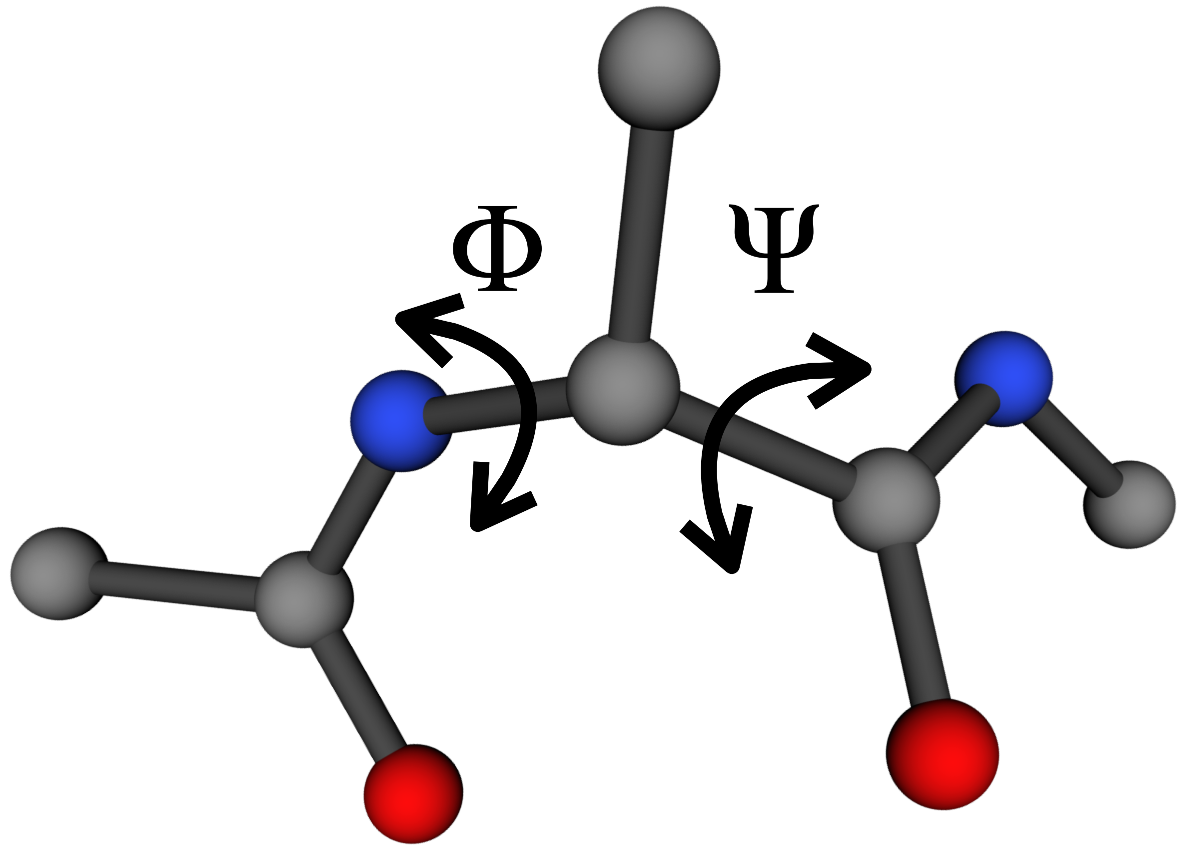
Neural ODE, Chen et al, 1806.07366, Monge-Ampère flow, Zhang et al 1809.10188

Li, Dong, Zhang, LW, PRX ‘20

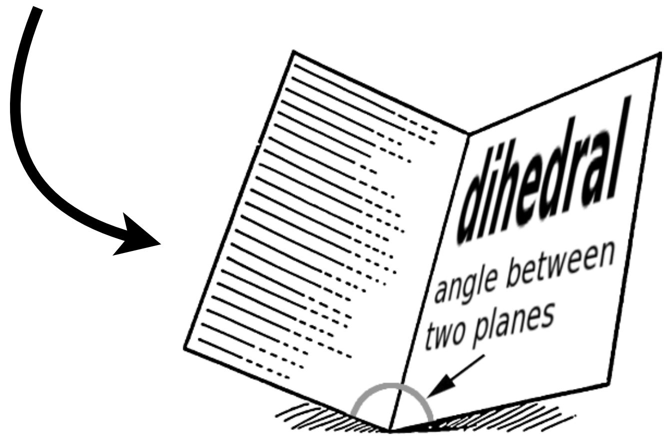


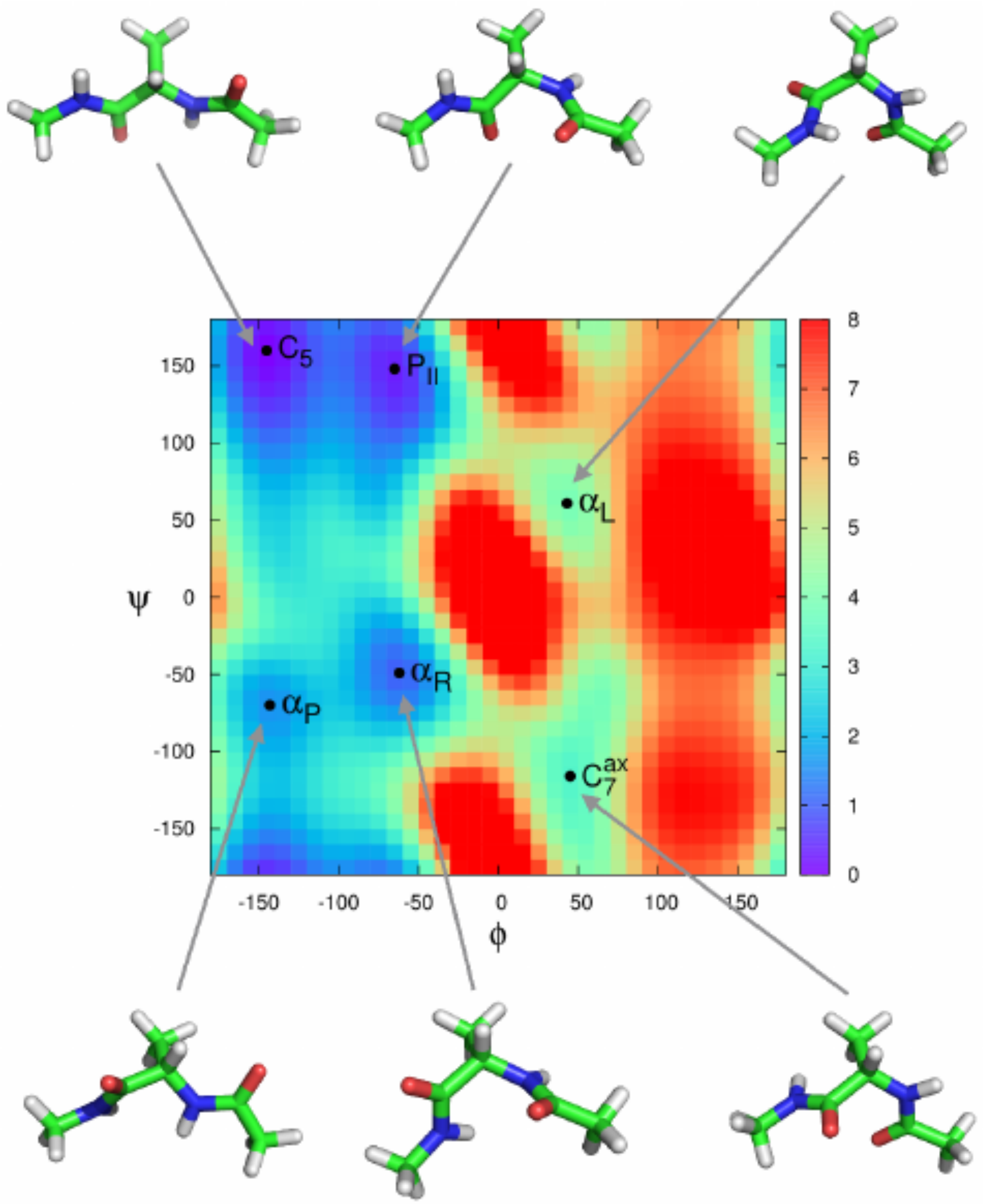


Neural canonical transformation identifies nonlinear slow modes



slow motion of the two torsion angles





Ramachandran plot for table conformations

Nonlinear dimension reduction to slow collective variables useful for control, prediction, enhanced sampling, cross interpolation...

check PRX '20 for more examples & applications

On identifiability, related to Gresele et al independent mechanism analysis 2106.05200

Entering the quantum world

"Canonical" transformations

classical world

Symplectic transformation

quantum world

Unitary transformation

PHYSICAL REVIEW VOLUME 85, NUMBER 4 FEBRUARY 15, 1952

Point Transformations in Quantum Mechanics

BRYCE SELIGMAN DEWITT*
Ecole d'Eté de Physique Théorique de l'Université de Grenoble, Les Houches, Haute Savoie, France
(Received September 14, 1951)

An isomorphism is shown to exist between the group of point transformations in classical mechanics and a certain subgroup of the group of all unitary transformations in quantum mechanics. This isomorphism is

The unitary representations of the point-transformation group may be obtained by determining the infinitesimal generators of the group. An infinitesimal point transformation may be expressed in the form

$$x'^i = x^i + \epsilon\Lambda^i(x), \tag{3.7}$$

$$p_i' = p_i - \tfrac{1}{2}\epsilon[(\partial/\partial x^i)\Lambda^j(x), p_j]_+, \tag{3.8}$$

"Quantizating" the point transformation

provides a unitary transformation $e^{-i\epsilon G} \equiv e^{-\frac{i}{2}\epsilon[\Lambda(x),p]_+}$

Canonical transformations

classical world

Symplectic transformation

Phase space density

$$\frac{\partial \rho}{\partial t} = \{G, \rho\}$$

Kullback-Leibler divergence

$$\mathbb{KL}\left(\rho \| \frac{e^{-\beta H}}{Z}\right)$$

quantum world

Unitary transformation

Density matrix

$$\frac{\partial \rho}{\partial t} = -i[G, \rho]$$

Quantum relative entropy

$$S\left(\rho \| \frac{e^{-\beta H}}{Z}\right)$$

The variational free energy principle

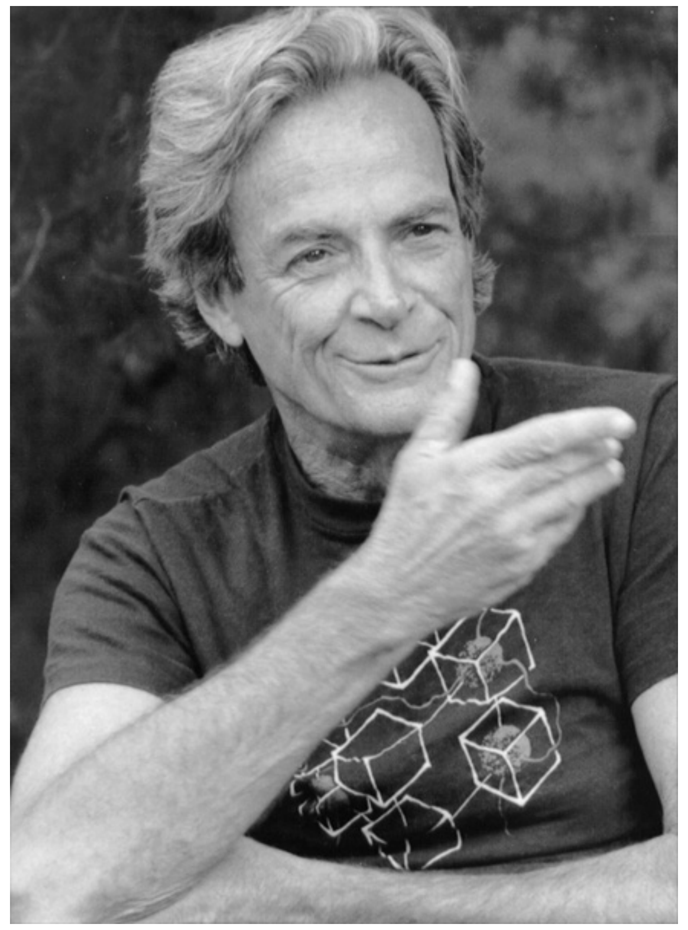
Gibbs–Bogolyubov-Feynman-Delbrück–Molière

$$\min \quad F[\rho] = \mathrm{Tr}(H\rho) + k_B T\, \mathrm{Tr}(\rho \ln \rho) \quad \geq F$$

↓ variational density matrix

↓ energy

↓ entropy



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

Richard P. Feynman

[1]transcript of Professor Feynman's talk in 1987

ρ ?

Generative models !

Variational density matrices as generative models

Learnable unitary transformation generated by point transformation

Learnable probabilistic model for ocuupation probability

$\sqrt{\text{flow}}$

JML '22, SciPost Physics'23

$$\rho = \sum_{\boldsymbol{n}} U |\boldsymbol{n}\rangle \, p_{\boldsymbol{n}} \, \langle \boldsymbol{n}| U^\dagger$$

VAN

PRL '19

See Cranmer et al 1904.05903
Saleh et al, 2308.16468
Siciliano et al 2407.03802

$$\mathrm{Tr}\rho = 1$$

$$\rho \succ 0$$

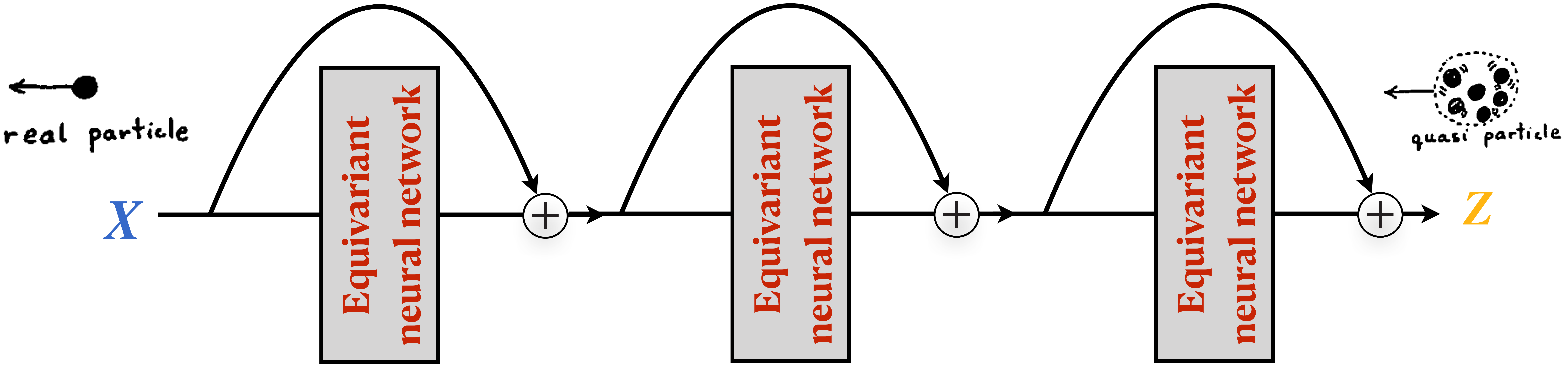
$$\rho^\dagger = \rho$$

$$S(\rho) = S(p_{\boldsymbol{n}})$$

Many-body "base" states e.g. Fermi sea, Hartree-Fock states, harmonic crystal, ...

The physics of $\sqrt{\text{flow}}$

$$\langle X | U | \boldsymbol{n} \rangle = \langle Z | \boldsymbol{n} \rangle \cdot \left| \det \left(\frac{\partial Z}{\partial X} \right) \right|^{\frac{1}{2}}$$



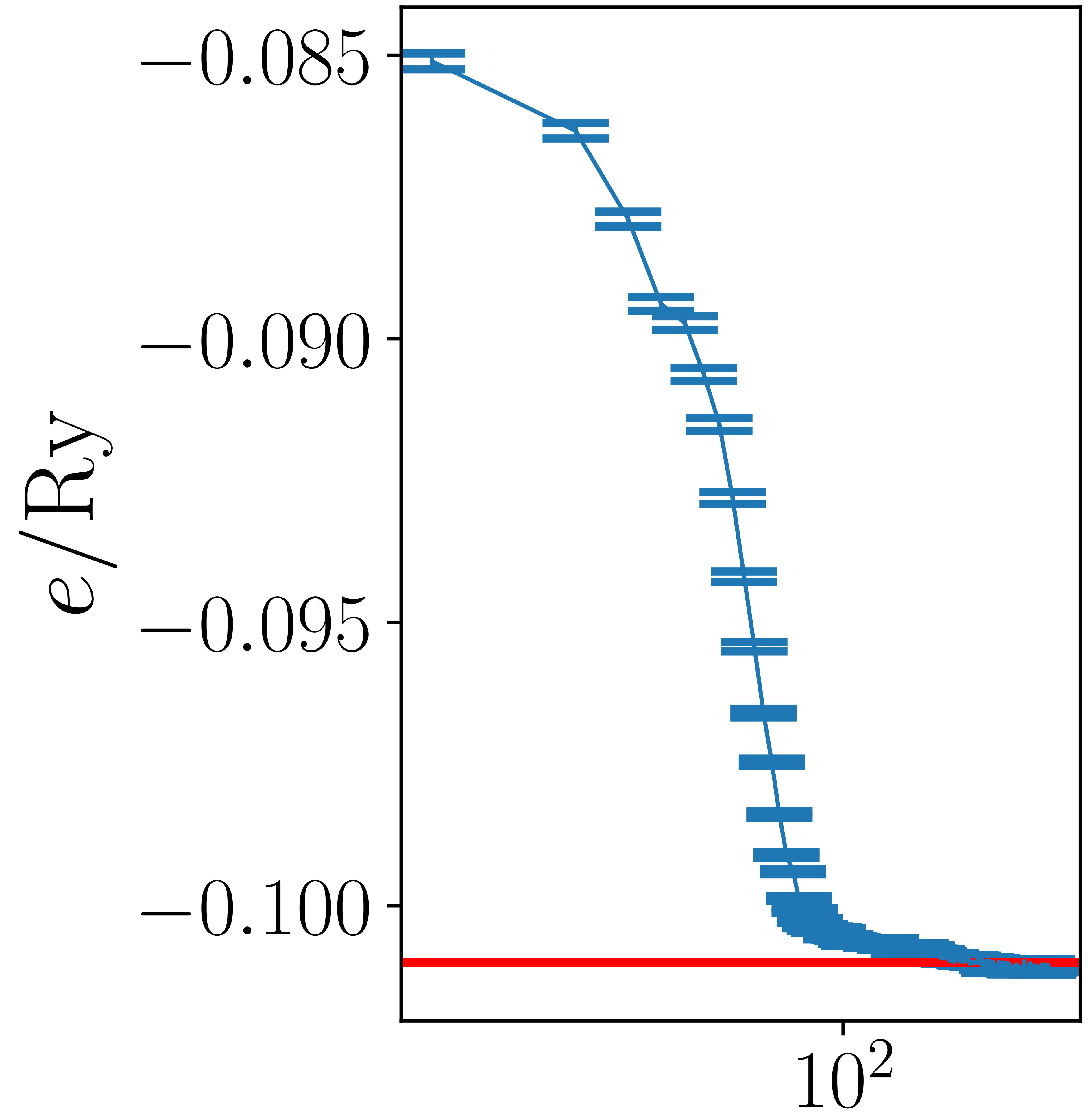
$X \leftrightarrow Z$: unitary backflow between particle and quasiparticle coordinates

Xie, Zhang, LW, JML '22, SciPost Physics '23

Benchmarks on uniform electron gas

Xie, Zhang, LW, SciPost Physics '23

$r_s = 10$, $T/T_F = 0.0625$, $N = 33$



metals: $2 < r_s < 6$

r_s	Θ	$\langle sign \rangle$	E_{tot}^{exact}	E_{tot}
4.0	0.0625	−0.00055(62)	−0.5(1)	−0.1023(7)
10.0	0.0625	−0.002(1)	−0.16(2)	−0.1010(1)

Brown et al, PRL '13 Restricted PIMC

see also Schoof et al PRL '15, Malone et al PRL '16

ANNALS OF PHYSICS: **24**, 63–88 (1963)

Point Transformations and the Many Body Problem*

M. EGER† AND E. P. GROSS

Brandeis University, Waltham, Massachusetts

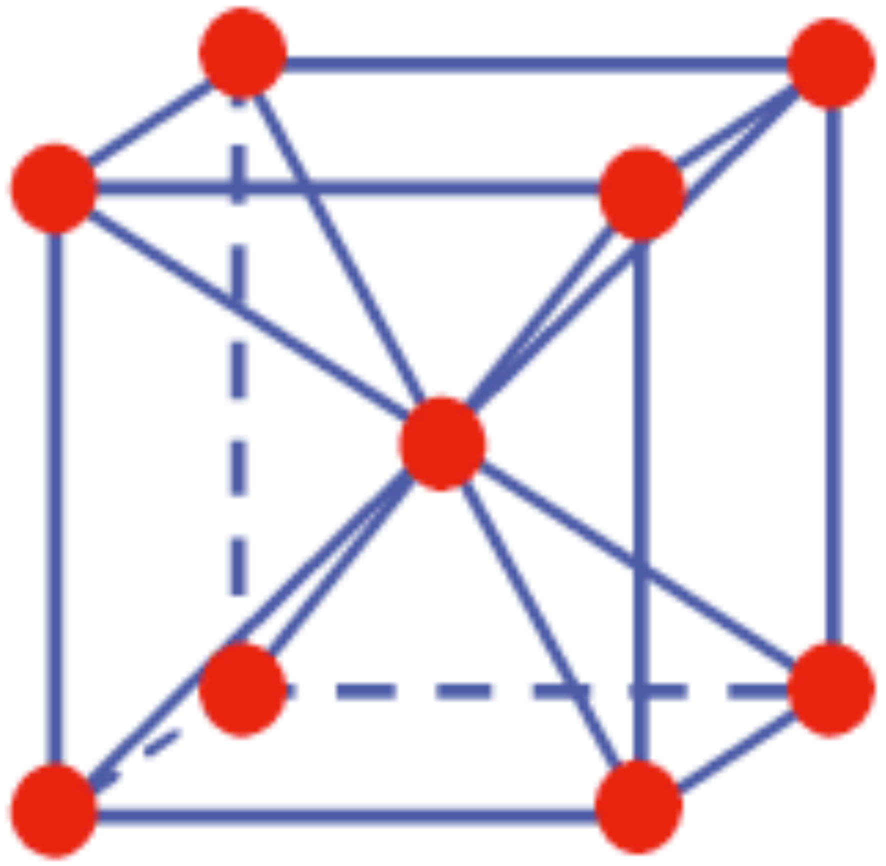
An investigation is made of possible uses of many dimensional coordinate transformations in the quantum many-body problem. The transformed Hamiltonian is quadratic in the momenta with a space dependent metric. The original potential energy undergoes alteration and an additional "metric" potential energy appears. A relatively complete analysis of the transformed original potential is made, and the coordinate transformation can be used to suppress undesirable features of the original potential. For bosons one can attempt to directly map a complete set of noninteracting states onto approximate eigenstates of the system with interactions. Contact is made with a theory of weakly interacting bosons. In the general case it emerges that a given transformation uniquely fixes all the spatial correlation functions, which can be explicitly computed. The extended point transform can then be used as a link between diverse experimental quantities. The full use of the transformation to compute from first principles requires adequate approximations to the Jacobian and the inverse transform. These problems are not studied.

√flow

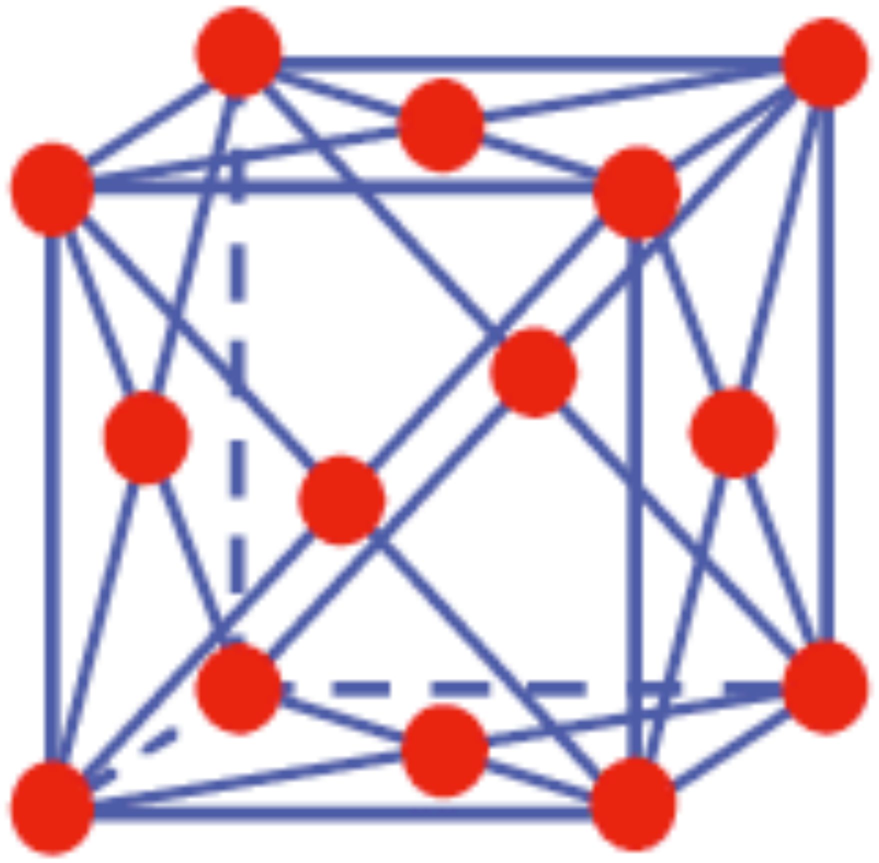
materializes this dream

Solid lithium: bcc or fcc?

bcc

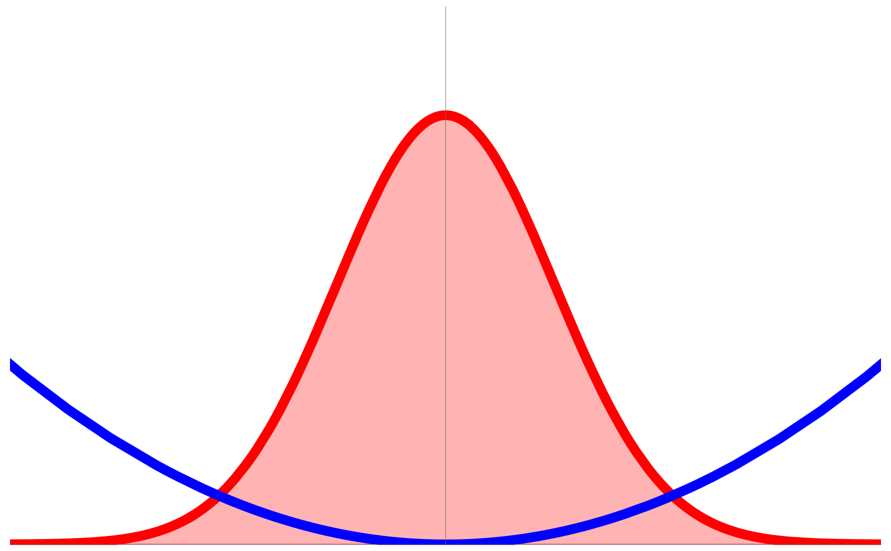


fcc



3
Li

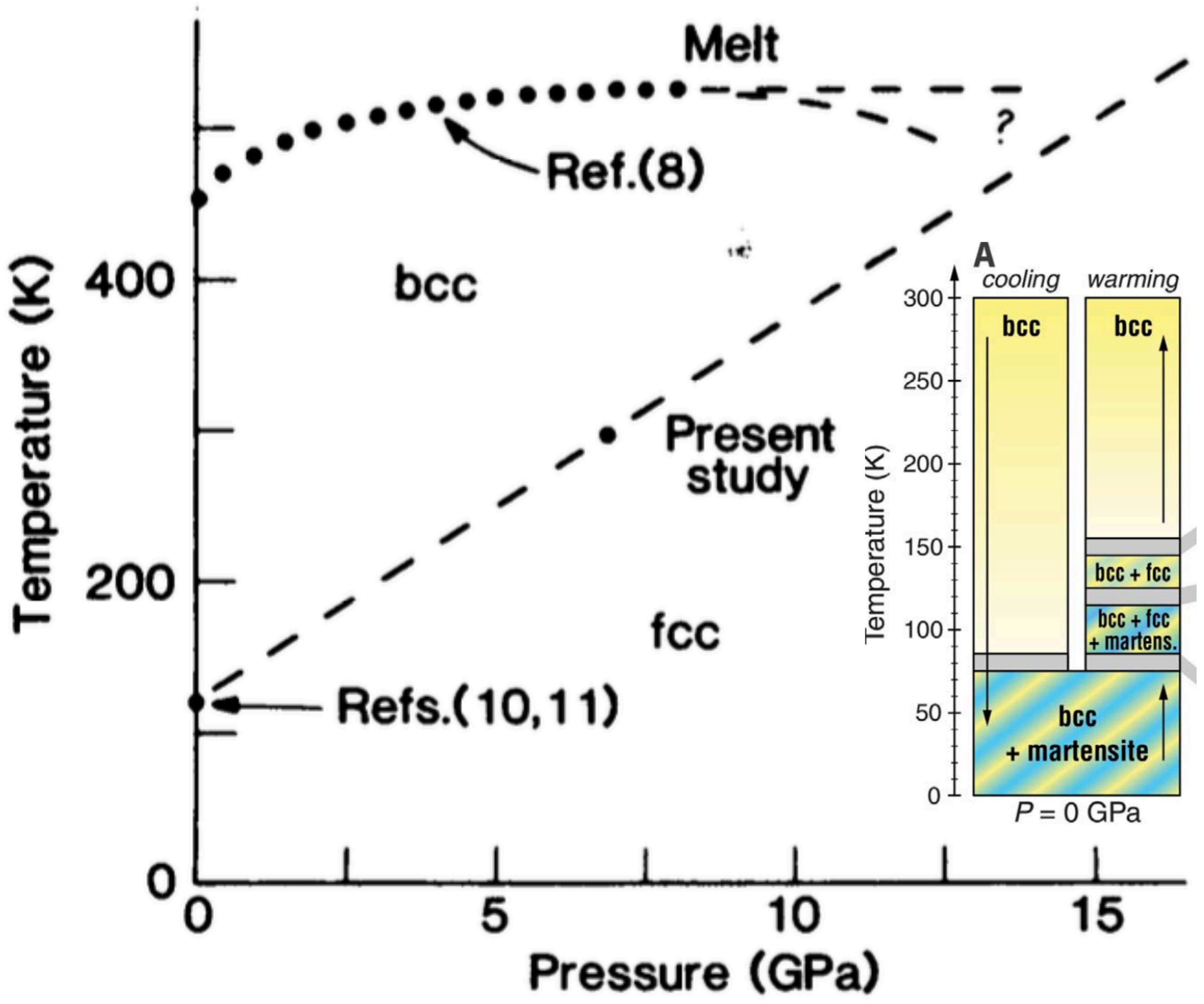
Light nuclei mass => large amplitude oscillation
quantum anaharmonicity plays a significant role



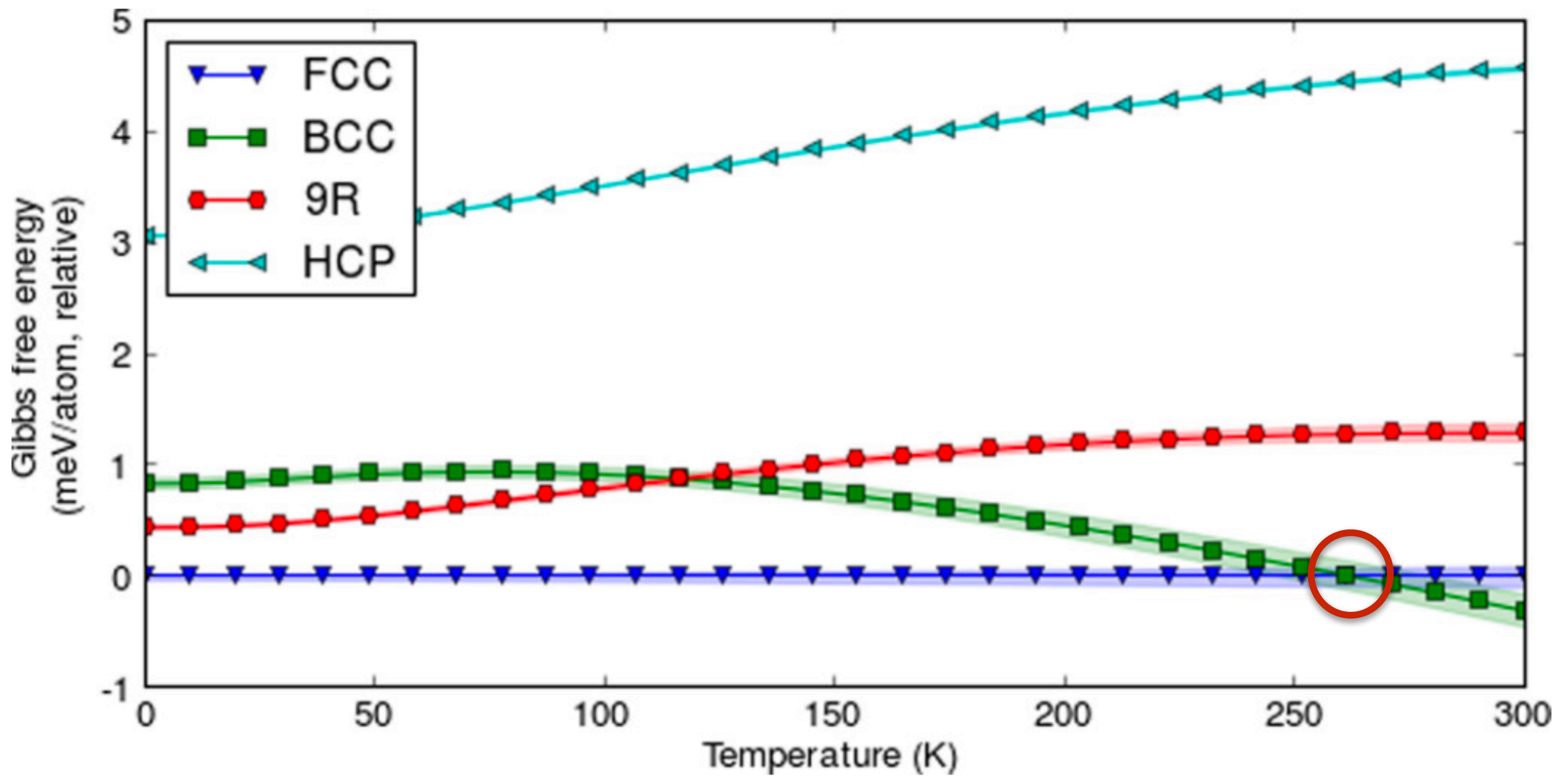
fcc is the groud state, Ackland et al, Science 2017

Temperature driven bcc to fcc transition

$$F = E - TS_{\mathrm{vib}}$$



Experiments:
Olinger et al Science 1983
Ackland et al, Science 2017



Vibrational self-consistent field calculation

Hutcheon, Needs, PRB 99,014111 (2019)

Neural canonical transformation for lattice dynamics

Zhang et al, 2412.12451

$$H = \sum_{i=1}^{N} \frac{-\nabla_i^2}{2M} + V(\boldsymbol{X})$$

ML PBE interatomic potential

Zhang et al PRL '18, Wang et al Nat.Comm '23

Classical: Ahmad 2111.01292, Wirnsberger, 2111.08696

$$F = \mathop{\mathbb{E}}_{\boldsymbol{n} \sim p_{\boldsymbol{n}}} \left[k_B T \ln p_{\boldsymbol{n}} + \langle \boldsymbol{n} | U^\dagger H U | \boldsymbol{n} \rangle \right]$$

$\boldsymbol{n} = n_1, n_2, \ldots, n_{3N-3}$

Phonon modes

$p_{\boldsymbol{n}}$

VAN/PSA

Wu et al, PRL '19

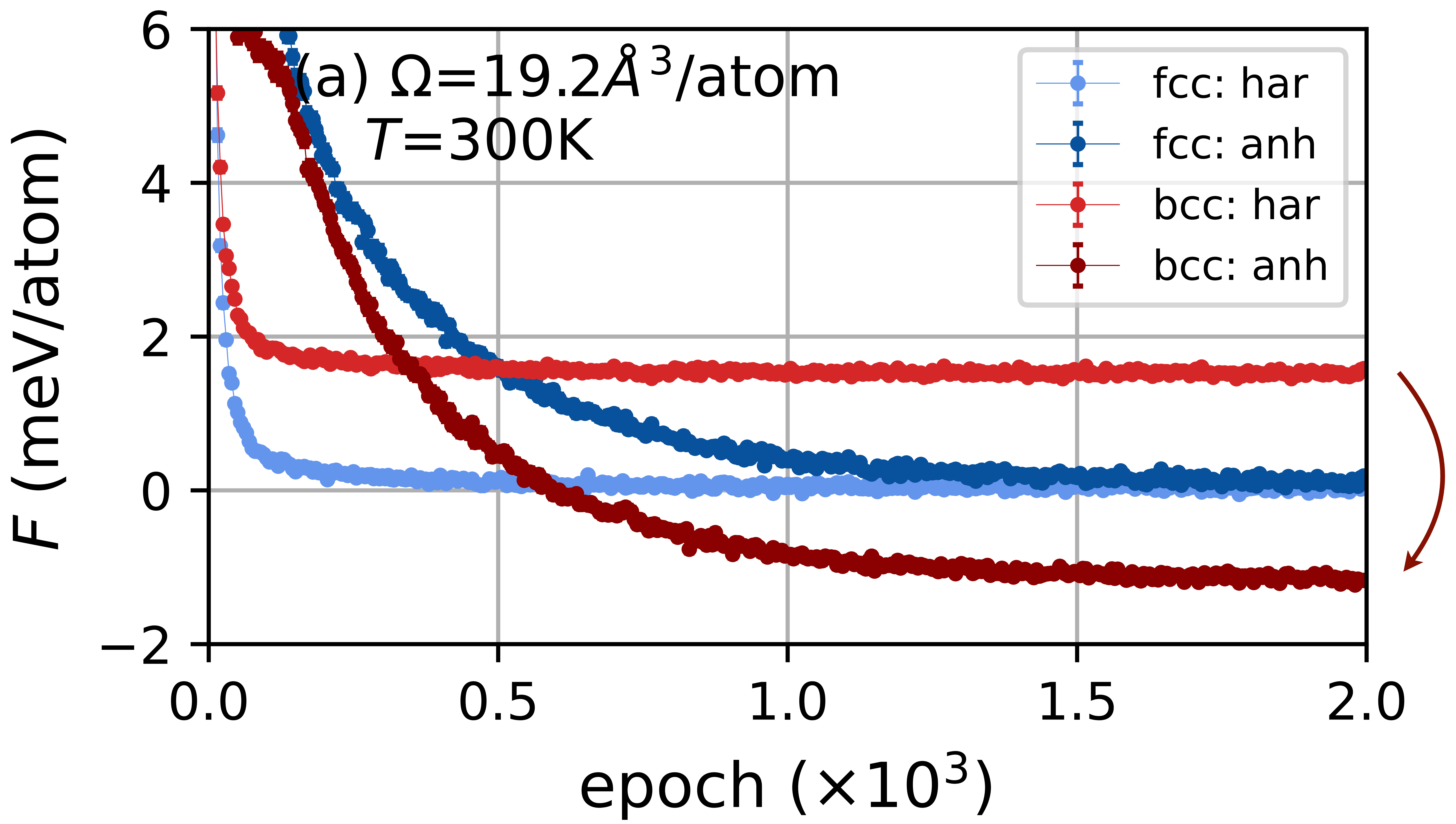
Martyn, Swingle, PRA '19

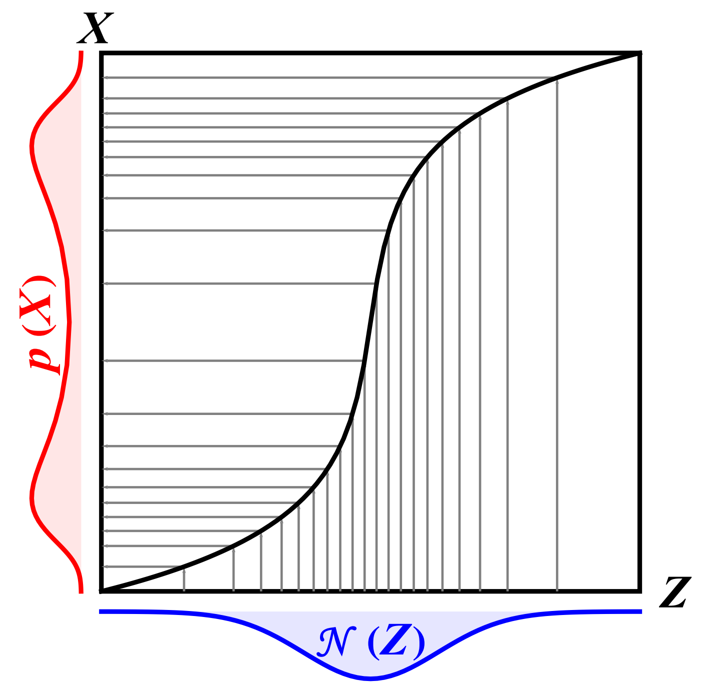
$U : \boldsymbol{X} \leftrightarrow \boldsymbol{Z}$

RealNVP flow

Dinh et al, 1605.08803

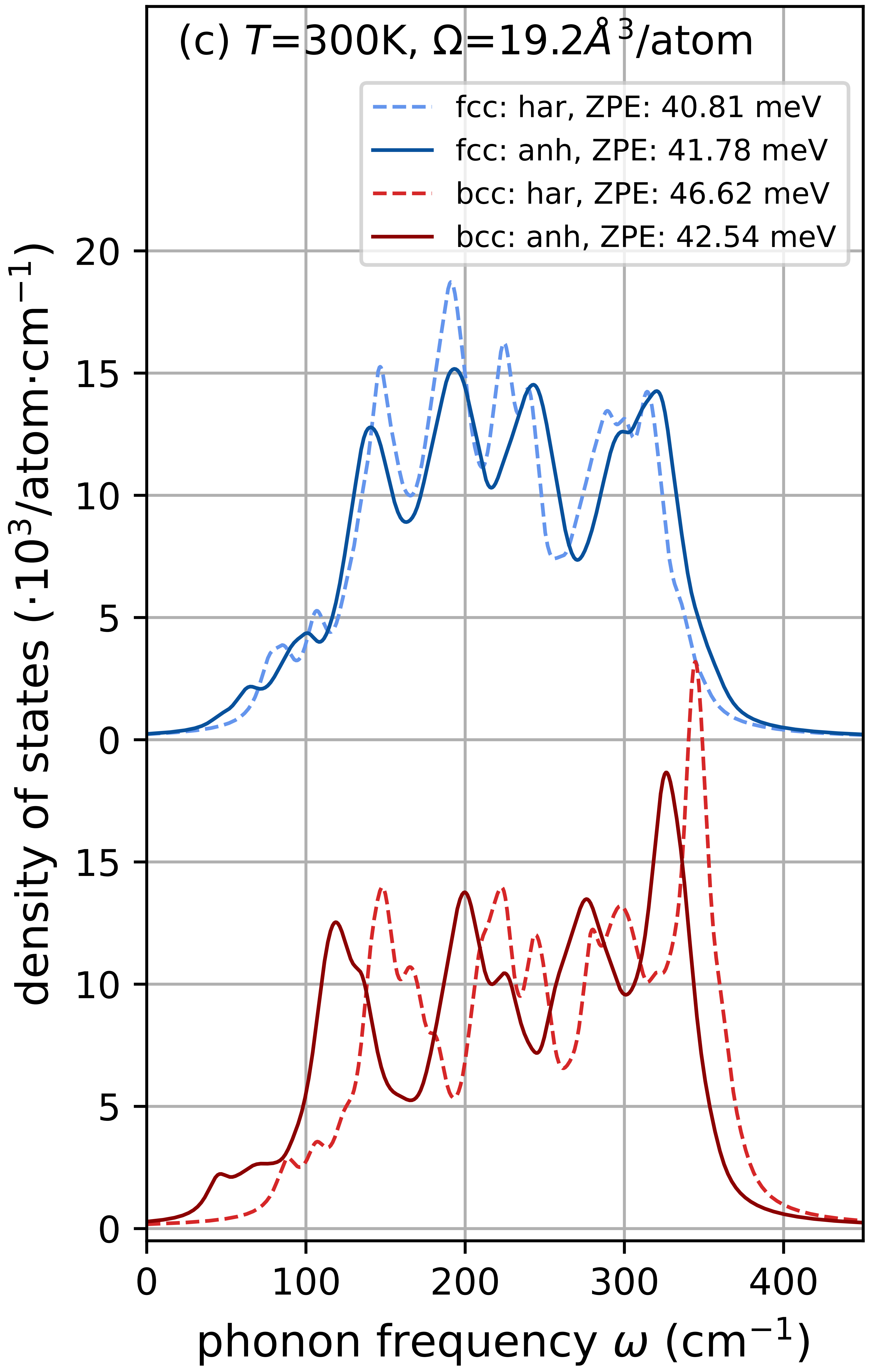
Optimization over ~10 million excited states of ~500 atoms



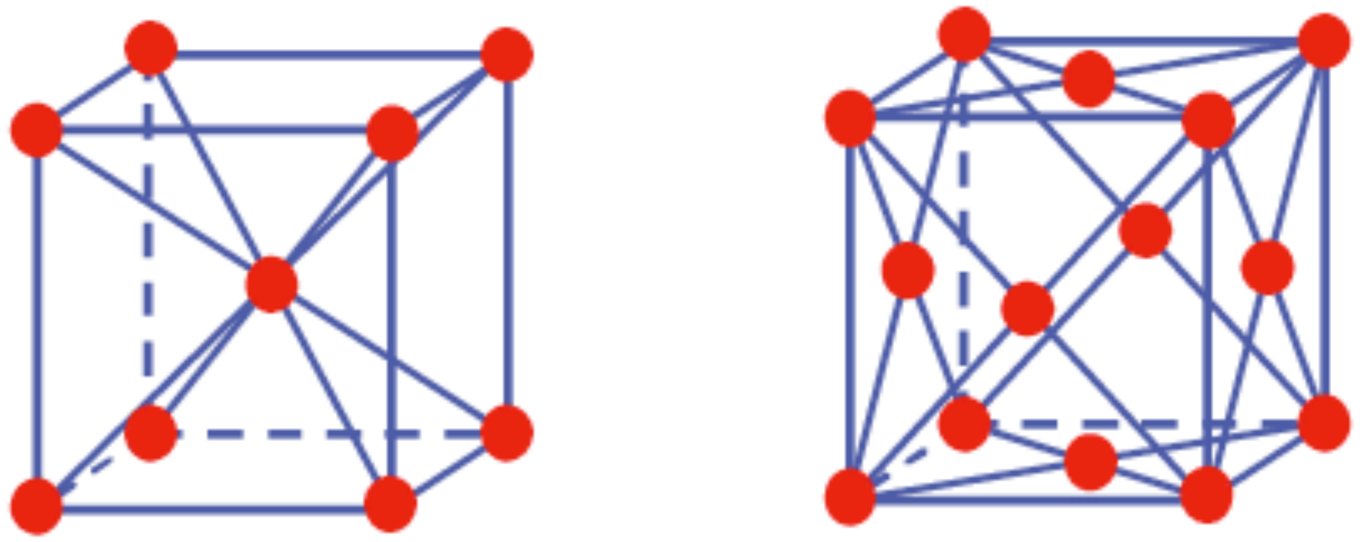


bcc structure
is stabilized
by quantum
anharmonicity

Zhang et al, 2412.12451



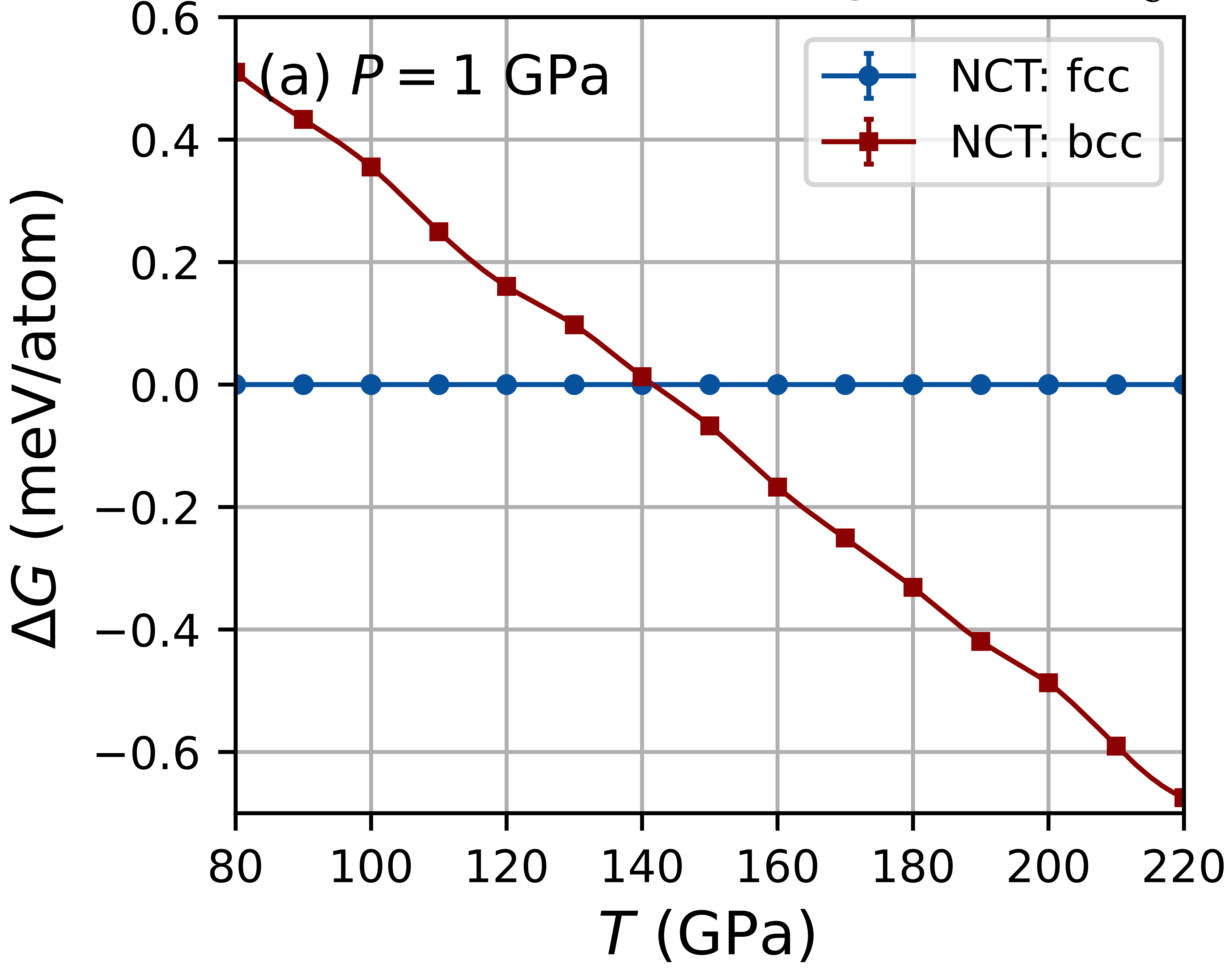
$$\omega_{\boldsymbol{n}} = \langle \boldsymbol{n} \,|\, U^{\dagger} H U \,|\, \boldsymbol{n} \rangle$$



Anharmonic softening of phonons in the bcc structure

Zhang et al, 2412.12451

Zhang et al, 2412.12451



Vibrational SCF: 260K

Hutcheon, Needs, PRB 2019

AIMD: 190K

Ackland et al, Science 2017

DeepMD: 185K

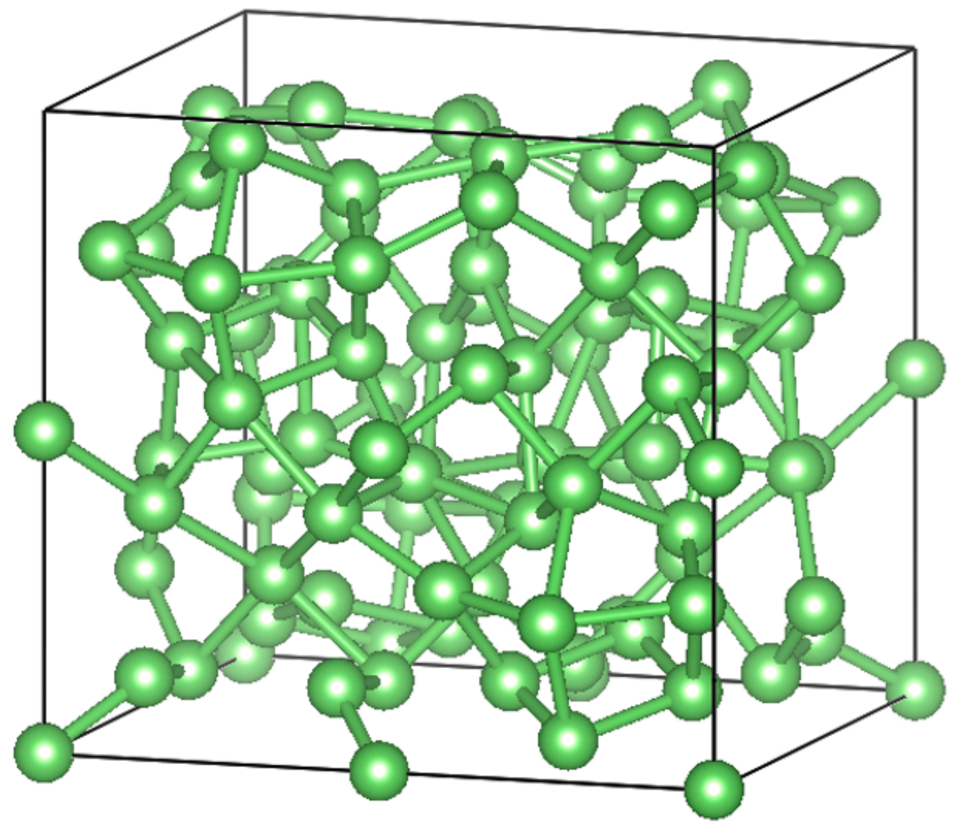
Wang et al, Nat.Comm 2023

Experiment: 100-160K

Ackland et al, Science 2017

Solid lithium: the story of Oc88 phase

Experiment observation at 70 GPa

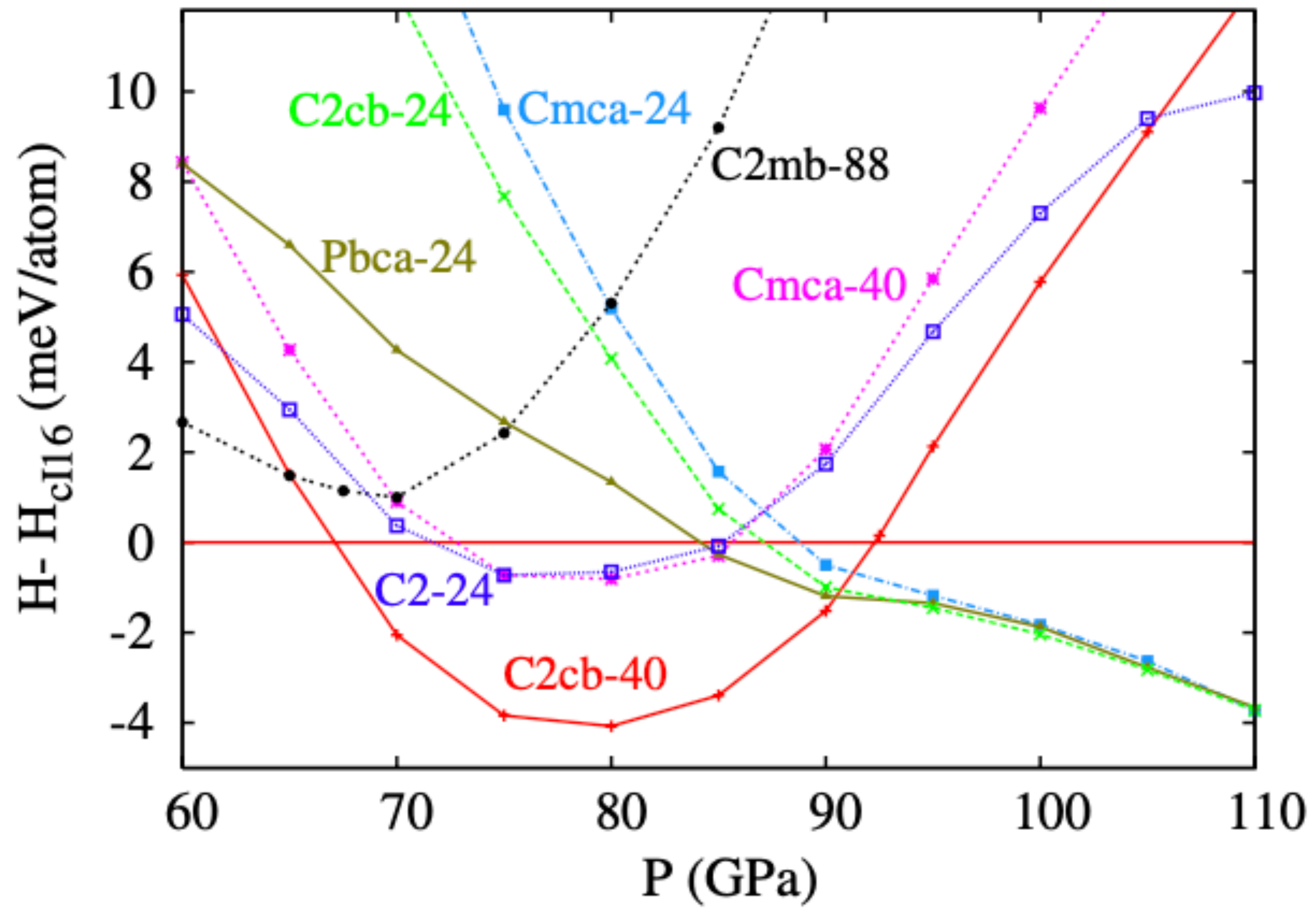


oC88 (Aem2, C2mb, No.39)

On further compression, the cI16 structure transforms into an orthorhombic C-face centred phase having 88 atoms per unit cell, oC88, with $a = 8.569(6)$ Å, $b = 9.282(8)$ Å, $c = 8.389(4)$ Å and unit

Guillaume et al, Nature physics, '11

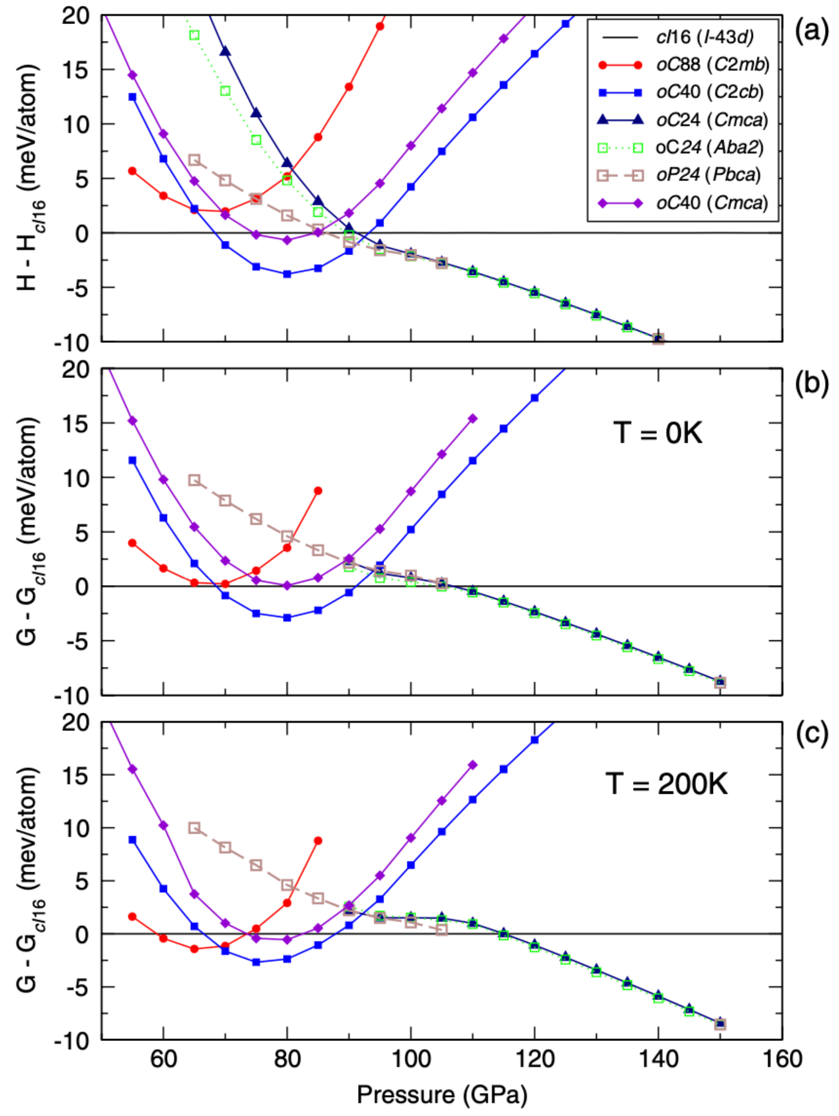
Missing in static lattice calculation



(Fig. 2). The difference is small, and the inclusion of dynamical effects, both zero-point and finite-temperature, could stabilize this *oC*88 structure against *cI*16. Thus AIRSS has revealed the structure, but some additional physics is needed to explain the thermodynamic stability of *oC*88. A peculiarity of the observed *oC*88 phase at very

Marqués et al, PRL '11

Stable in dynamic lattice calculation



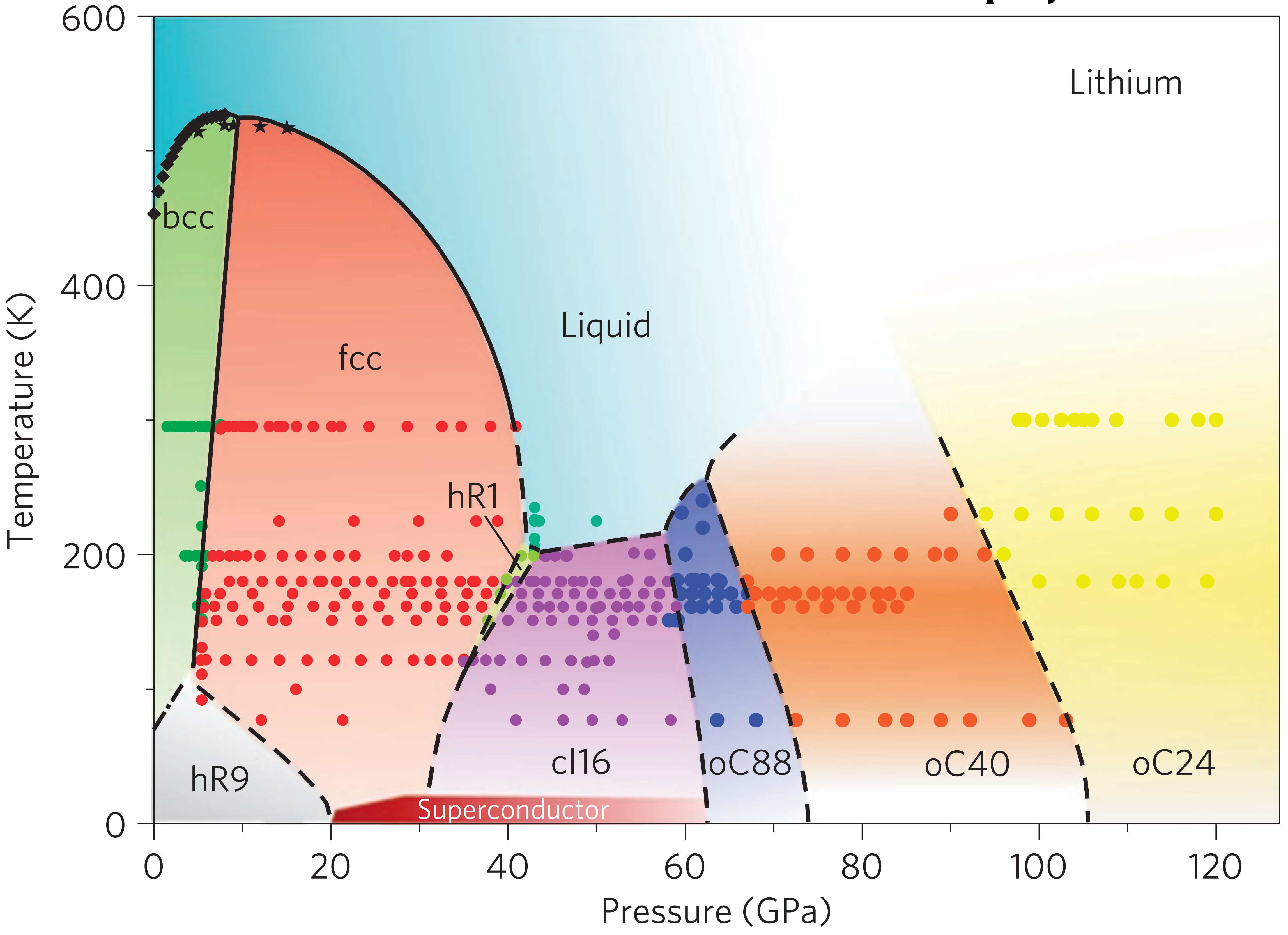
DFT enthalpy alone. The effect of ZPE is shown in Fig. 4(b), the Gibbs free energy of *oC*88 becomes just about equal to that of *cI*16 near 65 GPa; the differences are too small to allow us to conclude which structure is preferred. At finite *T*, however, *oC*88 becomes stable and its stability range increases with *T* in excellent agreement with the experimental measurements. It is worth noting, that the theoretical

Gorelli et al PRL '12

Happy ending ?

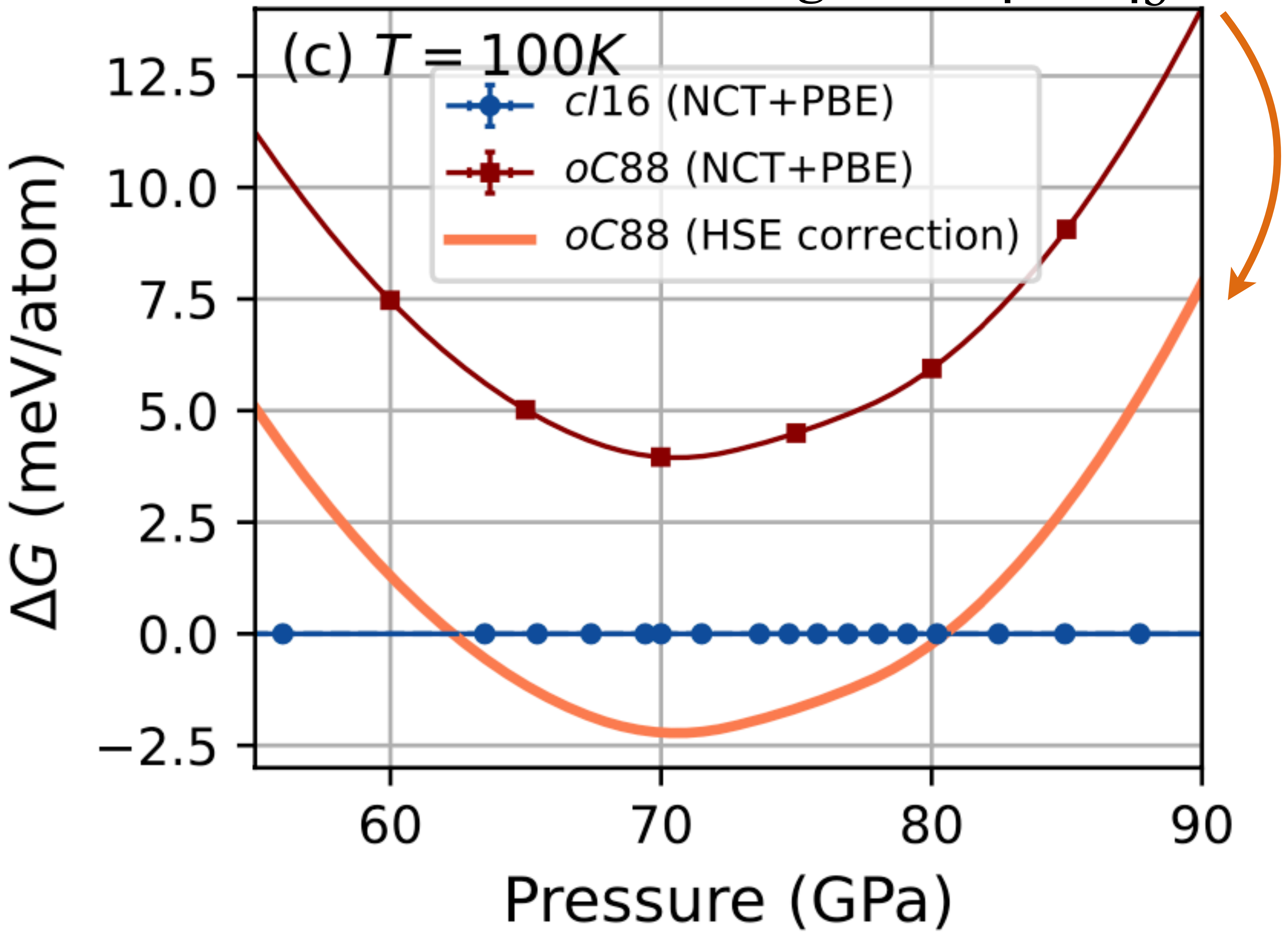
The story of Oc88 phase

Guillaume et al, Nature physics, 2011



Our calculation does **NOT** reproduce the experimentally observed Oc88 phase, which contradicts Gorelli et al PRL ’12

Zhang et al, 2412.12451

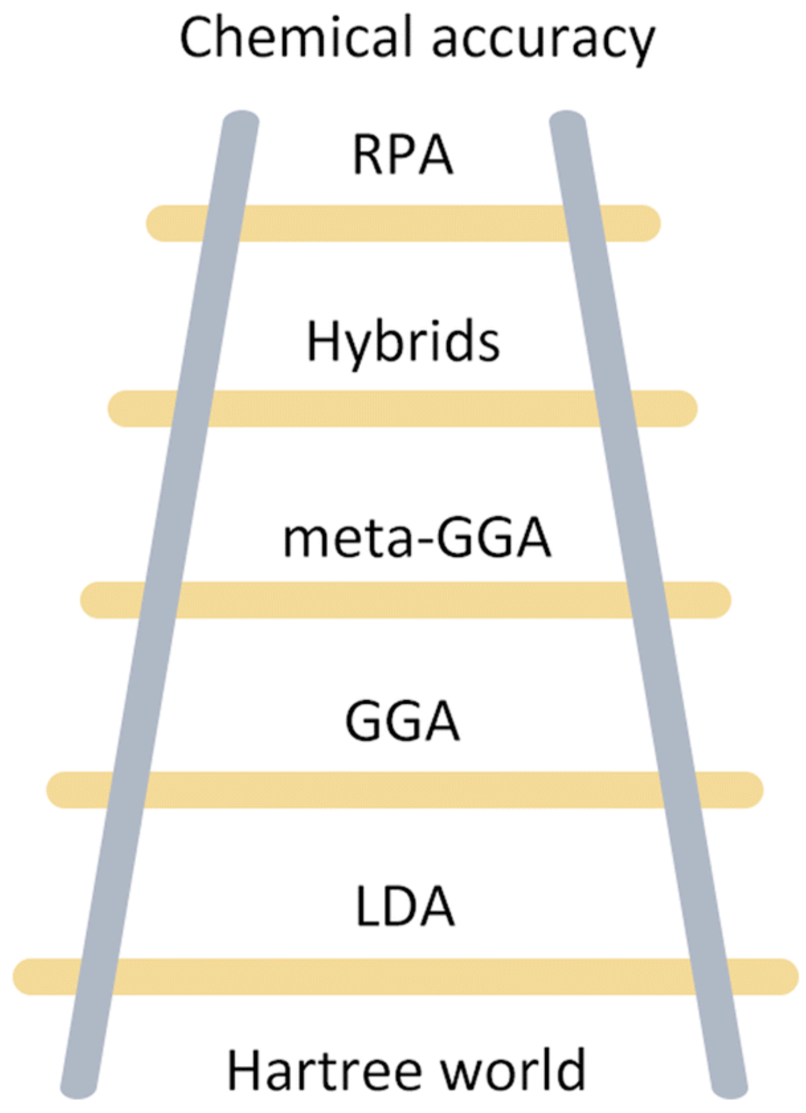


- ☑ Thermal entropy
- ☑ Quantum anharmonicity
- ☐ DFT functional

The story of Oc88 phase

Zhang et al, 2412.12451

Method	DP (VASP)	ABACUS	ABACUS	FHI-aims	FHI-aims
Functional	PBE	PBE	HSE06	PBE	HSE06
Basis	Plane Wave	DZP	DZP	intermediate	intermediate
Pseudopotential	PAW	Dojo-NC-FR	Dojo-NC-FR	-	-
ΔH *oC88 - cI16*	+1.68	+2.44	−3.73	+3.44	−4.23
ΔG *oC88 - cI16*	+3.96	+3.96	−2.21	+3.96	−3.71



The Oc88 phase is stablized by high-precision density functionals

NOT thermal effect, NOT nuclear quantum effect

Reflections

Why do we need higher-order functional ?

Oc88 is a *poor metal*, which iccurs localization error

Why not ten years ago ?

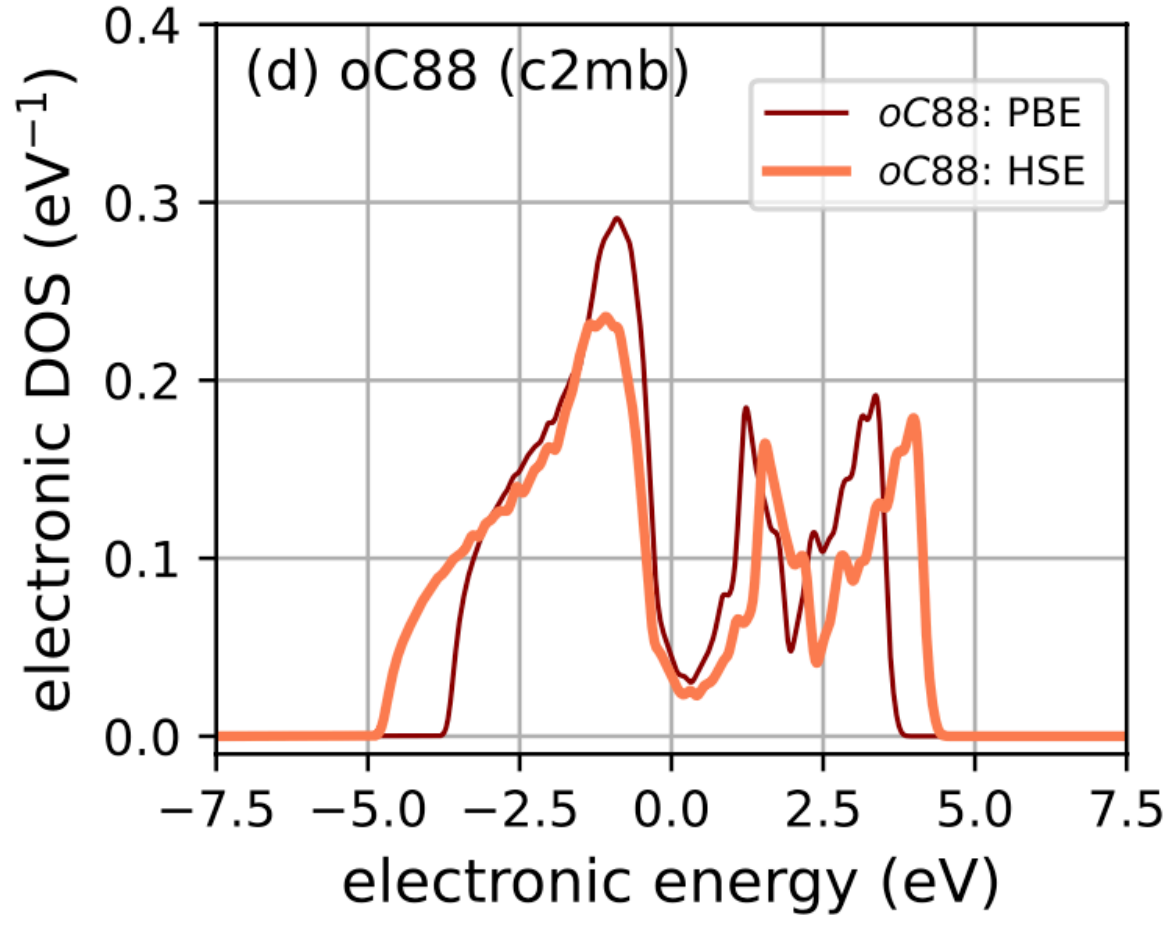
HSE is 100 times more expensive, but Oc88 is large

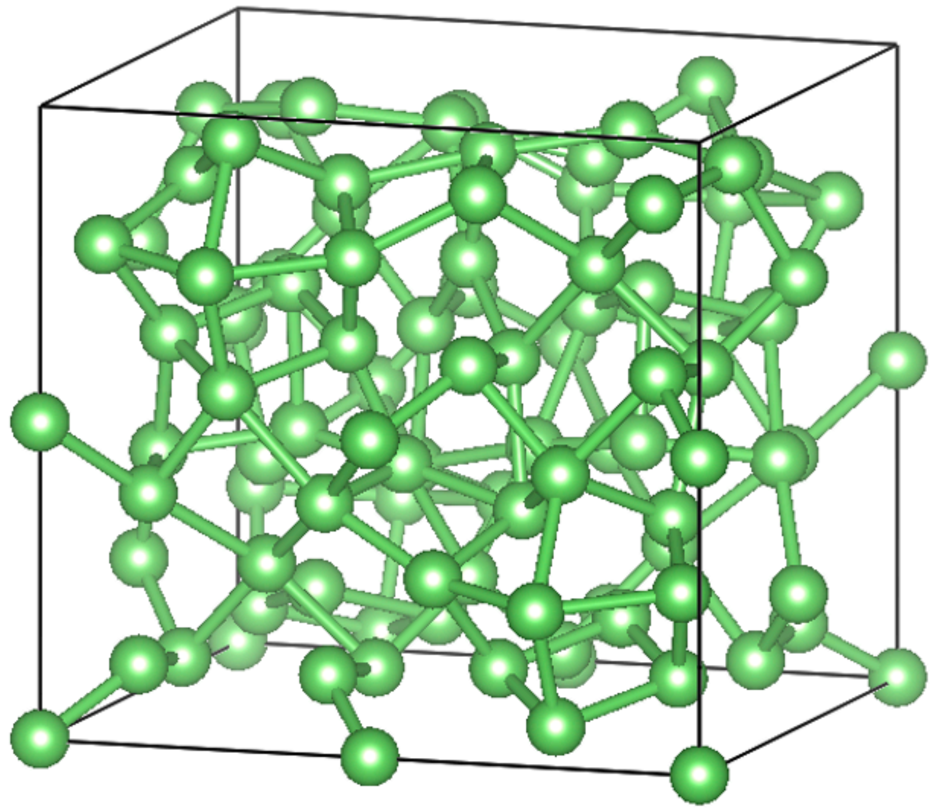
(Sociologically, entropy or nuclear quantum effect sounds fancier than changing DFT functional)

With neural canonical transformation, we are now confident in the Gibbs free energy

(whatever remains when you have eliminated the impossible)

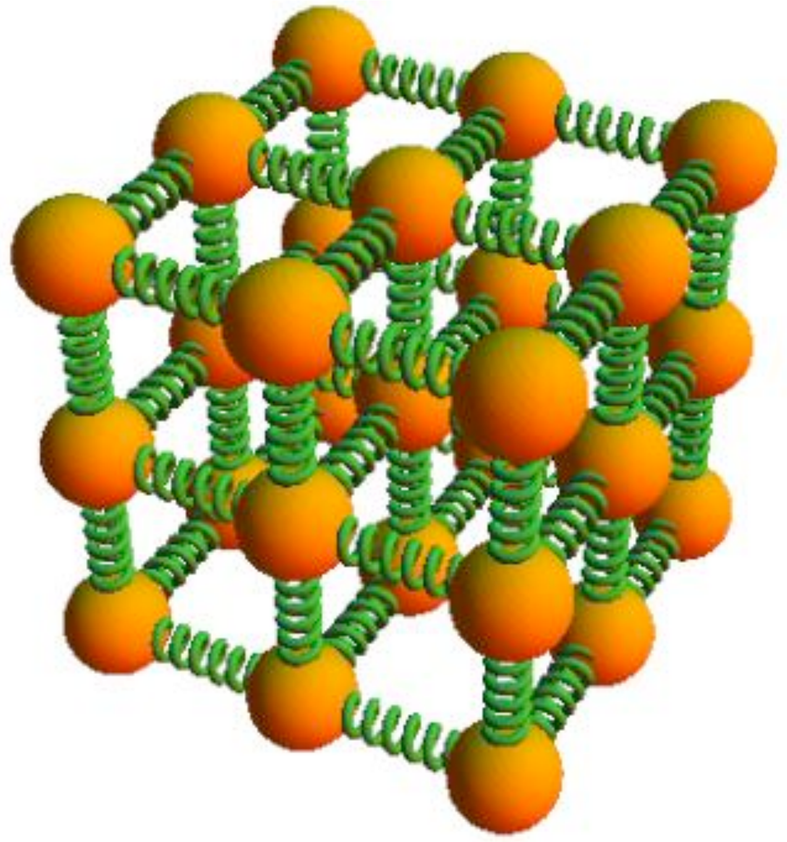
Zhang et al, 2412.12451





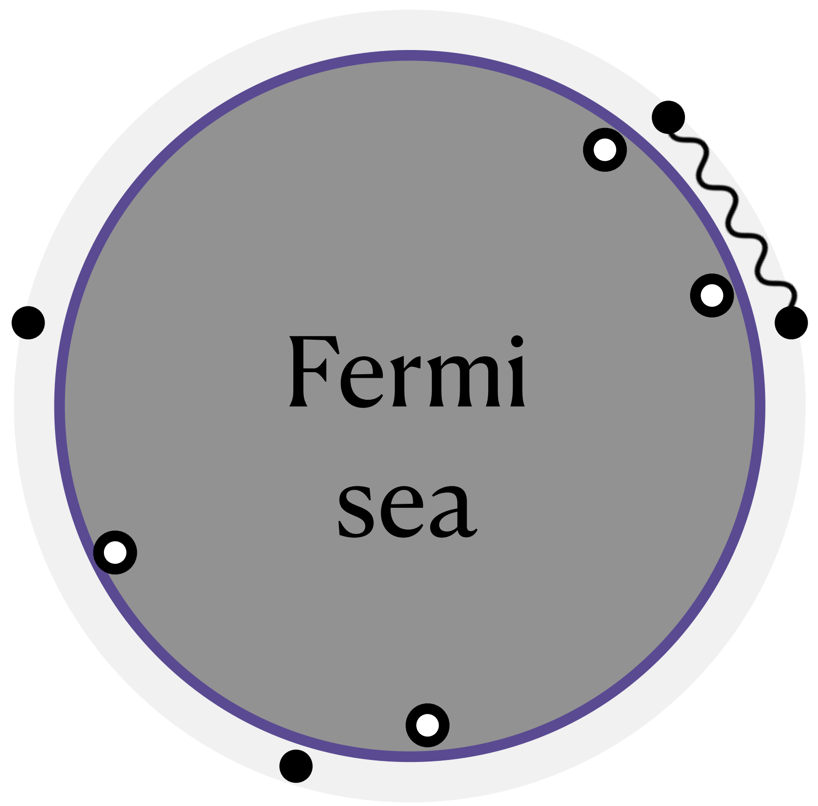
Neural canonical transformation for atoms and electrons

Harmonic oscillators
↕
Anharmonic crystal



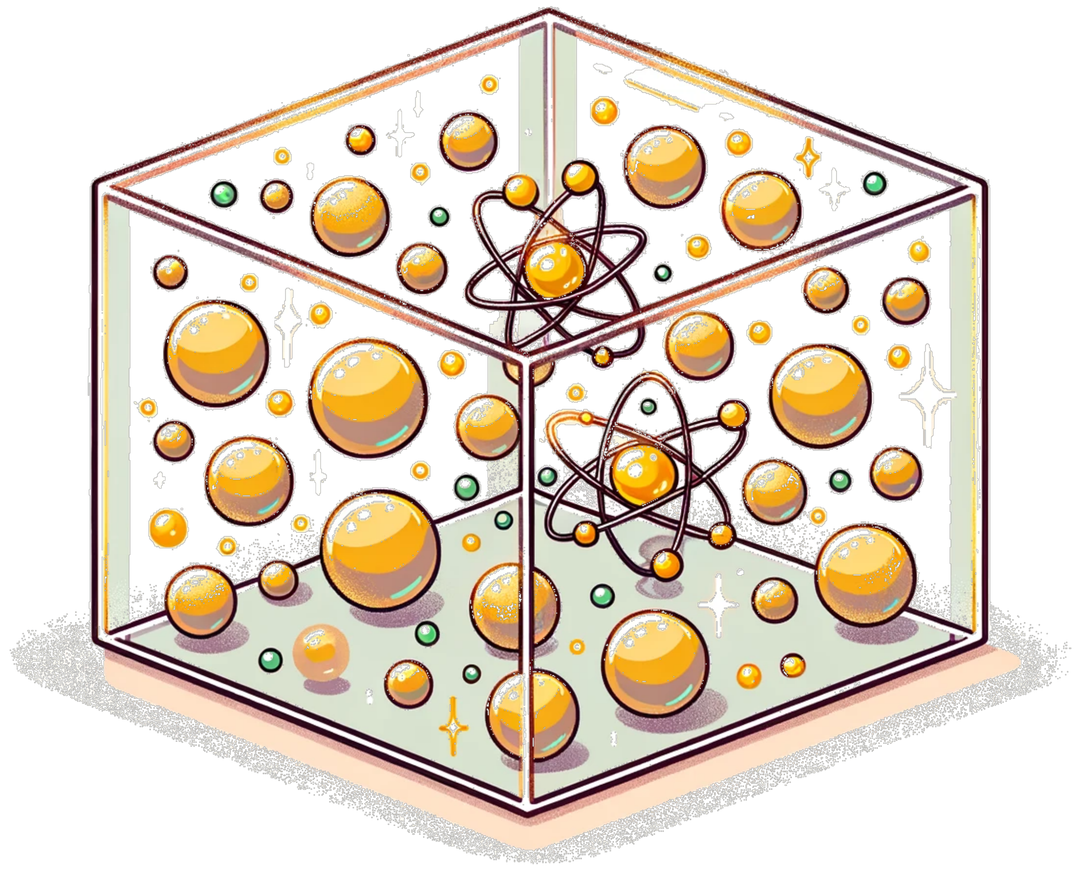
Vibrational spectra of
molecules and solids
JCP ’24 and 2412.12451
(~500 atoms)

Ideal Fermi gas
↕
Fermi liquid



Low-temperature properties
of Coulomb gas
JML ’22 and SciPost Physics ’23
(~50 electrons)

Hartree-Fock states
↕
Interacting electrons



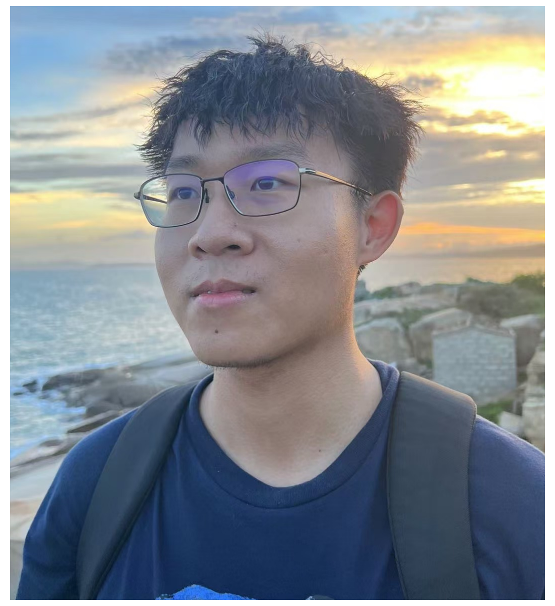
Equation of states of
dense hydrogen
PRL ’23 and ongoing
(~50 e-p pairs)

Thank you!

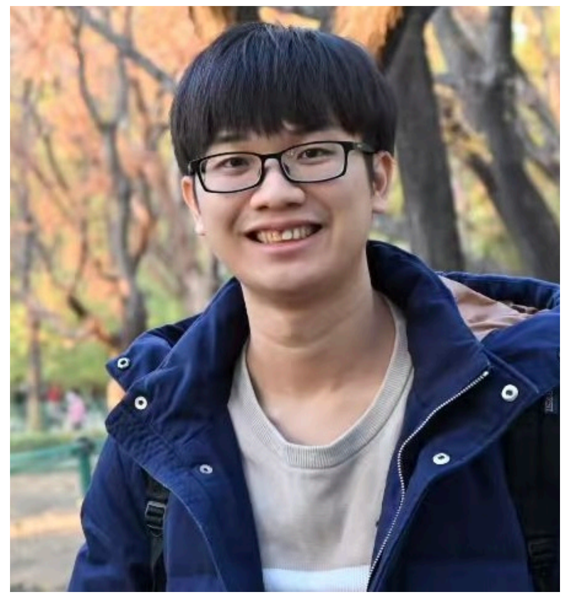
Neural canonical transformations for identifying slow modes, solving interacting electrons and quantum solids, and more!

Shuo-Hui Li
IOP →HKUST

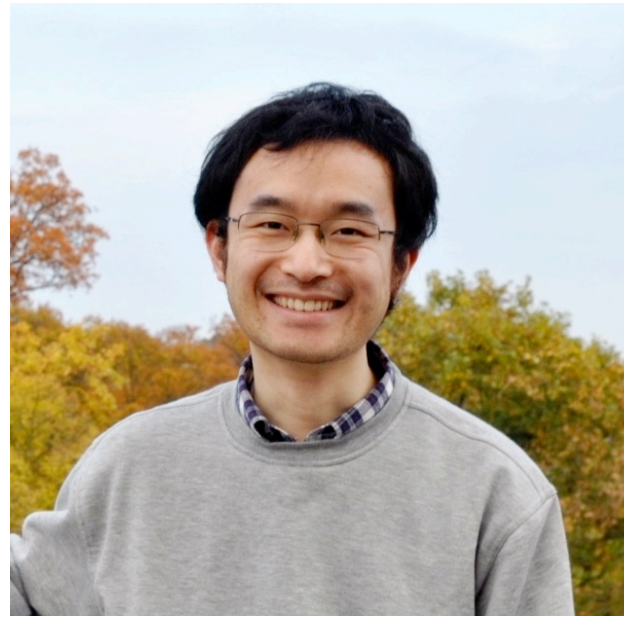
Hao Xie
IOP →UZH



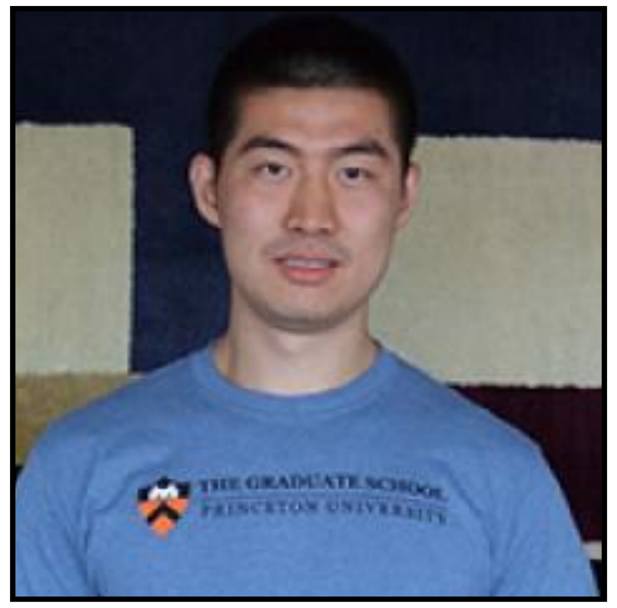
Rui-Si Wang
IOP



Qi Zhang
IOP



Han Wang
IAPCM



Linfeng Zhang
DP/AISI

1910.00024, PRX '20
2105.08644, JML '22
2201.03156, SciPost '23
2412.12451

li012589/neuralCT
FermiFlow/fermiflow
FermiFlow/CoulombGas
zhangqi94/lithium