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Impacts of Large Low Shear Velocity Provinces on the Heat Flux from the Earth's Core: Insights from the Thermal Conductivity of Bridgmanite and Post-perovskite

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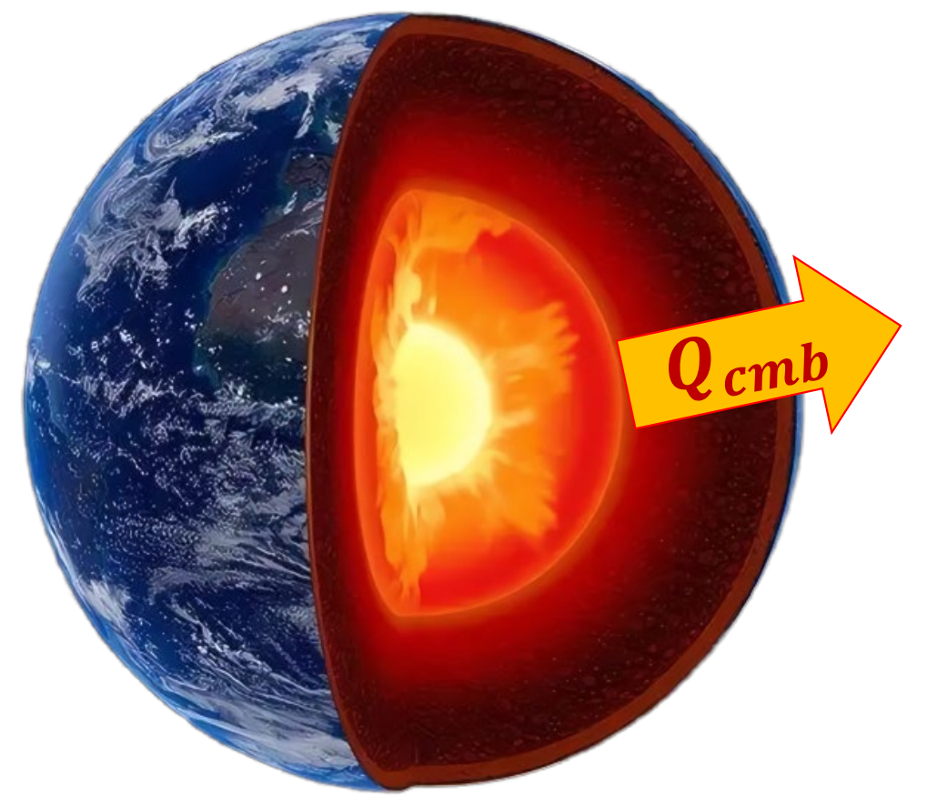
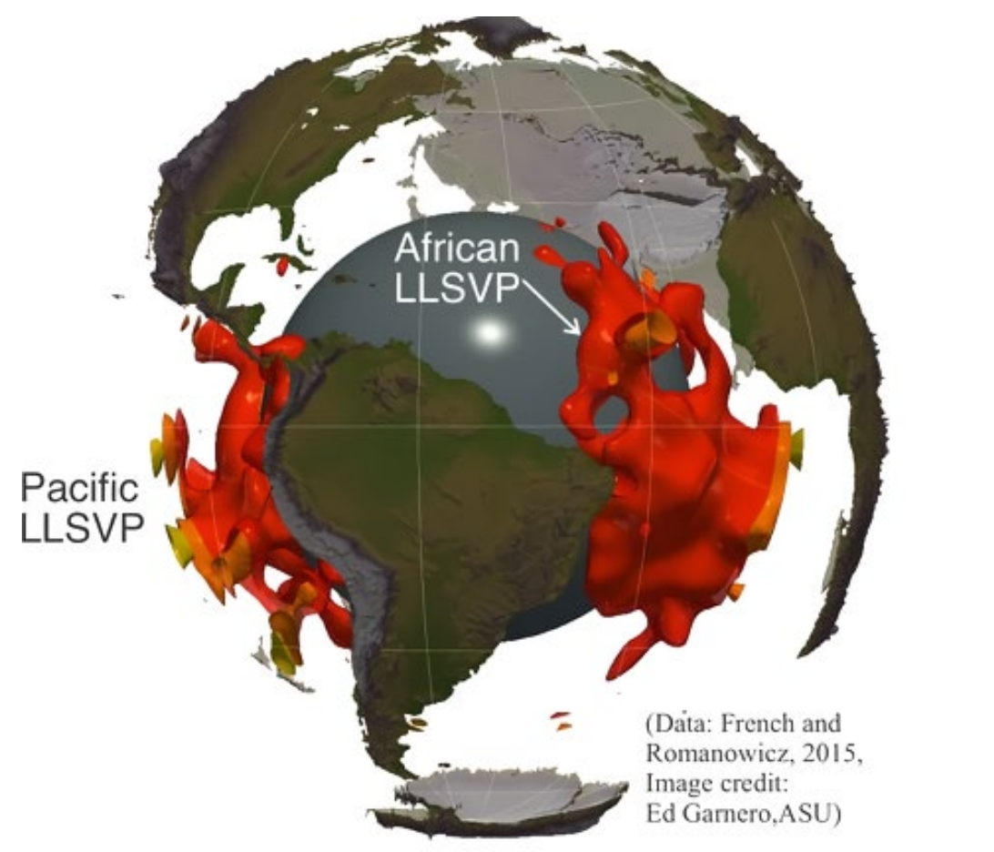
Introduction



The heat flux from the core (Q_{cmb}) is crucial for understanding:

- The growth and structure of the Earth's core
- The intensity and reversal frequency of the geomagnetic field
- Plume size, and so on.

Large low shear velocity provinces (LLSVPs) with compositional and thermal anomalies should have a large impact on Q_{cmb}



(Data: French and Romanowicz, 2015, Image credit: Ed Garnero,ASU)

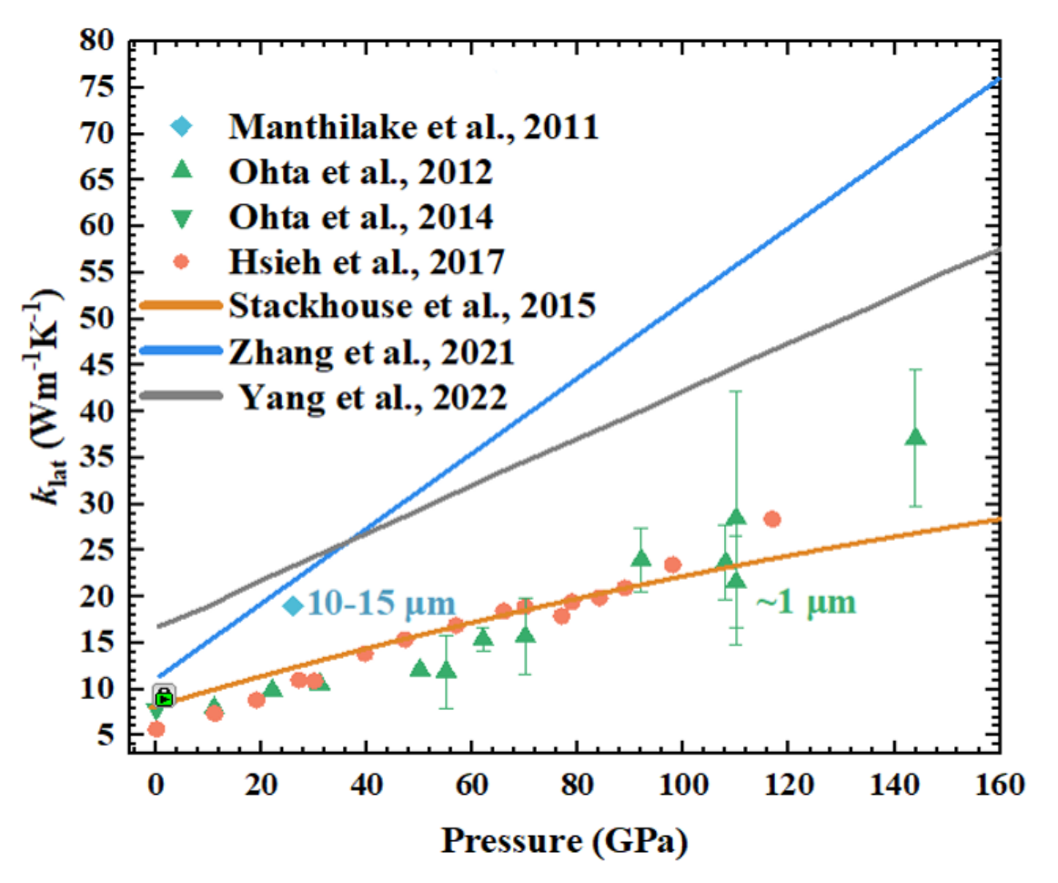
Determining the heat flux in the LLSVPs regions requires the thermal conductivity of the main minerals in the LLSVPs

$$Q = k\frac{\partial T}{\partial x}$$

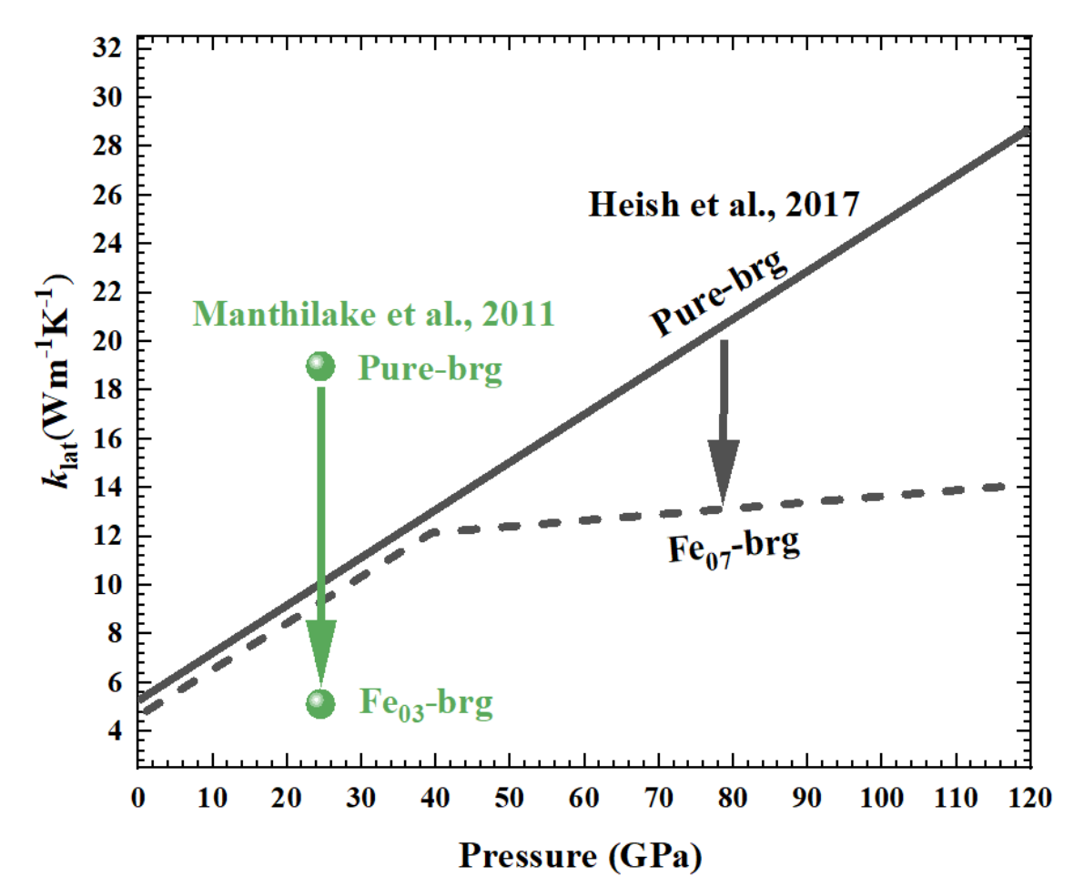
k: thermal conductivity
$\frac{\partial T}{\partial x}$: temperature gradients

The thermal conductivity of the potential main minerals (bridgmanite and post-perovskite) in the LLSVPs are highly debated

e.g. Pure bridgmanite (Brg) at 300 K



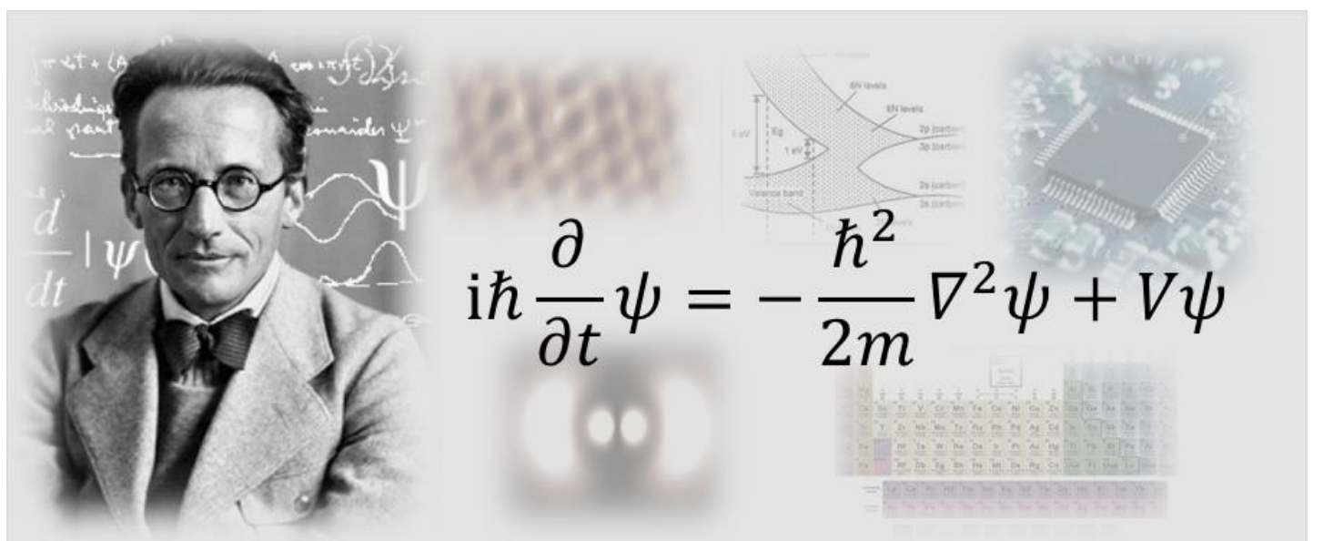
The effect of Fe is also controversial



Challenges in determining k at mantle conditions

Experiments: In-situ measurements are challenging
Theoretical calculations: Finite size effect

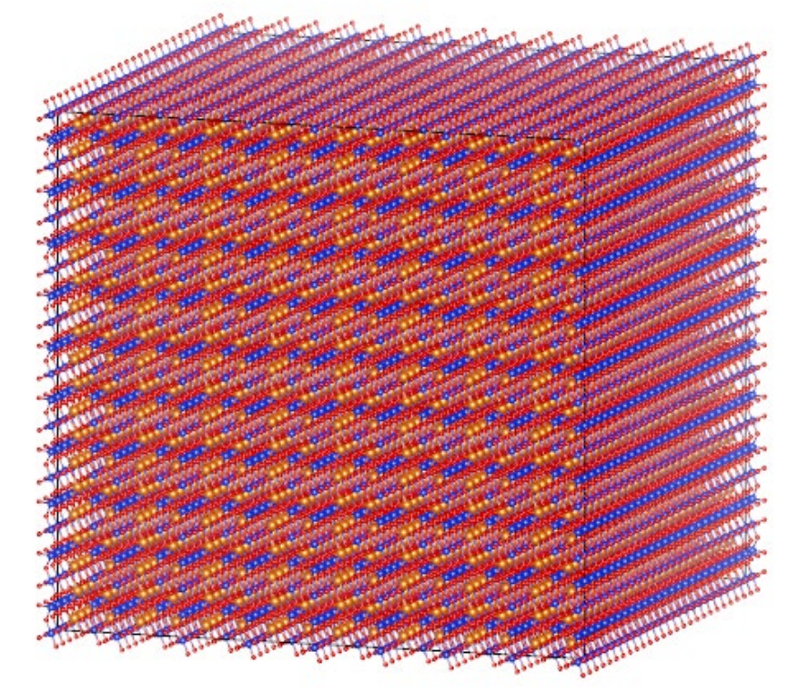
Impossible for first-principles calculations due to computational costs



$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$$

Cost $\propto N^3$, N: number of atoms

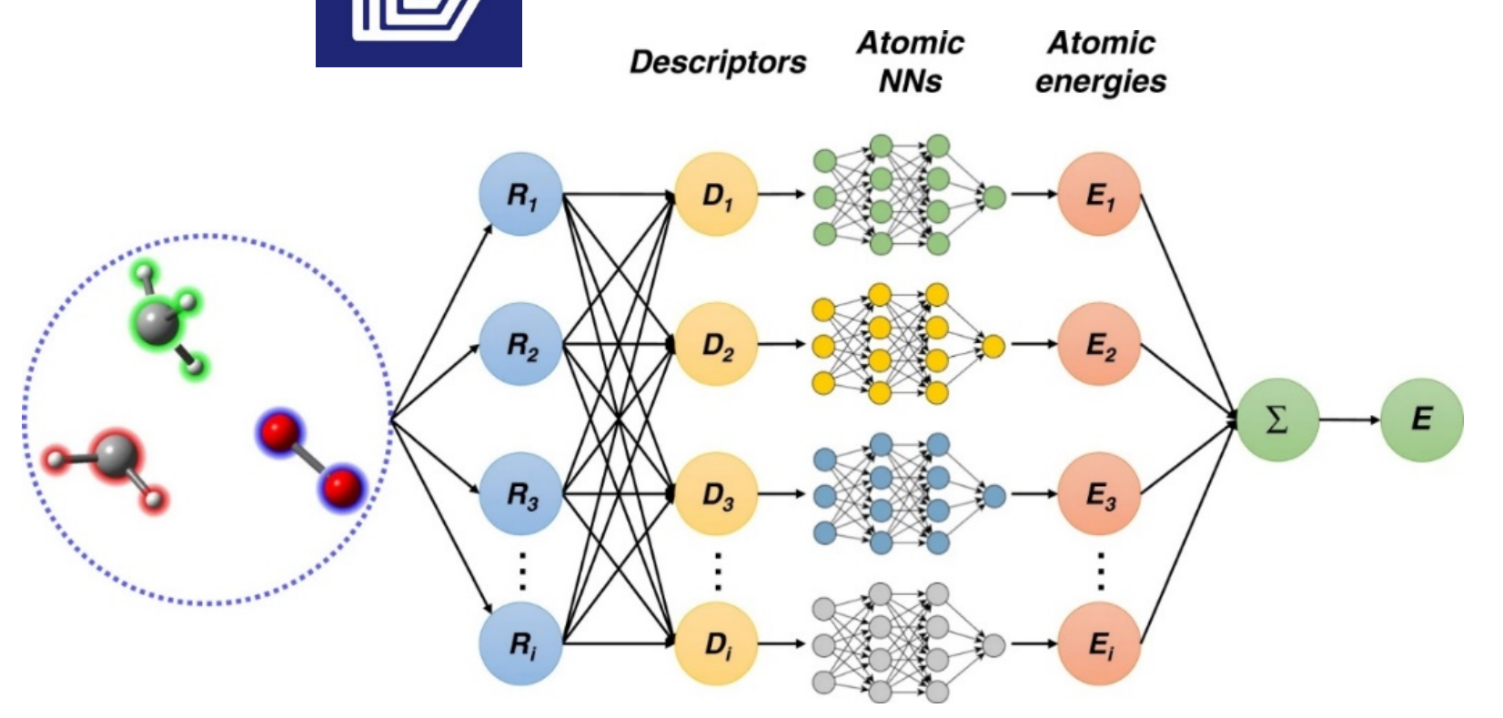
Calculations on huge systems are required



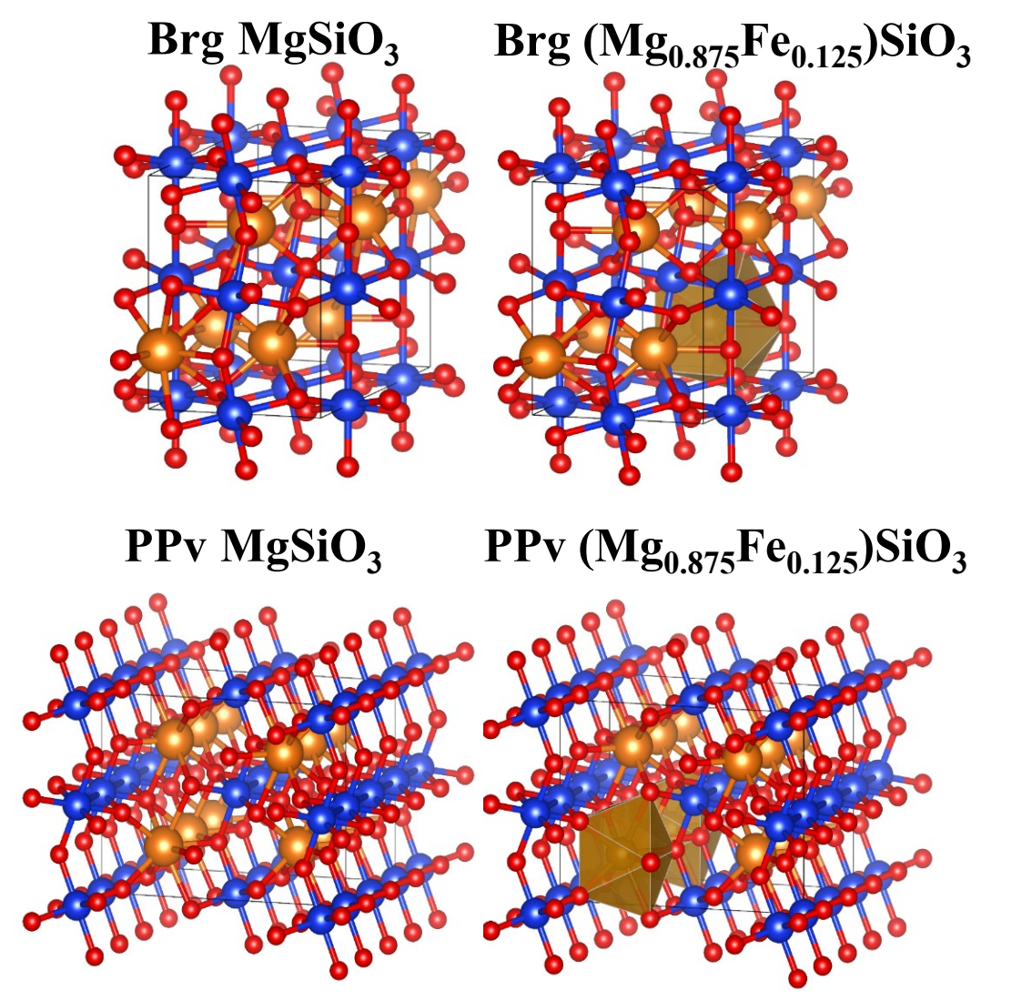
Computational Methods

1、We trained a machine learning potential (MLP) for Fe-free and Fe-bearing bridgmanite（Brg）and post-perovskite（PPv）based on first-principles data

DeePMD-kit

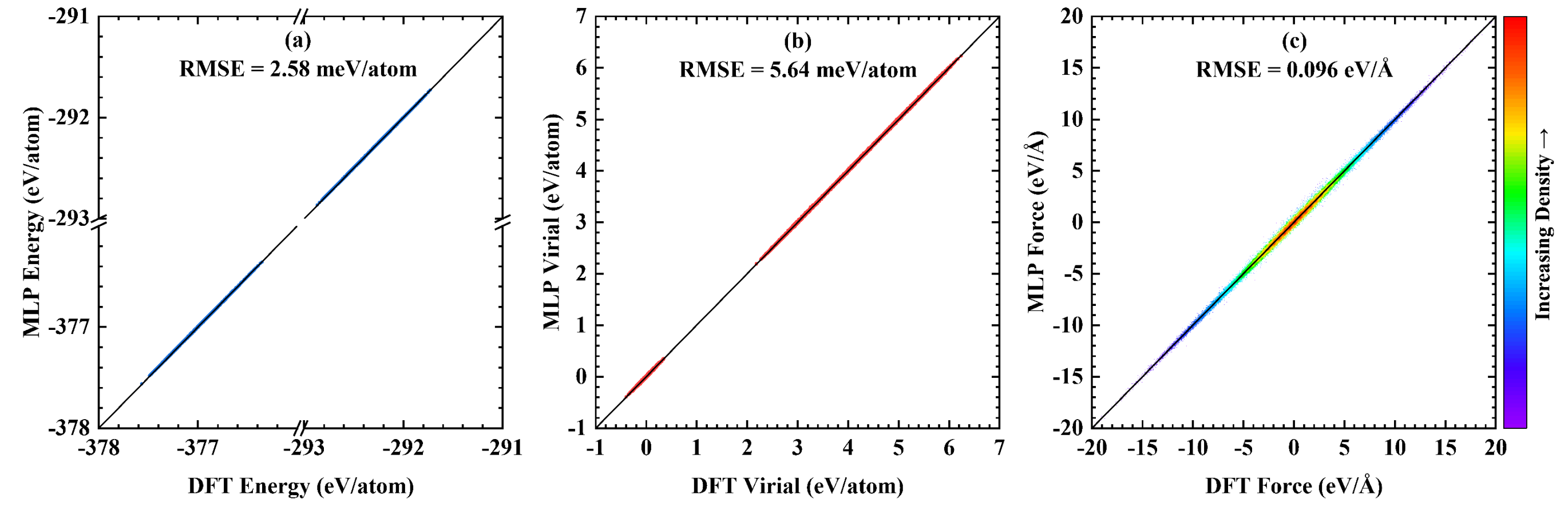


$$L(P_\epsilon, P_f, P_\xi) = \frac{P_\epsilon}{N}\Delta\epsilon^2 + \frac{P_f}{3N}\sum_i |\Delta \boldsymbol{F}_i|^2 + \frac{P_\xi}{9N}\|\Delta\Xi\|^2$$



- There are four structures under current consideration. All Fe remains in the high spin state as Si-site Fe was not considered.
- The size of the training set is ~200,000.

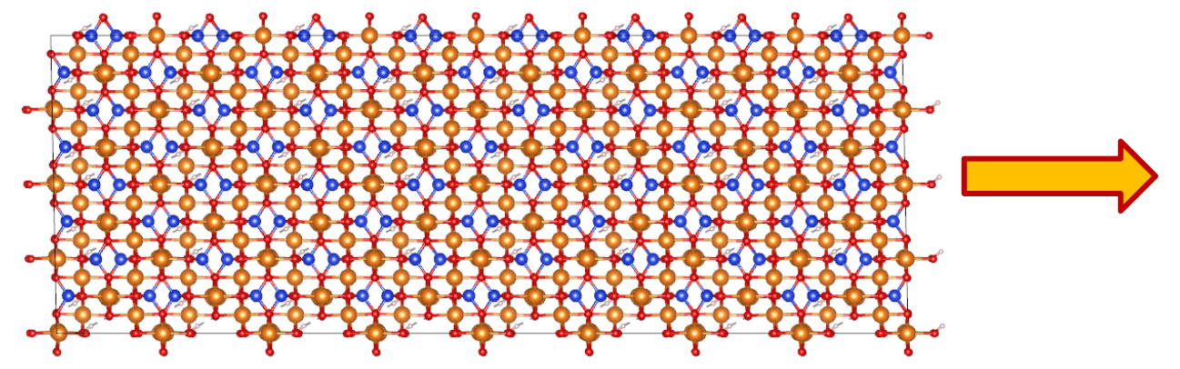
2、The test error of the MLP

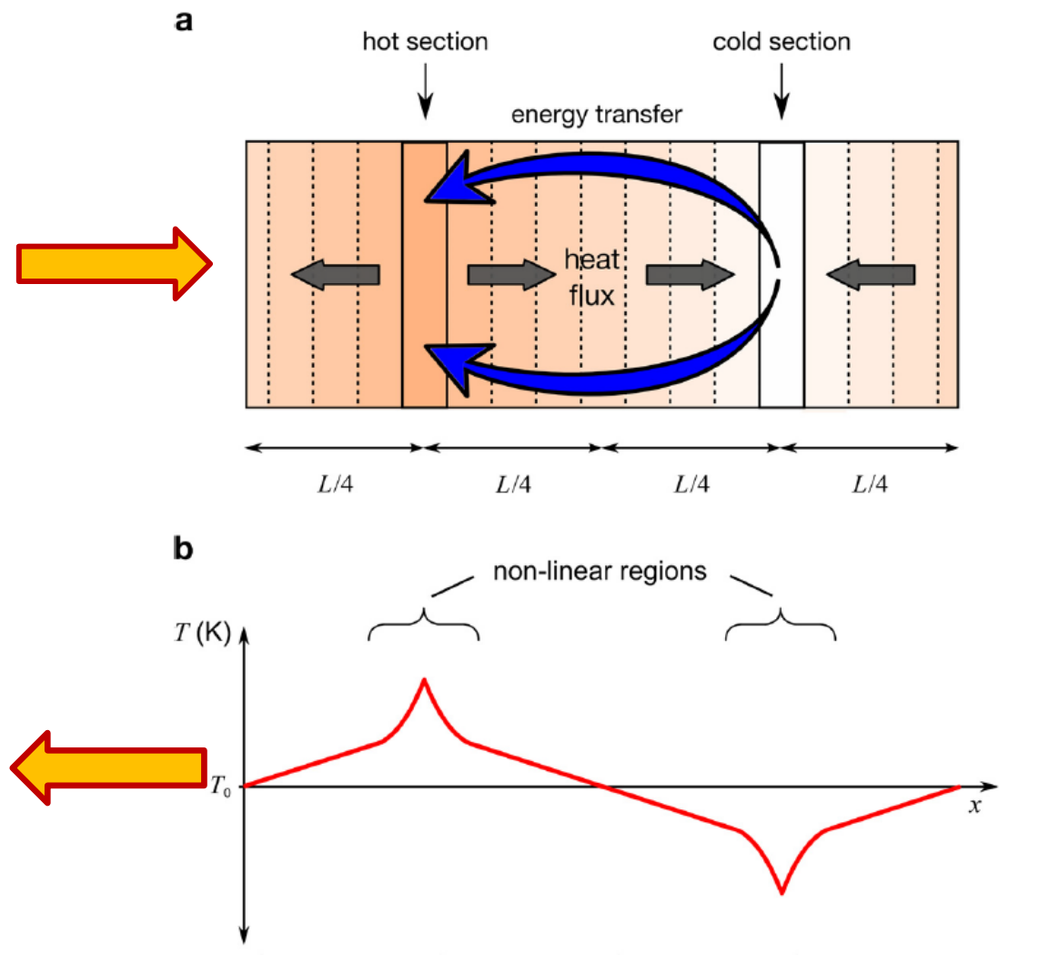


- The test set contains ~9,000 randomly selected data.
- The root-mean-square error of energies, forces and virial stresses are 2.58 meV/atom, 0.096 eV/Å, and 5.64 meV/atom, respectively.

3、Using Non-equilibrium molecular dynamics based on the MLP, we predicted the lattice thermal conductivity (k_{lat}) of Fe-free and Fe-bearing Brg and PPv in large cells

Non-equilibrium molecular dynamics (An experiment-like approach)



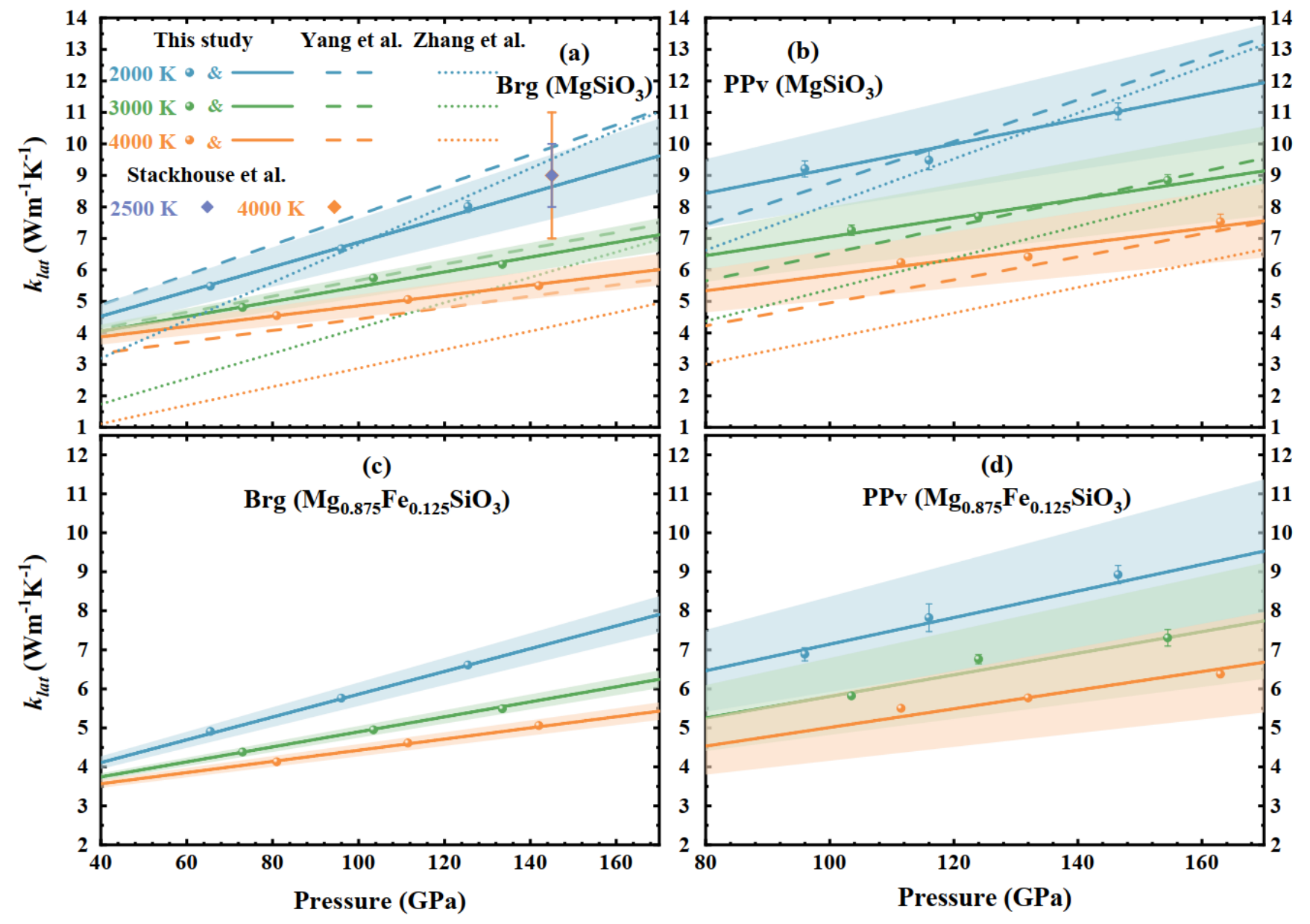


$$k = q\left(\frac{\partial T}{\partial x}\right)^{-1}$$

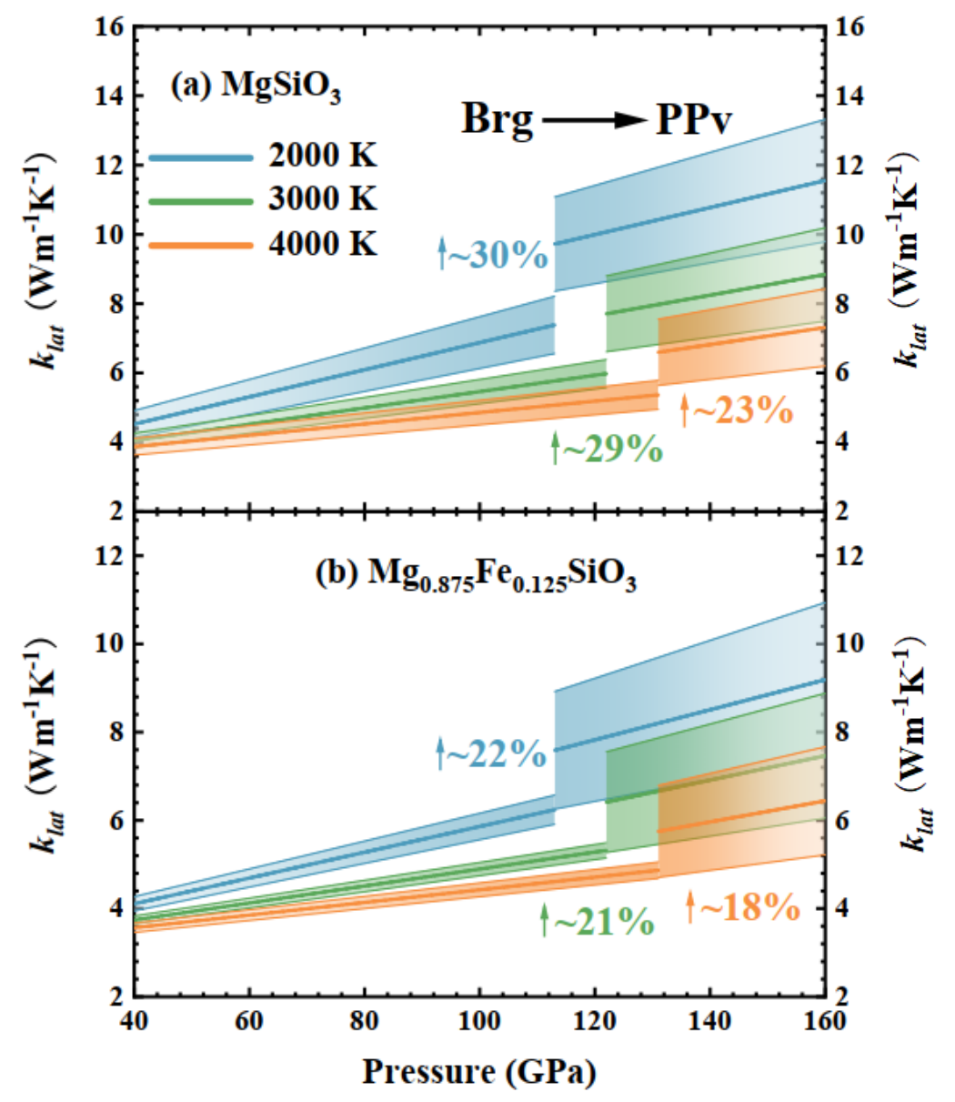
- We divided the cell into 32 regions of equal size, and exchanged the velocities of two atoms between the first and seventeenth regions every n steps.
- Over time, a steady heat flow was established and a linear temperature profile was induced. The thermal conductivity can be calculated from Fourier's law.

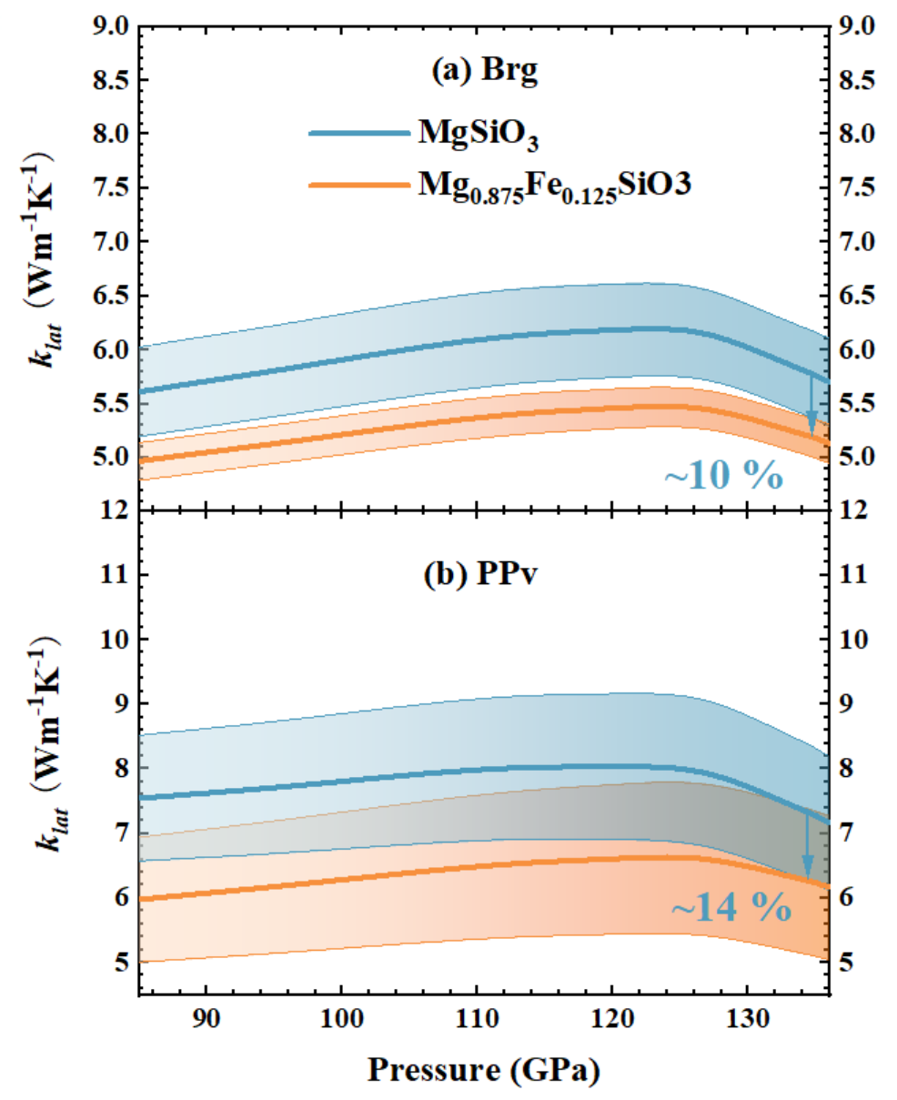
Results and Discussion

The k_{lat} of bridgmanite and post-perovskite



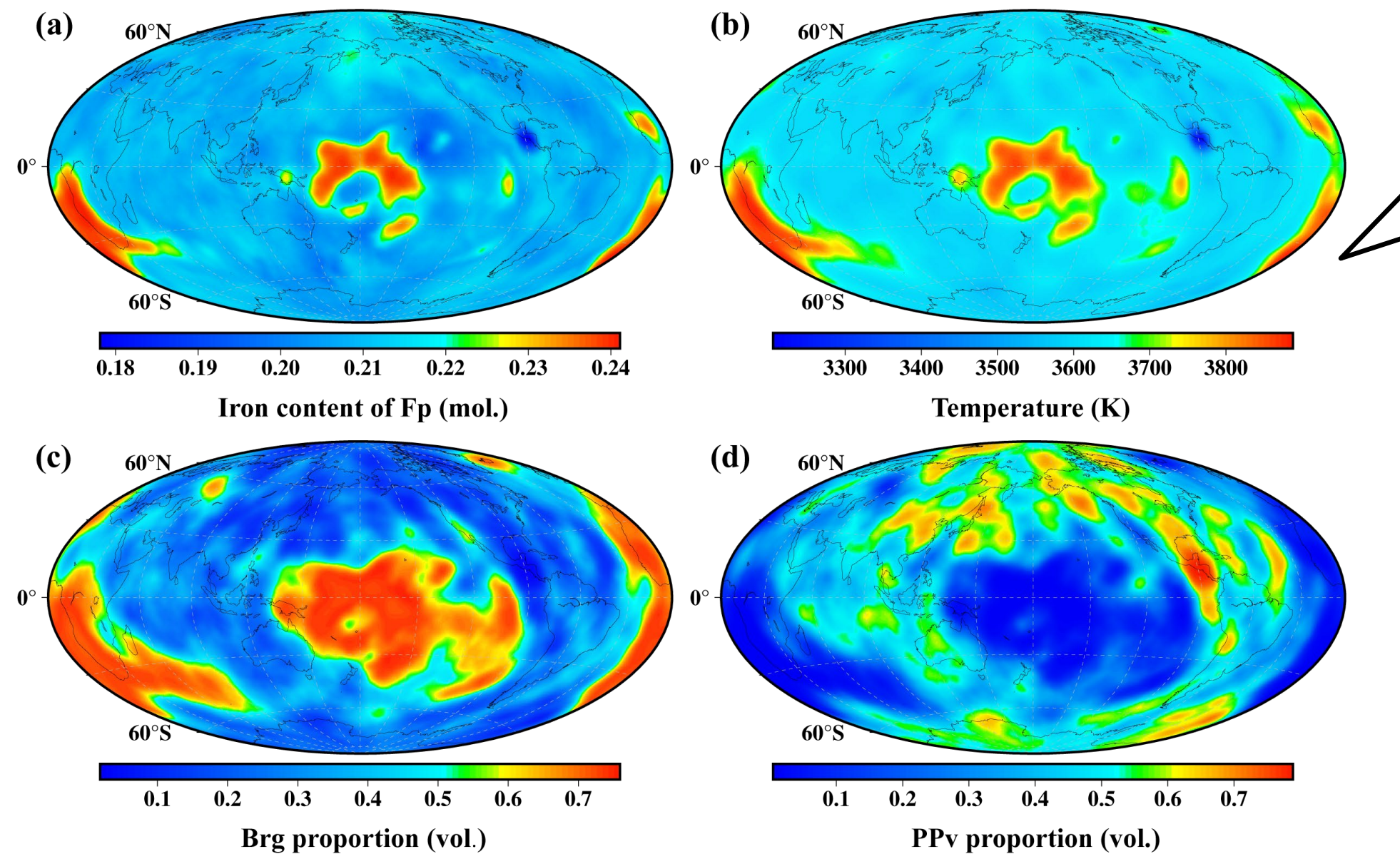
- The lattice thermal conductivities (k_{lat}) of Fe-free Brg and PPv are agree with those calculated by the Green-Kubo method (Yang et al., 2023) based on the MLP.
- The BTE theory (Zhang et al.,2021) tends to underestimate the contribution of diffusion-like phonons (mean free paths shorter than the Loffe-Regel limit), especially at high temperatures and low pressures where their mean free paths are shorter (Luo et al., 2020).





- The phase transition from Brg to PPv increases the k_{lat} by 20%-30%.
- 12.5 mol% Fe in the lowermost mantle decreases the k_{lat} of Pv and PPv by ~10% and ~14%, respectively.

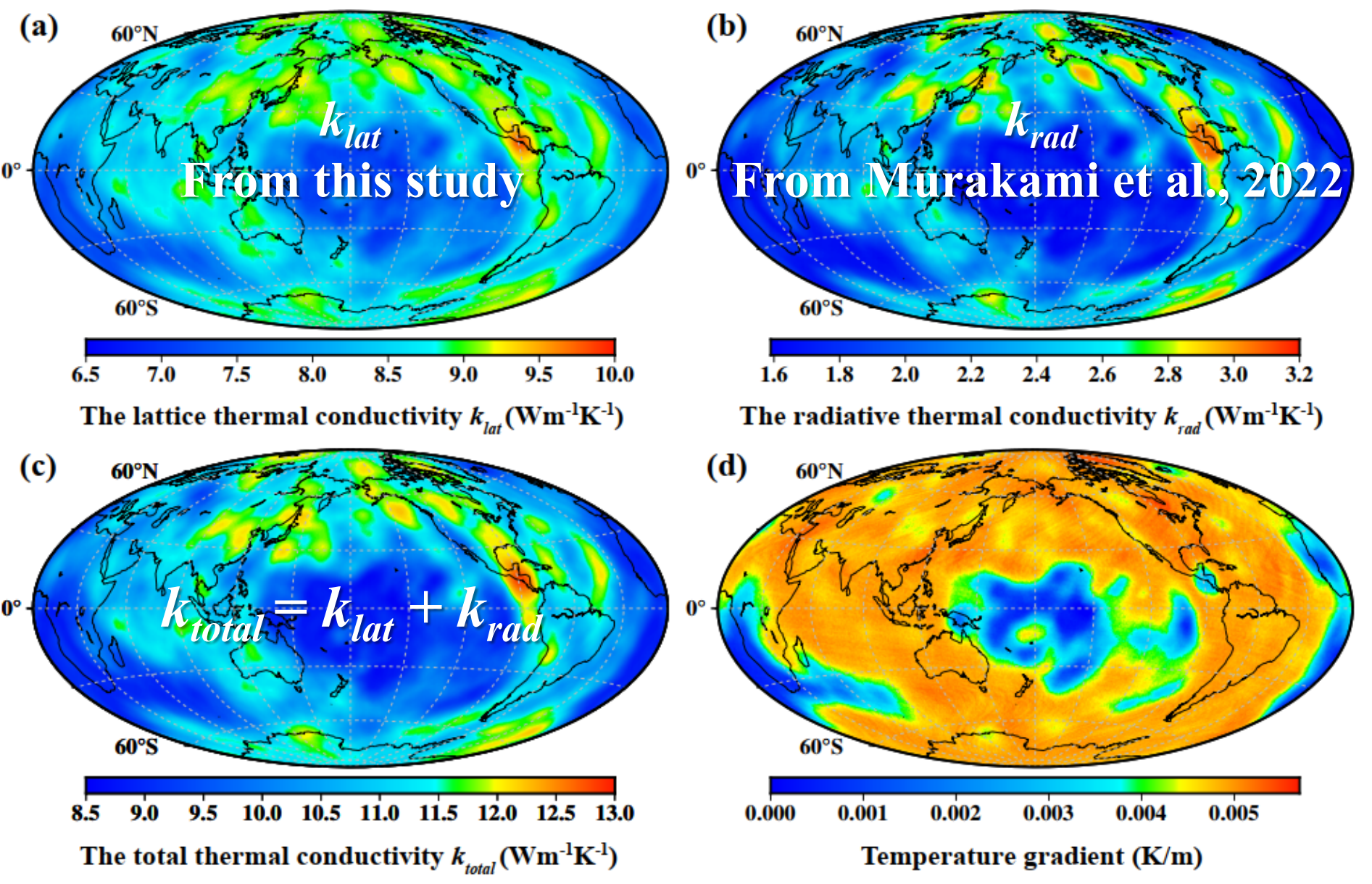
Compositional and thermal state of the lowermost mantle



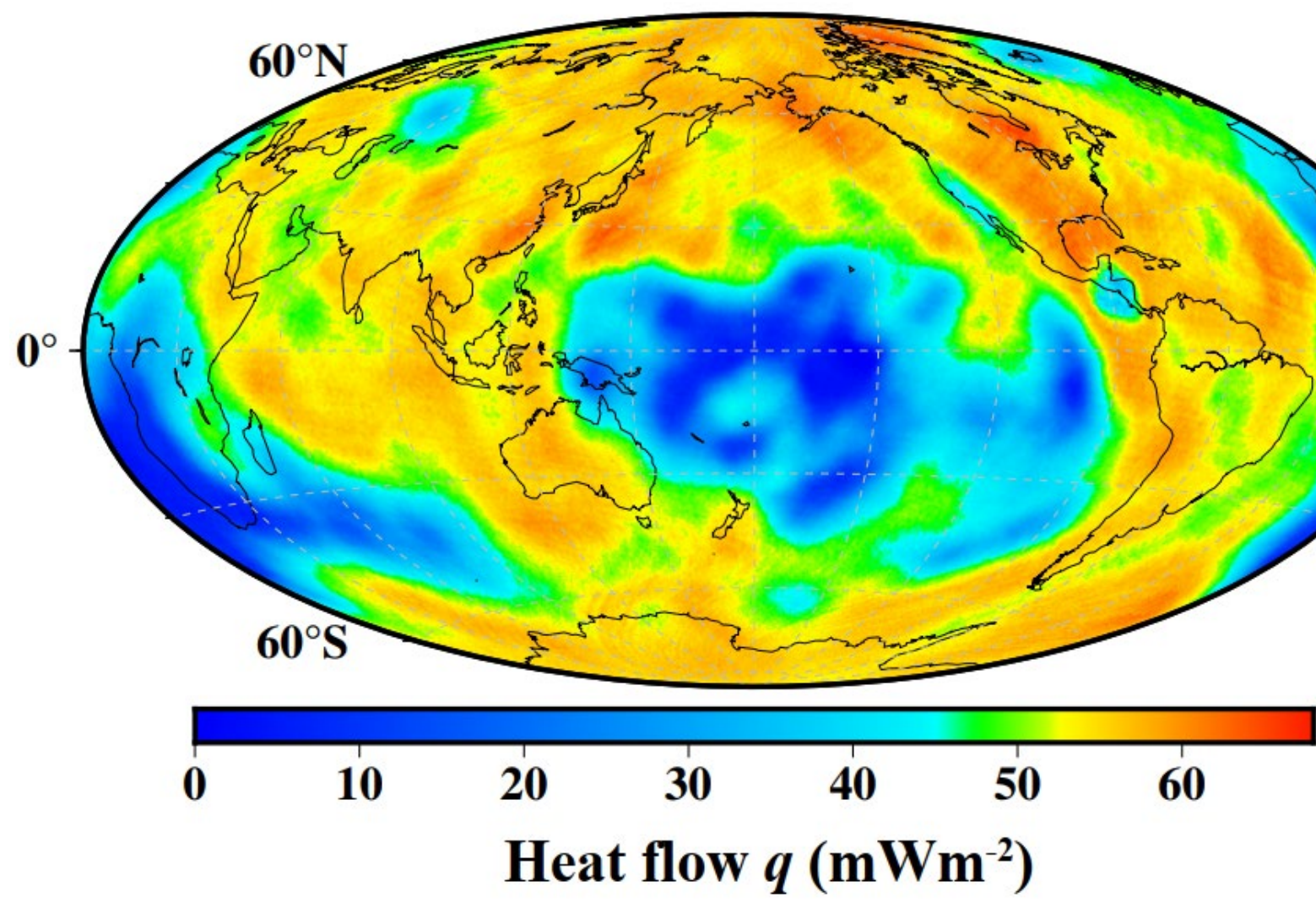
- The inversion based on mineral elasticity and seismic tomography models revealed that the LLSVPs regions are enriched in iron-rich Brg (Deng et al., 2023).

- The thermal conductivity is relatively low in the LLSVPs regions due to higher temperatures and lower PPv content within the LLSVP regions.
- The temperature gradients are relatively low in the LLSVPs regions due to the high temperature there.
- The k_{lat} of davemaoite and ferropericlase are from previous studies (Zhang et al., 2021; Hsieh et al., 2018; Manthilake et al., 2011).

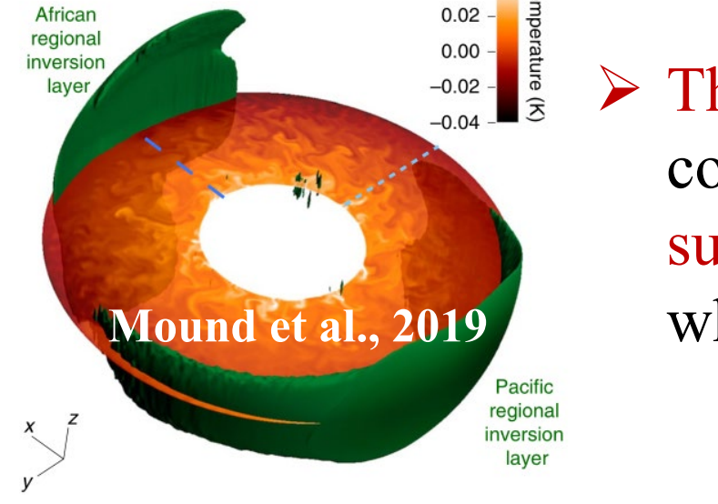
The k and temperature gradient at the lowermost mantle



The heat flux from the Earth's core

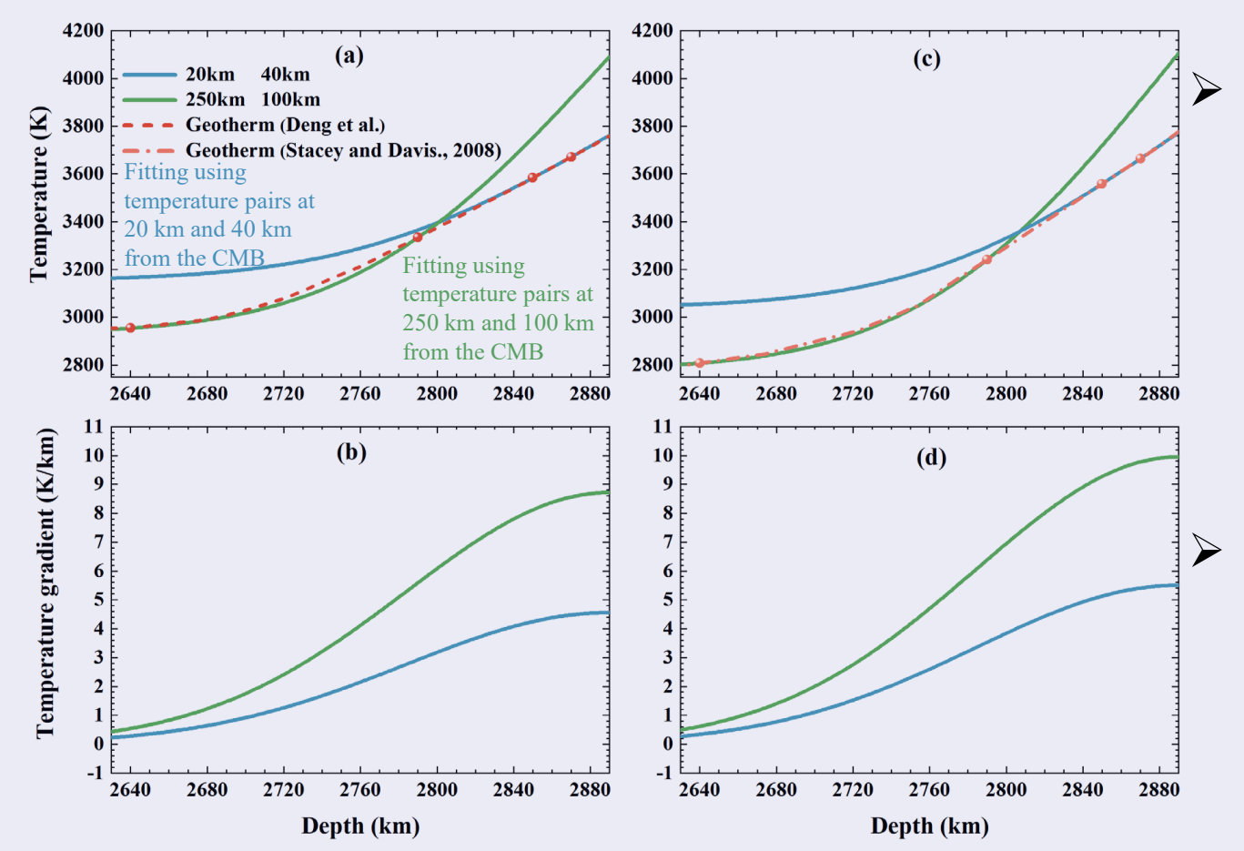


- The heat flux in the LLSVPs regions is extremely low due to the lower temperature gradient and thermal conductivity there, which leads to large lateral variations ($q^* = \frac{Q_{max}-Q_{min}}{2\times Q_{average}} = 1$).



- Thermal convection in the Earth's core below the LLSVPs regions is suppressed by the lower heat flux, which affects the geomagnetic field.
- Total heat flow from the Earth's core is 7.1±0.5 TW, which is sufficient to sustain geodynamo (Nimmo, 2015), but lower than previous estimates from the double crossing of the Brg-PPv phase boundary (Lay et al., 2006; van der Hilst et al.,2007).

The double crossing method overestimates the temperature gradients



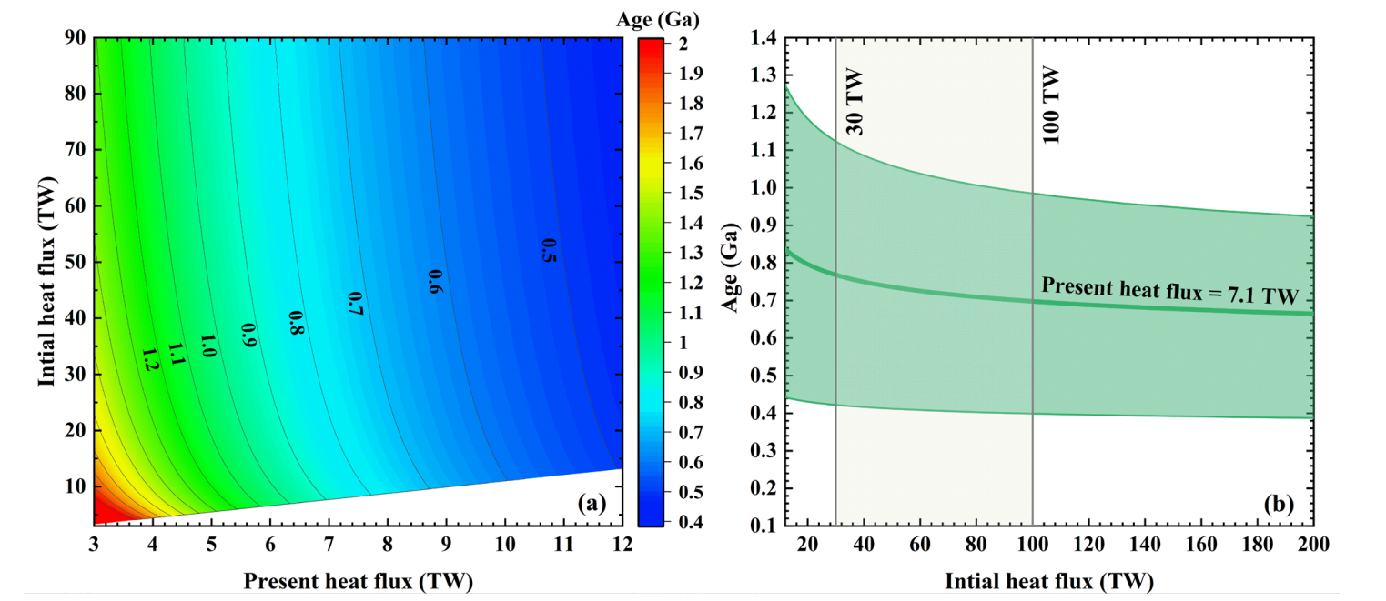
- The simple functions derived from the half-space cooling model cannot be used to describe the geotherm at the CMB and significantly overestimate the temperature gradients in the case that the double-crossing is far from the CMB (~50-350 km) (Lay et al., 2006; van der Hilst et al., 2007).
- The temperature gradients in our model were directly derived from temperatures within 50 km of the CMB.

	Thermal conductivity	Temperature gradients	Total heat flow
This study	10.4 W/m/K	4.4 K/km	7.1 ± 0.5 TW
Double crossing	10 W/m/K	6-16 K/km	12 ± 5 TW

Age of the inner core

$$\int_{-Age}^{0} Q(t)dt = \boxed{Q_C + Q_L + Q_G + Q_H}$$

The total energy released since the onset of the crystallization of the inner core (Labrosse et al., 2001).



$$Q_{intial} = 30 \text{ to } 100\text{TW}$$

$$Q(t) = Q_{intial}\exp(-t/\tau_Q)$$

0.75 ± 0.35 Ga

Summary

- We trained an **MLP** for Fe-free and Fe-bearing Brg and PPv with data from first-principles calculations, then investigated their lattice thermal conductivity at mantle conditions in the large cells with **finite-size effects well considered.**
- The phase transition from **Brg to PPv increases the lattice thermal conductivity by 20%-30%.**
- Above the CMB, the presence of **12.5 mol% Fe decreases** the thermal conductivity of **Brg and PPv by ~10% and ~14%**, respectively.
- The **LLSVPs regions** with extremely **low heat flux hinder the cooling and thermal convection of the core.**
- The total heat flow from the Earth's core was estimated to be **7.1 ± 0.5 TW**, which supports a geologically **young inner core of 0.75 ± 0.35 Ga**.

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