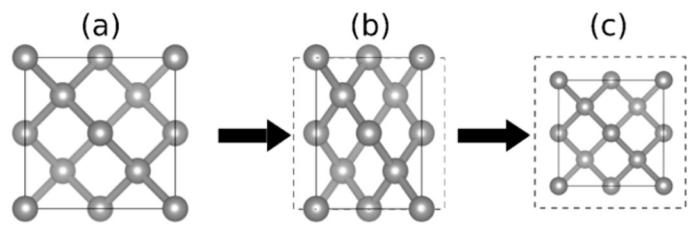


# A model for ramp compression from ab initio calculations



Felipe González

B.K. Godwal, R. Jeanloz, B. Militzer, K. Driver (LLNL)

Department of Earth and Planetary Science  
University of California, Berkeley

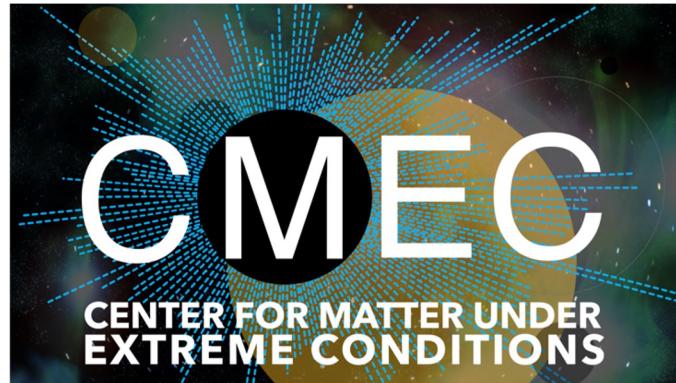
07/14/2022



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DOE-NNSA  
(DE-NA0003842)



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Scientific Computing Center

## Collaborators:

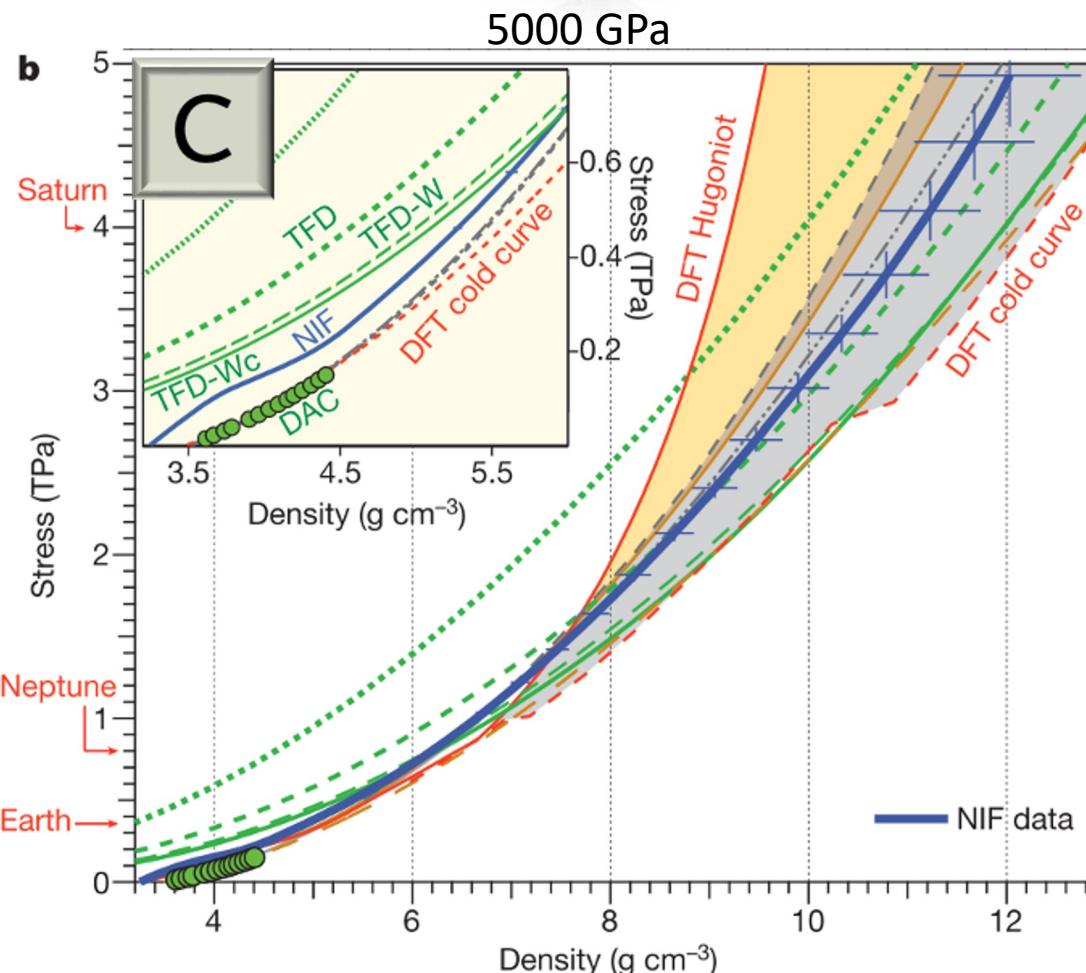
B. Militzer (UCB)  
R. Jeanloz (UCB)  
B.K. Godwal (UCB)  
K. Driver (LLNL)

# Motivation

Diamond



Understanding ramp compression



Smith+ Nature (2014)

$$\text{Plastic work} = \int \beta dW_p$$

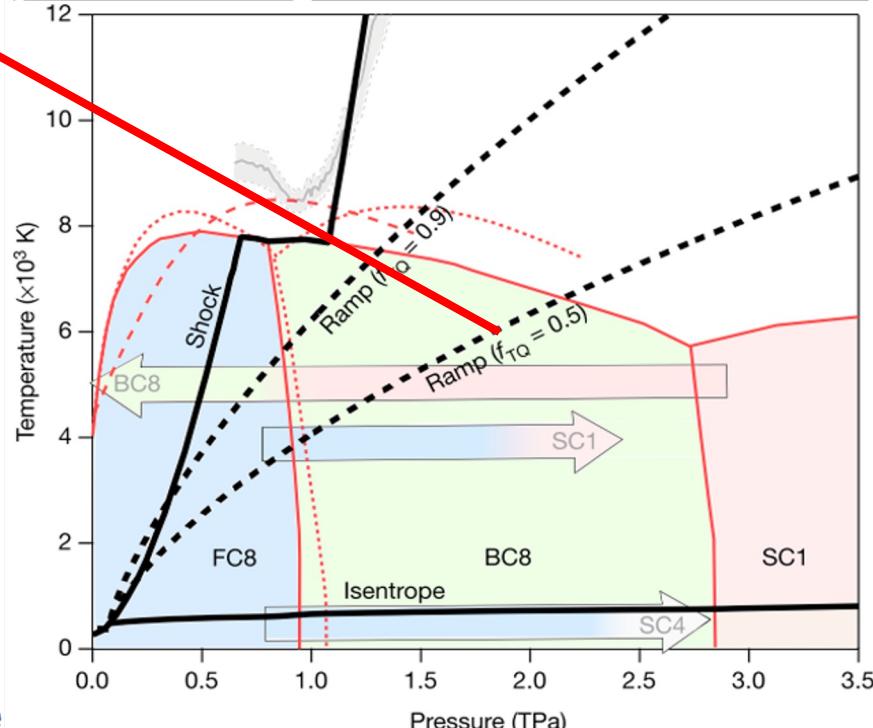
2000 GPa

A. Lazicki+, Nature (2021)

Article

## Metastability of diamond ramp-compressed to 2 terapascals

<https://doi.org/10.1038/s41586-020-03140-4>  
Received: 1 June 2020  
Accepted: 26 October 2020  
Published online: 27 January 2021

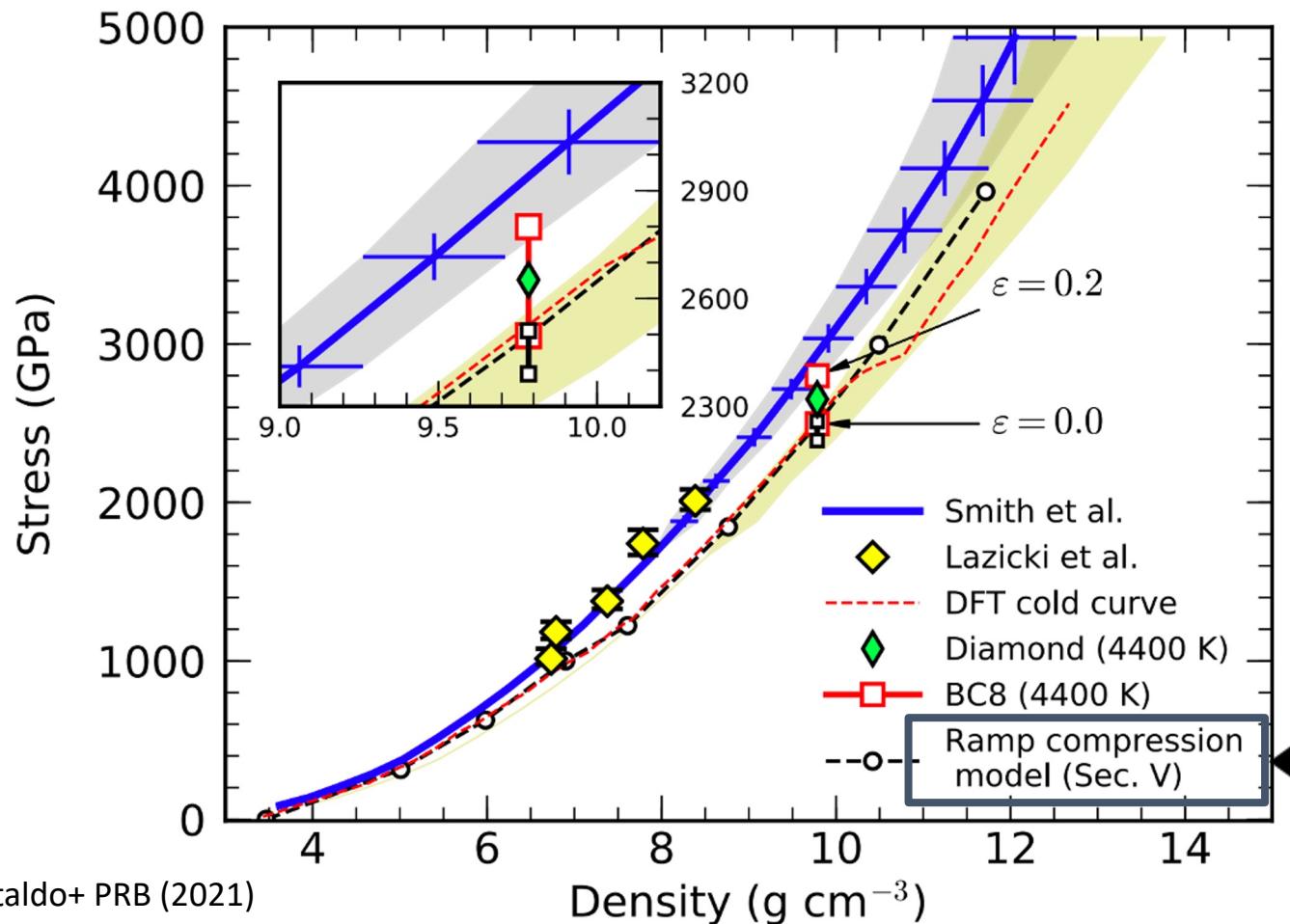


# Reconciling exp. & simulations

Diamond



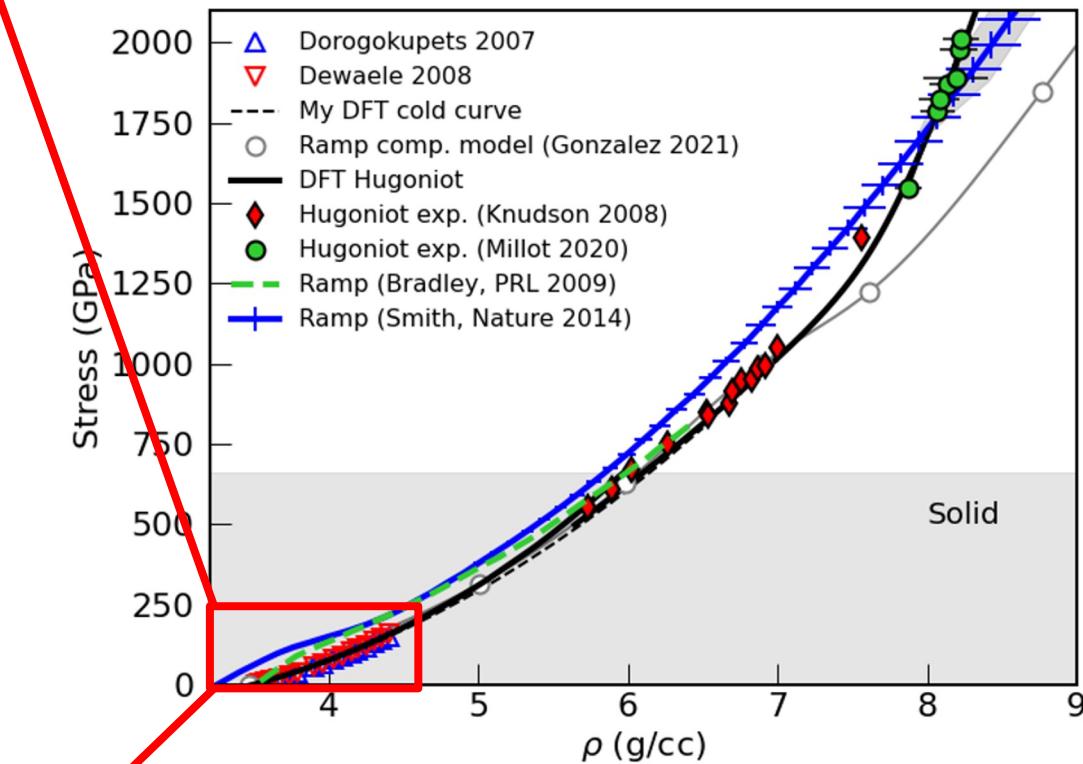
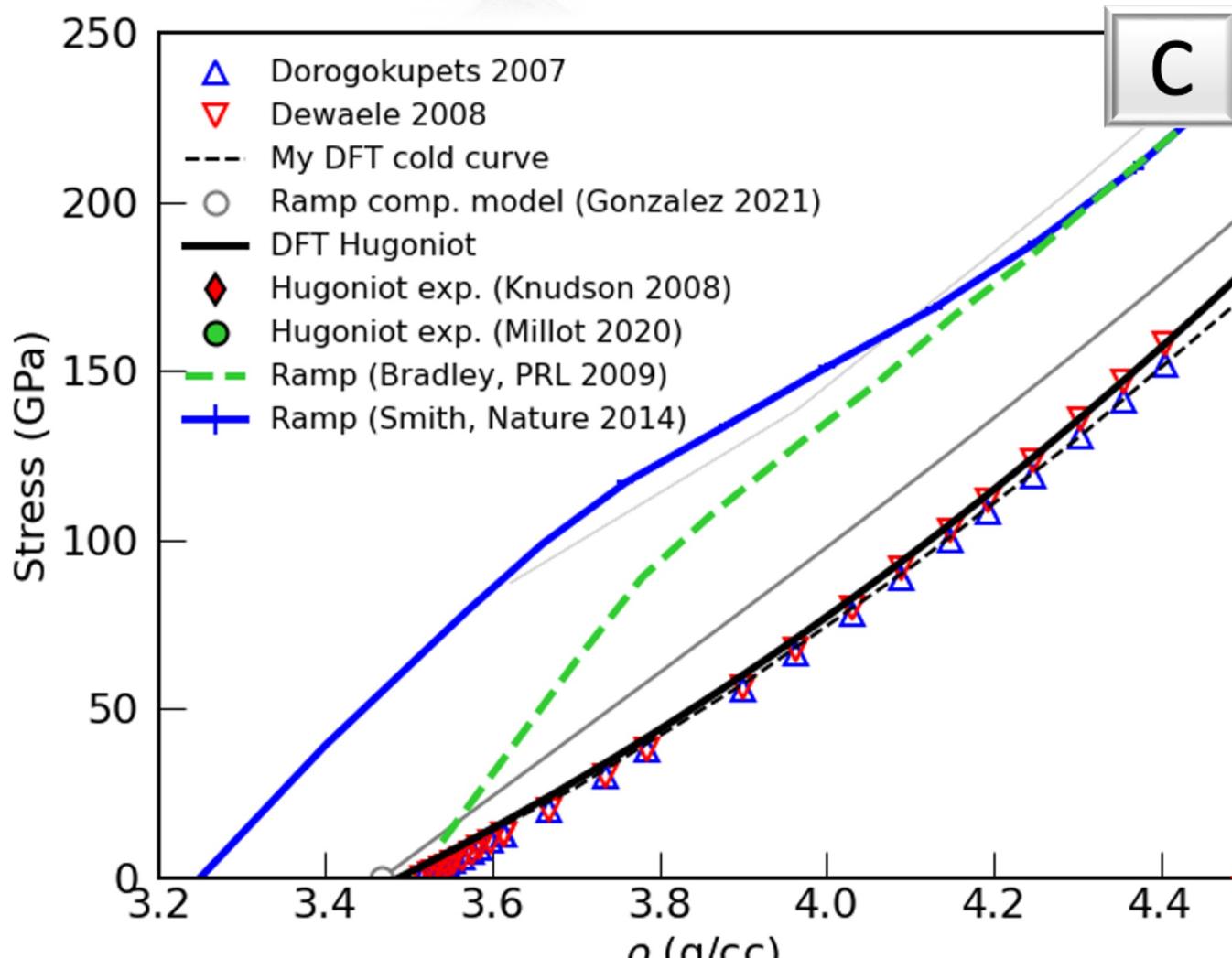
Understanding ramp compression



Our Model

# Reconciling exp. & simulations

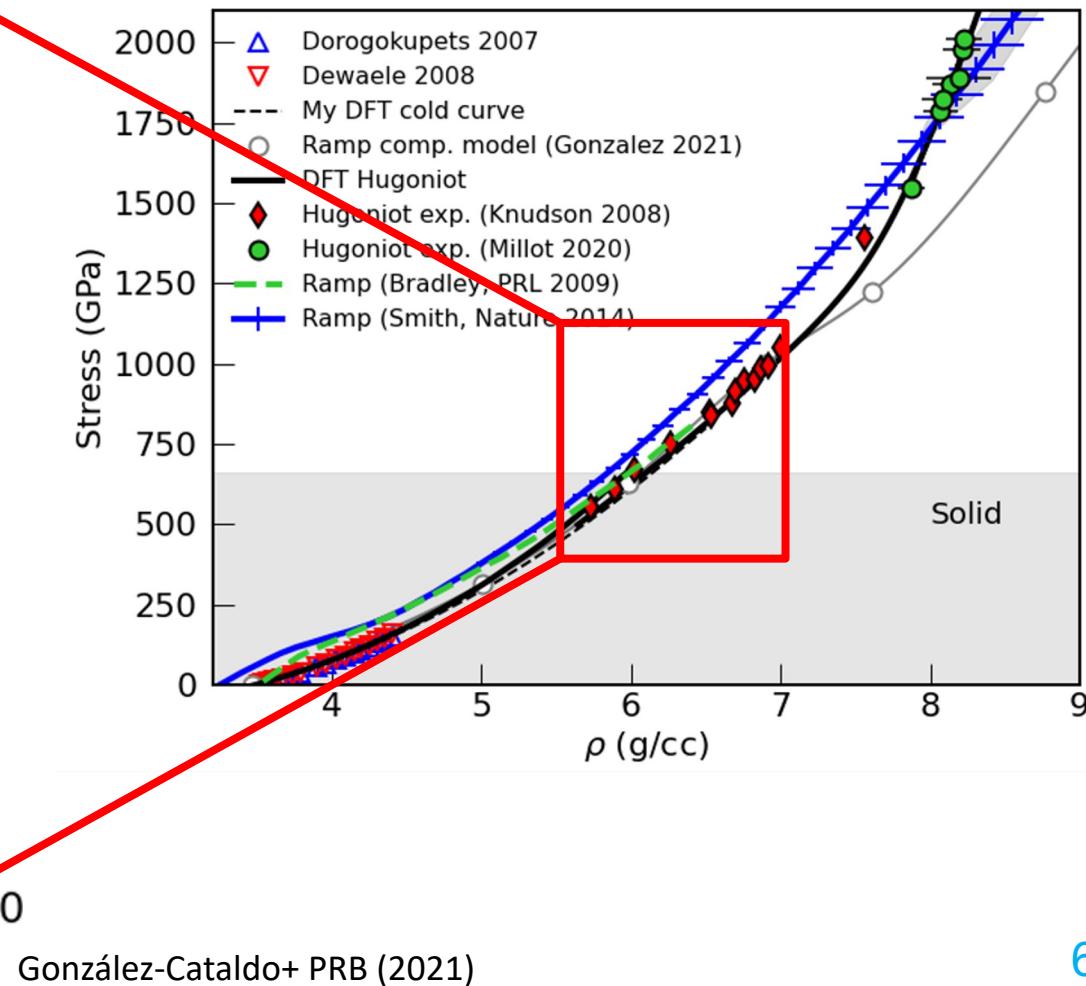
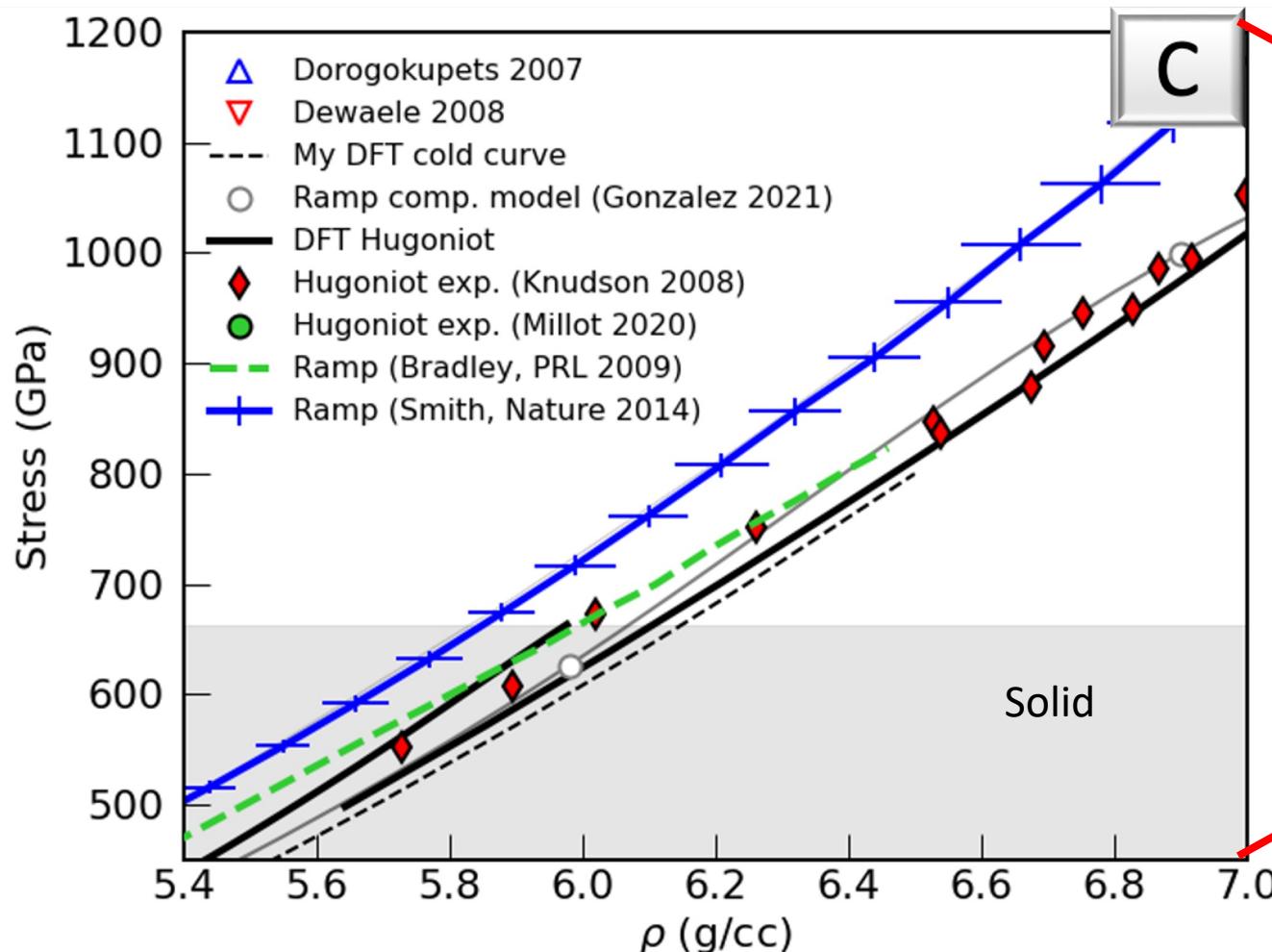
Diamond



González-Cataldo+ PRB (2021)

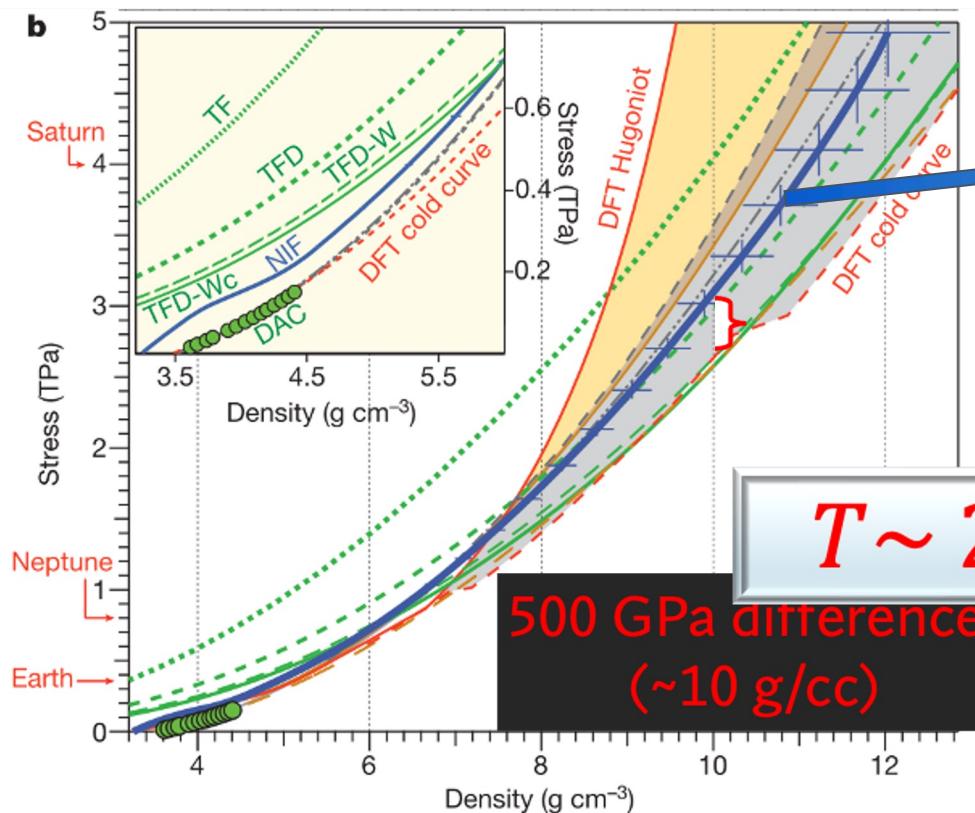
# Reconciling exp. & simulations

## Diamond

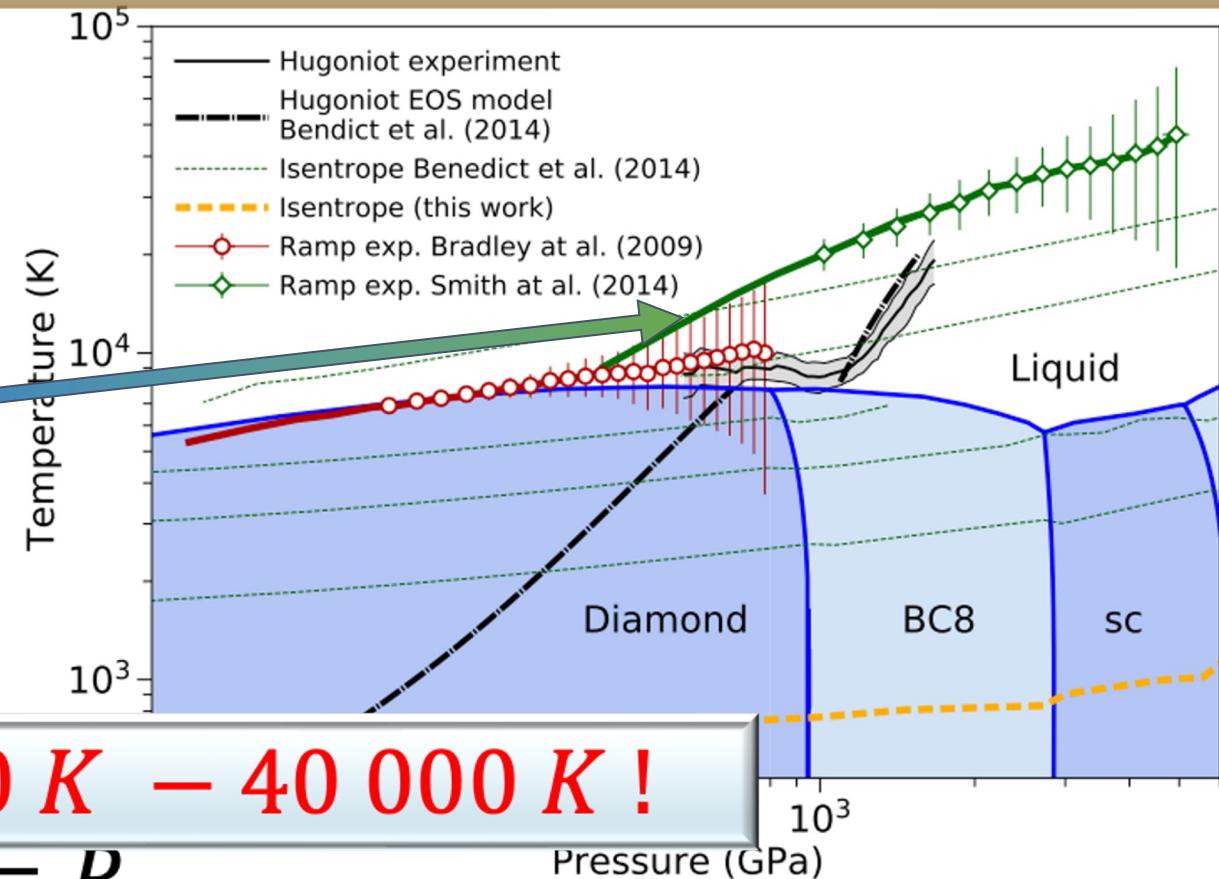


# Reconciling exp. & simulations

EOS of Liquid C:

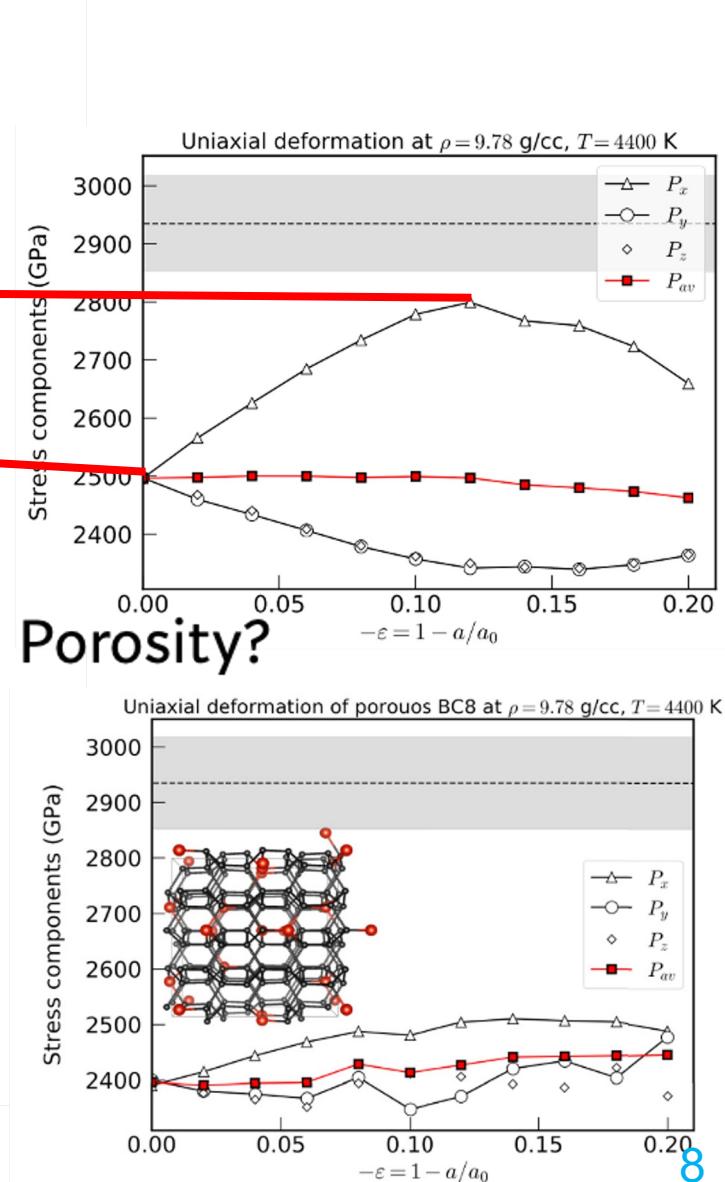
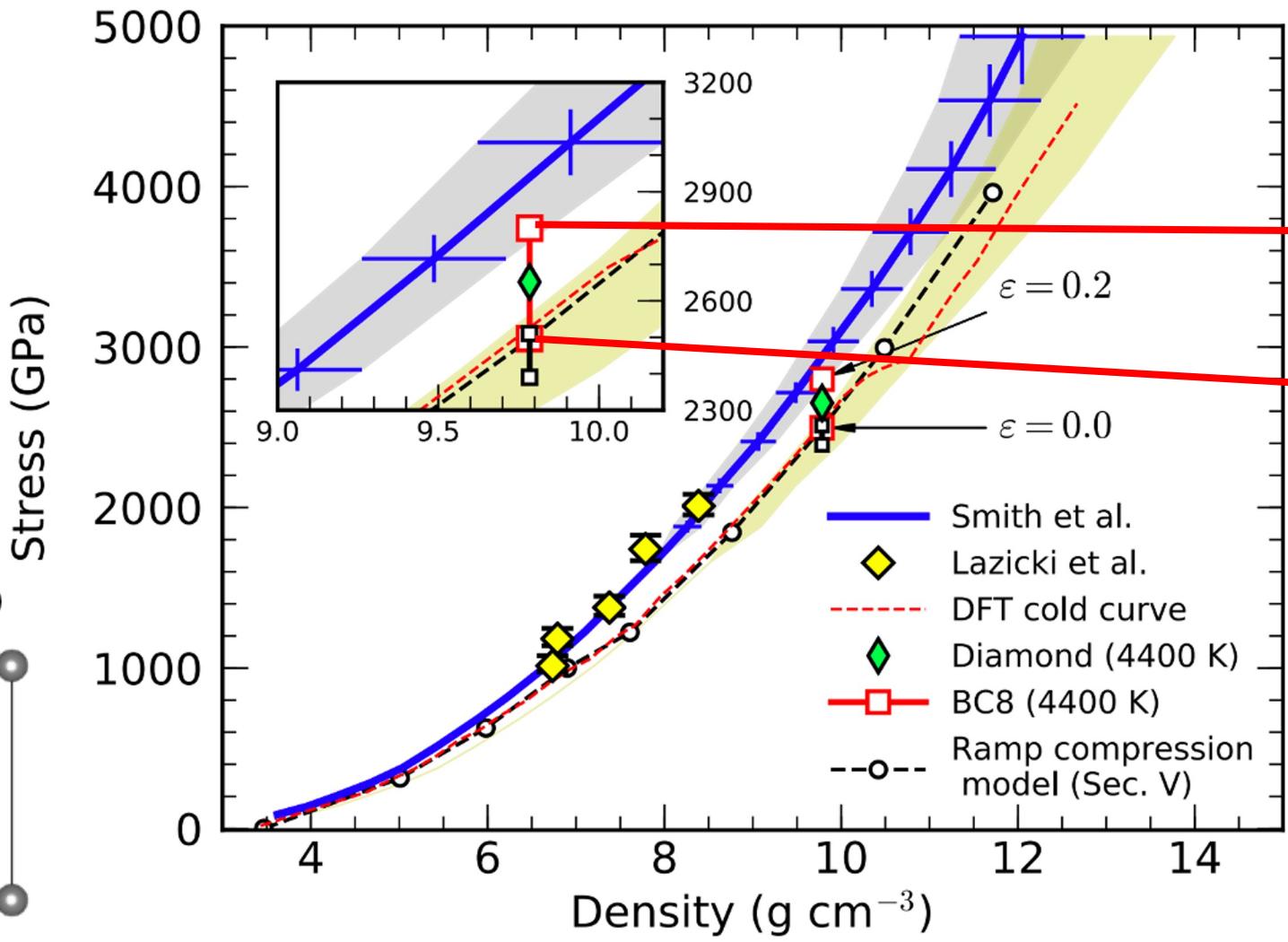
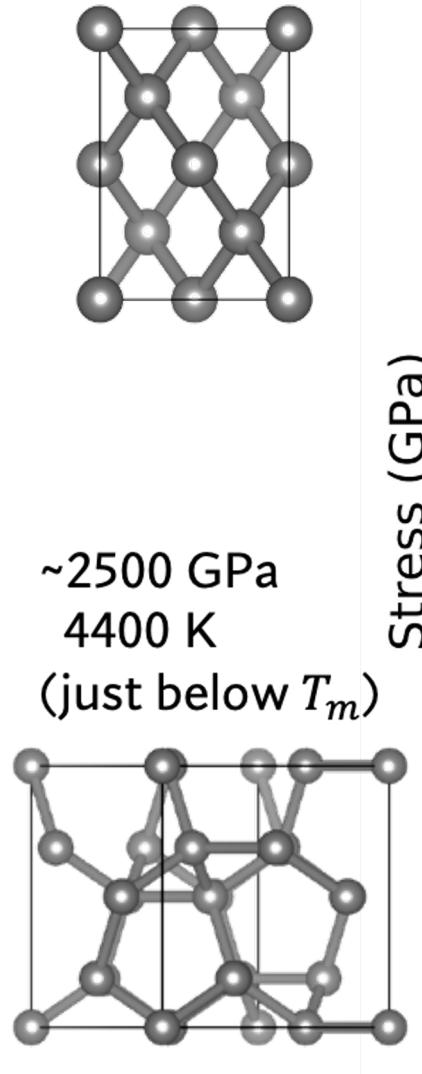


- $P_x = P$
- $P = P(\rho, T)$
- $T = T(\rho, P)$



$$T \sim 20\,000 \text{ K} - 40\,000 \text{ K} !$$

# Reconciling exp. & simulations



# Ramp compression

Diamond



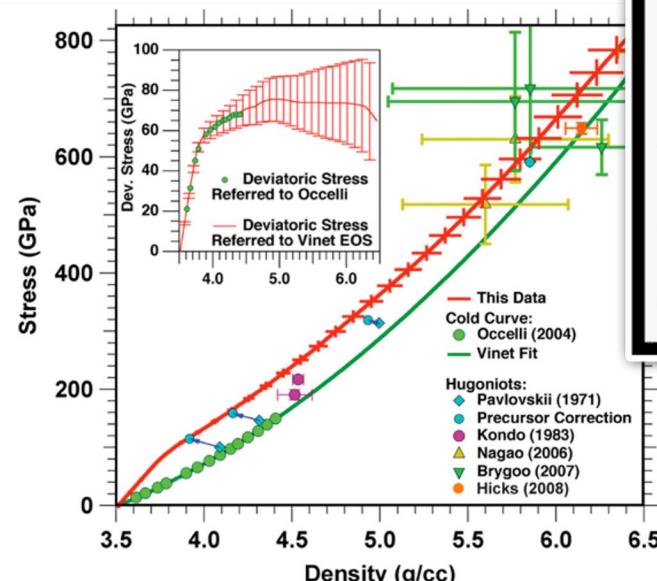
800 GPa

PRL 102, 075503 (2009)

PHYSICAL REVIEW LETTERS

Diamond at 800 GPa

D. K. Bradley, J. H. Eggert, R. F. Smith, S. T. Prisbrey,  
A. V. Hamza, R. E. Rudd, and  
Lawrence Livermore National Laboratory, P.O. Box 8000  
(Received 6 January 2008; published 20 March 2009)



LETTER

5000 GPa

doi:10.1038/nat

Article

Metastability of diamond ramp-compressed to 2 terapascals

2000 GPa

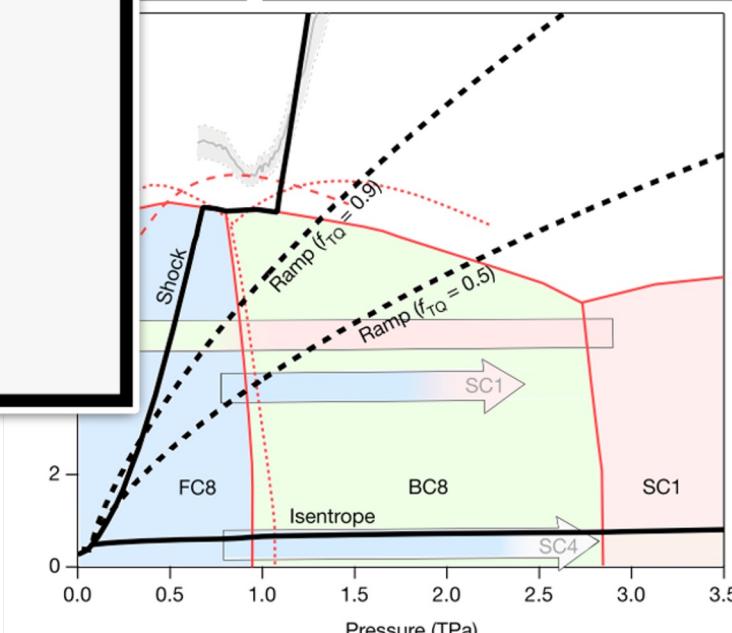
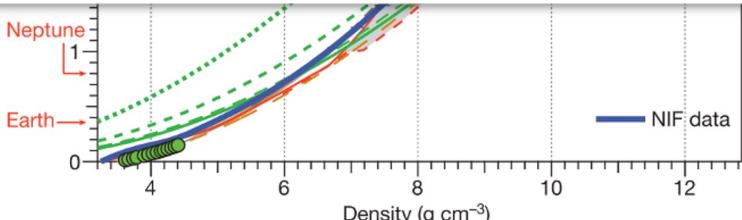
s41586-020-03140-4 A. Lazicki<sup>1,2</sup>, D. McGonegle<sup>2</sup>, J. R. Rygg<sup>3,4,5</sup>, D. G. Braun<sup>1</sup>, D. C. Swift<sup>1</sup>, M. G. Gorman<sup>1</sup>, R. F. Smith<sup>1</sup>, P. G. Heighway<sup>2</sup>, A. Higginbotham<sup>6</sup>, M. J. Suggit<sup>7</sup>, D. E. Franduono<sup>6</sup>, F. Coppari<sup>8</sup>, C. E. Wehrenberg<sup>9</sup>, R. G. Kraus<sup>9</sup>, D. Erskine<sup>9</sup>, J. V. Bernier<sup>9</sup>, J. M. McNamee<sup>9</sup>, R. E. Rudd<sup>1</sup>, G. W. Collins<sup>3,4,5</sup>, J. H. Eggert<sup>1</sup> & J. S. Wark<sup>2</sup>

020

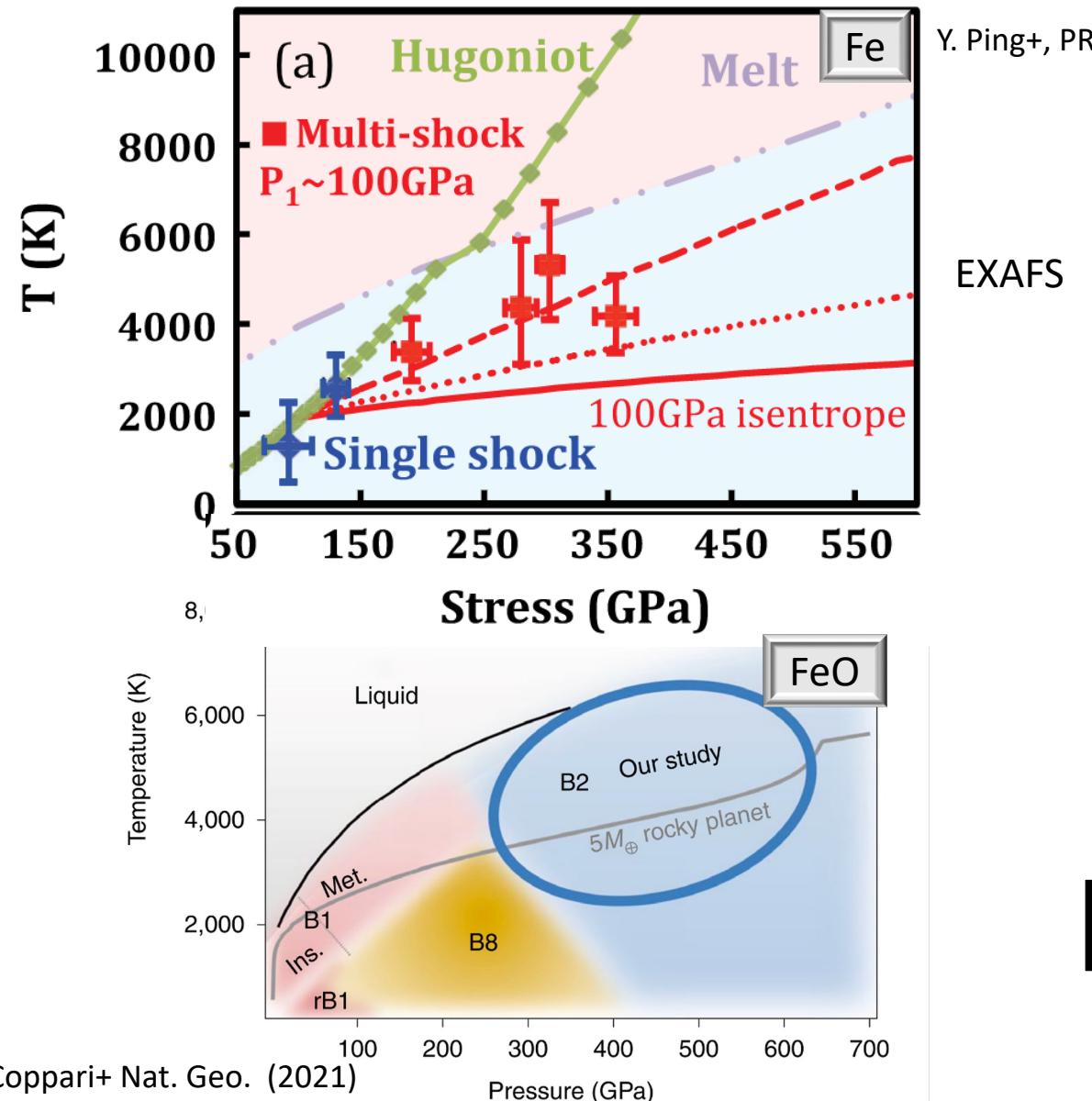
January 2021

## Open questions

- Equation of state (EOS)?
- Strength effects (Stress = Pressure)?
- Plastic work?
- Isentropic compression?
- Thermal state:  $T(\rho, P)$ ?



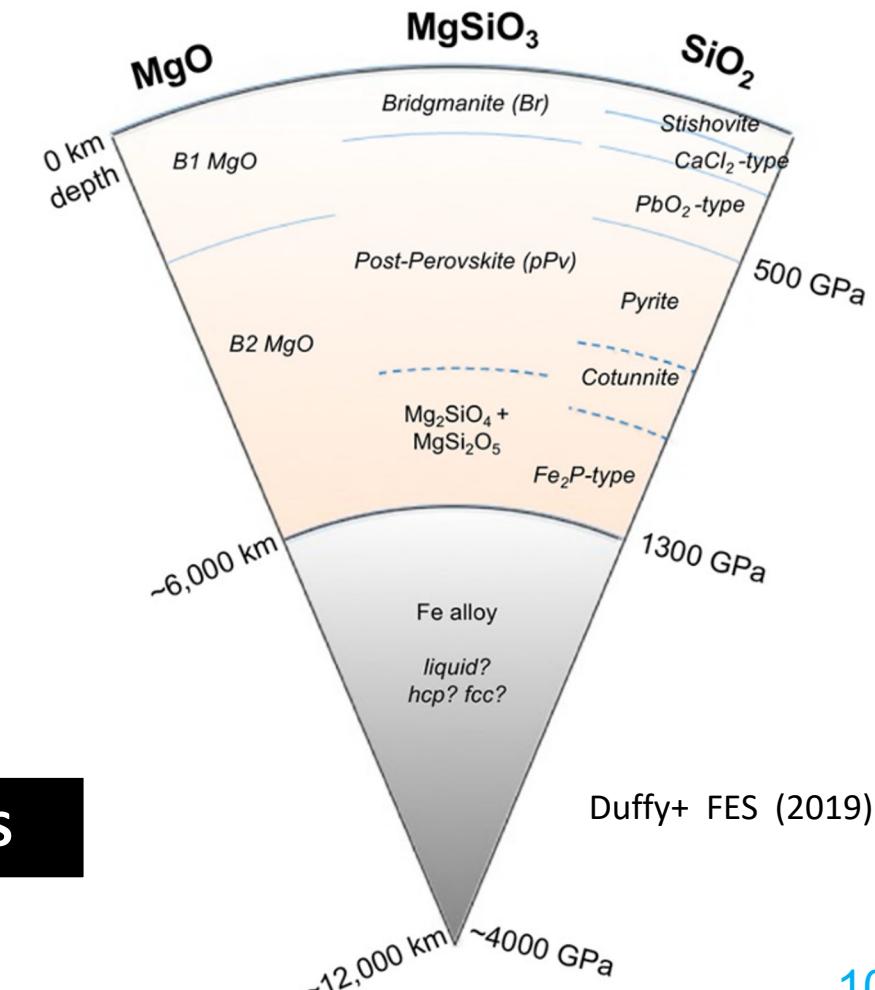
# Shock vs. ramp compression



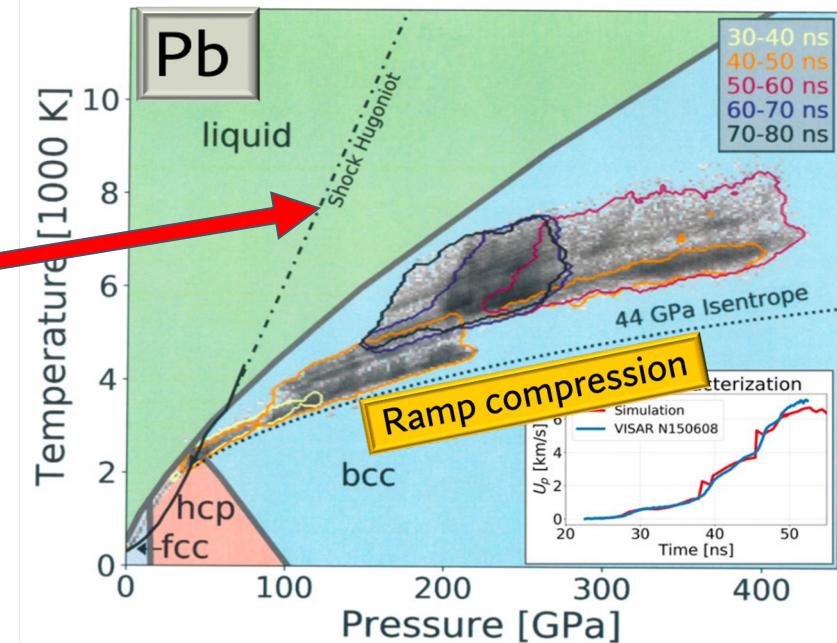
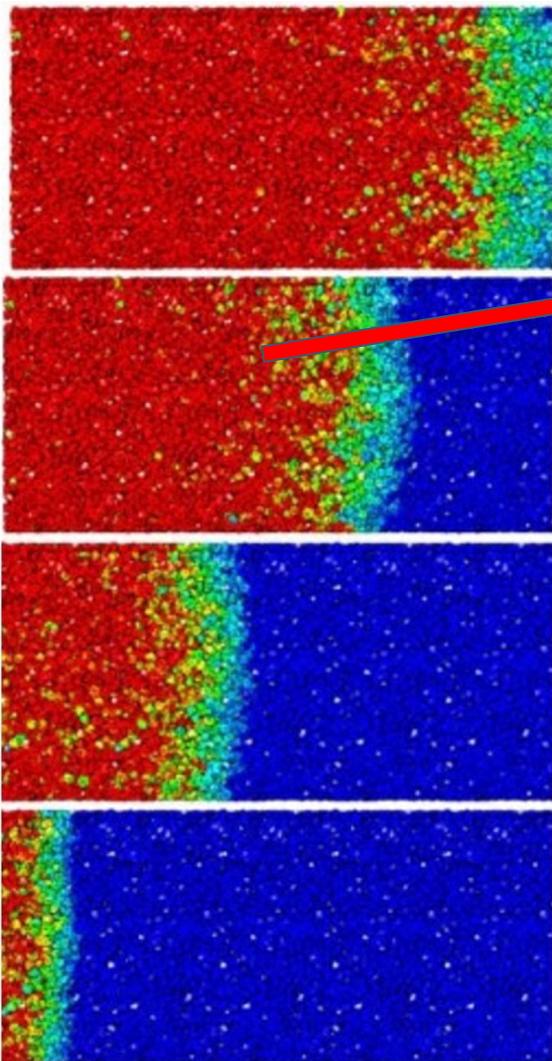
Y. Ping+, PRL (2013)

EXAFS

SUPER EARTHS



# Shock vs. ramp compression



Temperature measurements  
not available

Rankine-Hugoniot equations

$$H(V, T) = (\mathbf{E} - E_0) + \frac{1}{2} (\mathbf{P} + P_0)(V - V_0) = 0$$

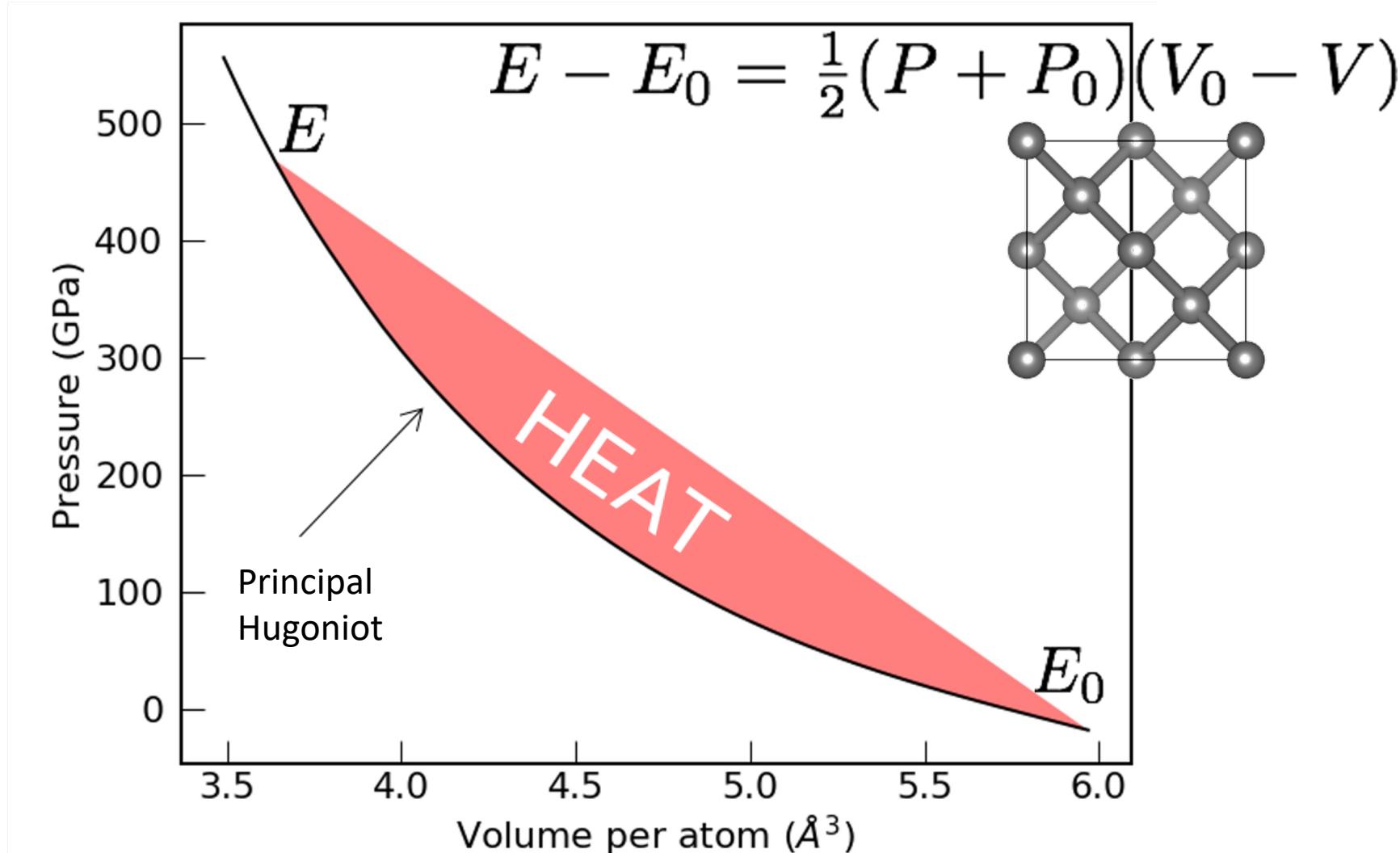
# Ramp compression model from *ab initio* simulations

PHYSICAL REVIEW B **104**, 134104 (2021)

**Model of ramp compression of diamond from *ab initio* simulations**

F. González-Cataldo<sup>1,\*</sup> B. K. Godwal,<sup>1</sup> K. Driver,<sup>1,2</sup> R. Jeanloz,<sup>1,3,4</sup> and B. Militzer<sup>1,3</sup>

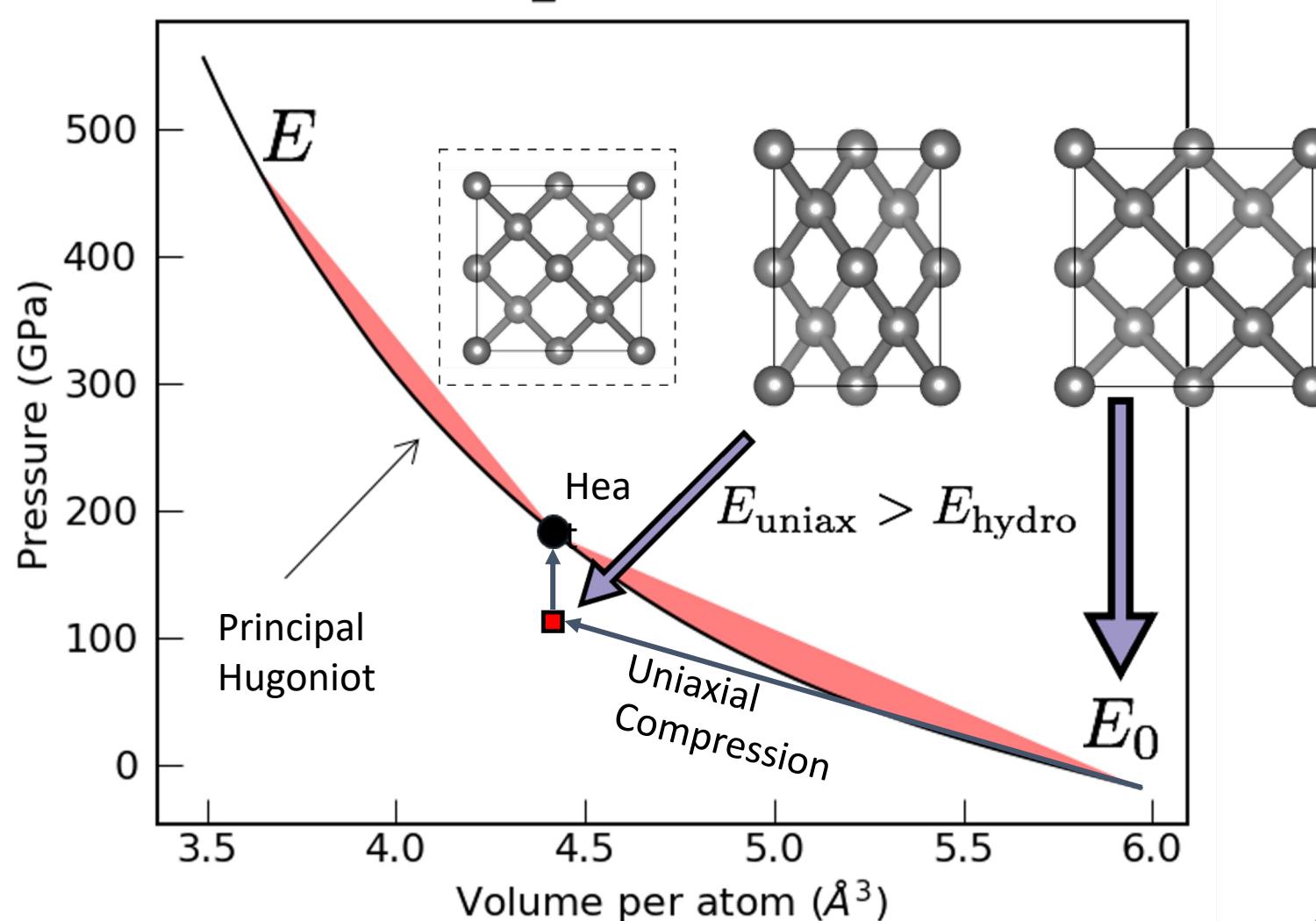
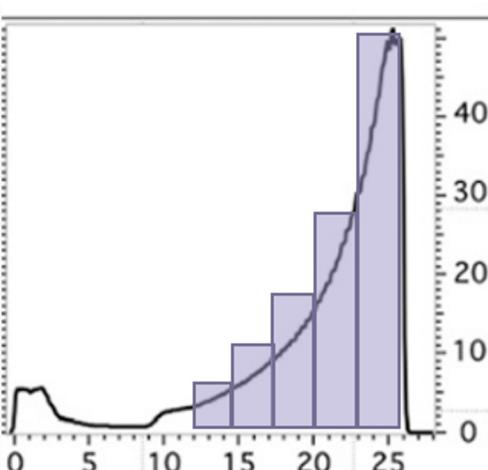
# Ramp $\sim$ multishocks



# Ramp $\sim$ multishocks

$$E - E_0 = \frac{1}{2}(P + P_0)(V_0 - V)$$

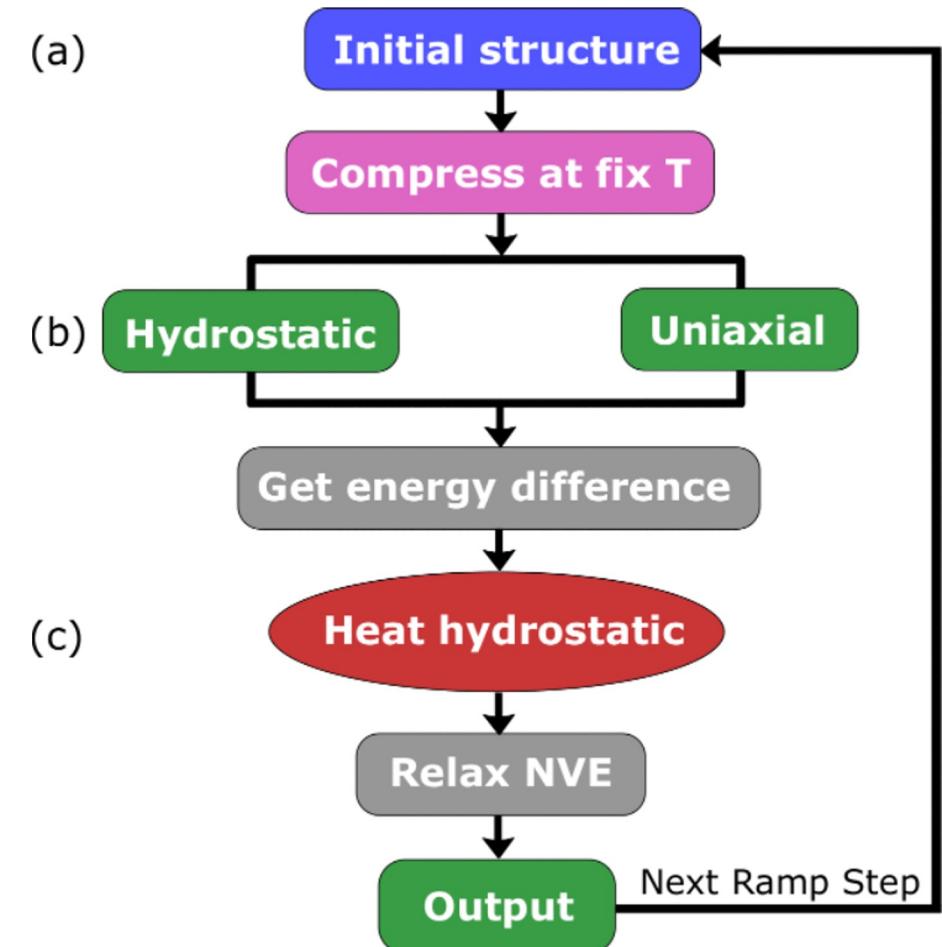
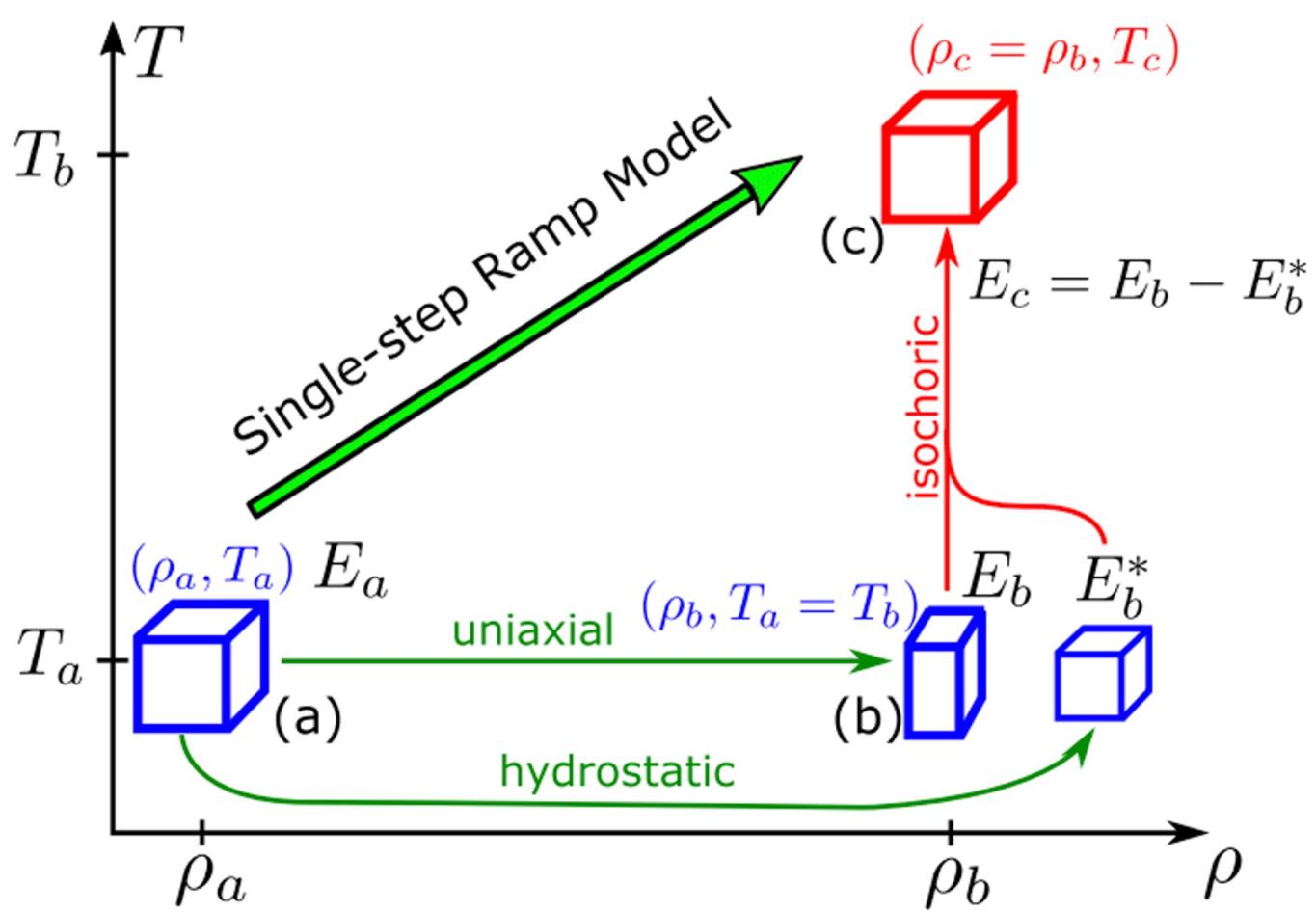
Ramp  $\sim$  Multishock



$\Delta E \rightarrow K$  14

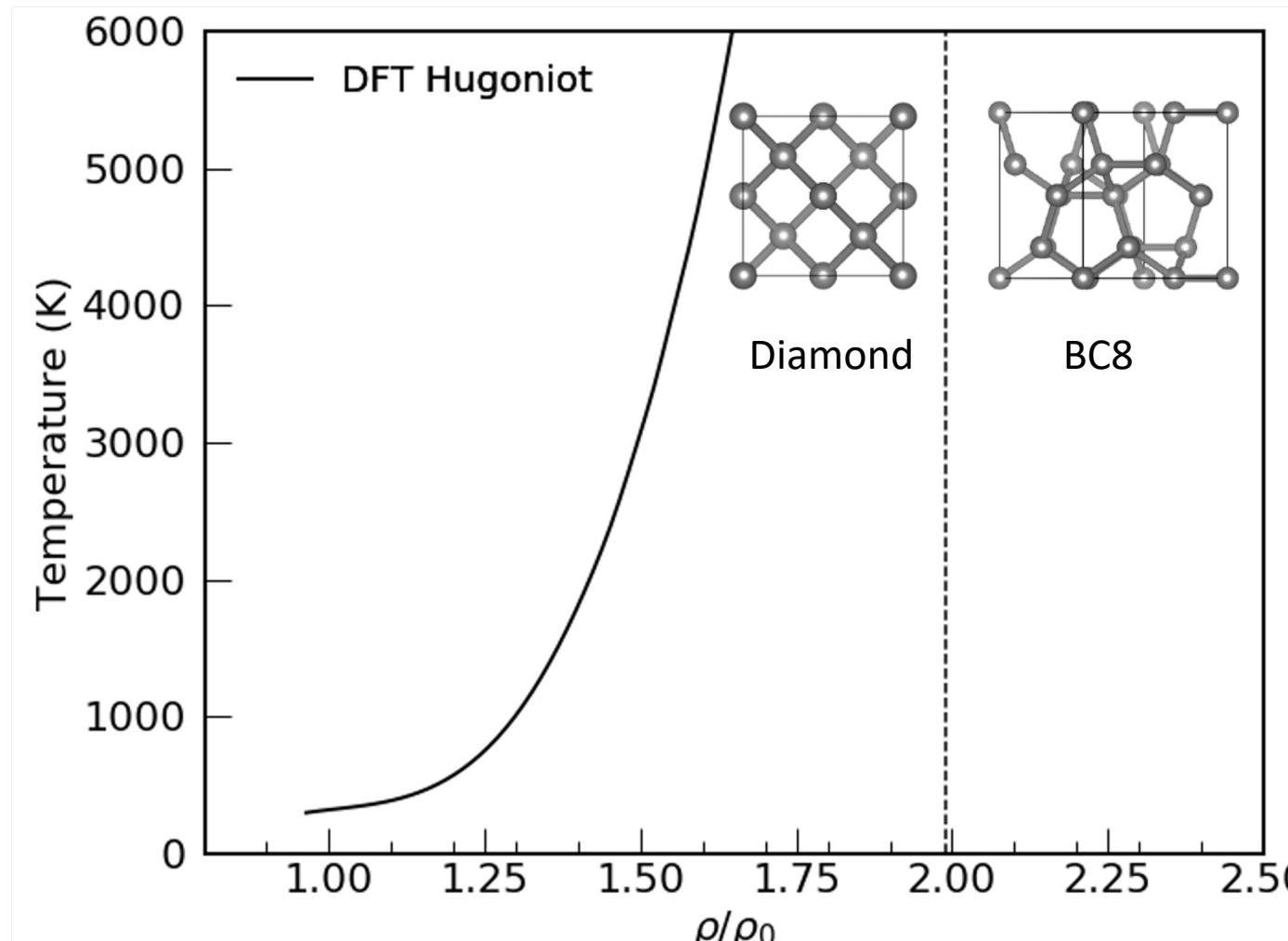
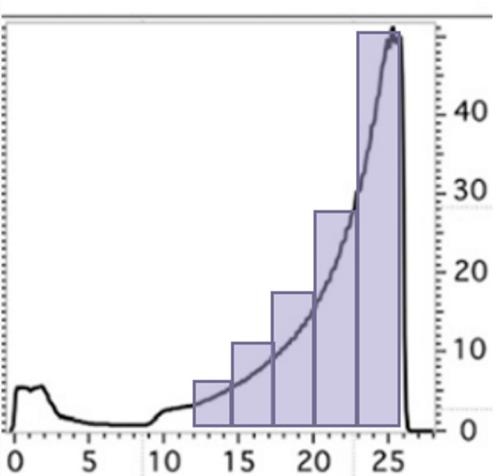
# OUR MODEL

for ramp compression from ab initio simulations



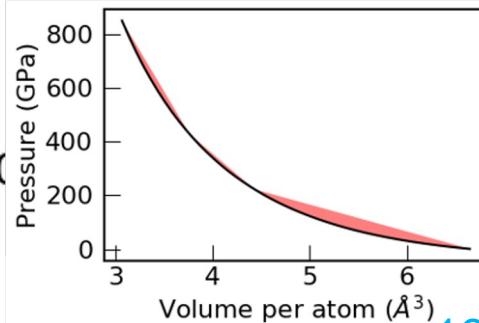
# OUR MODEL

3 steps



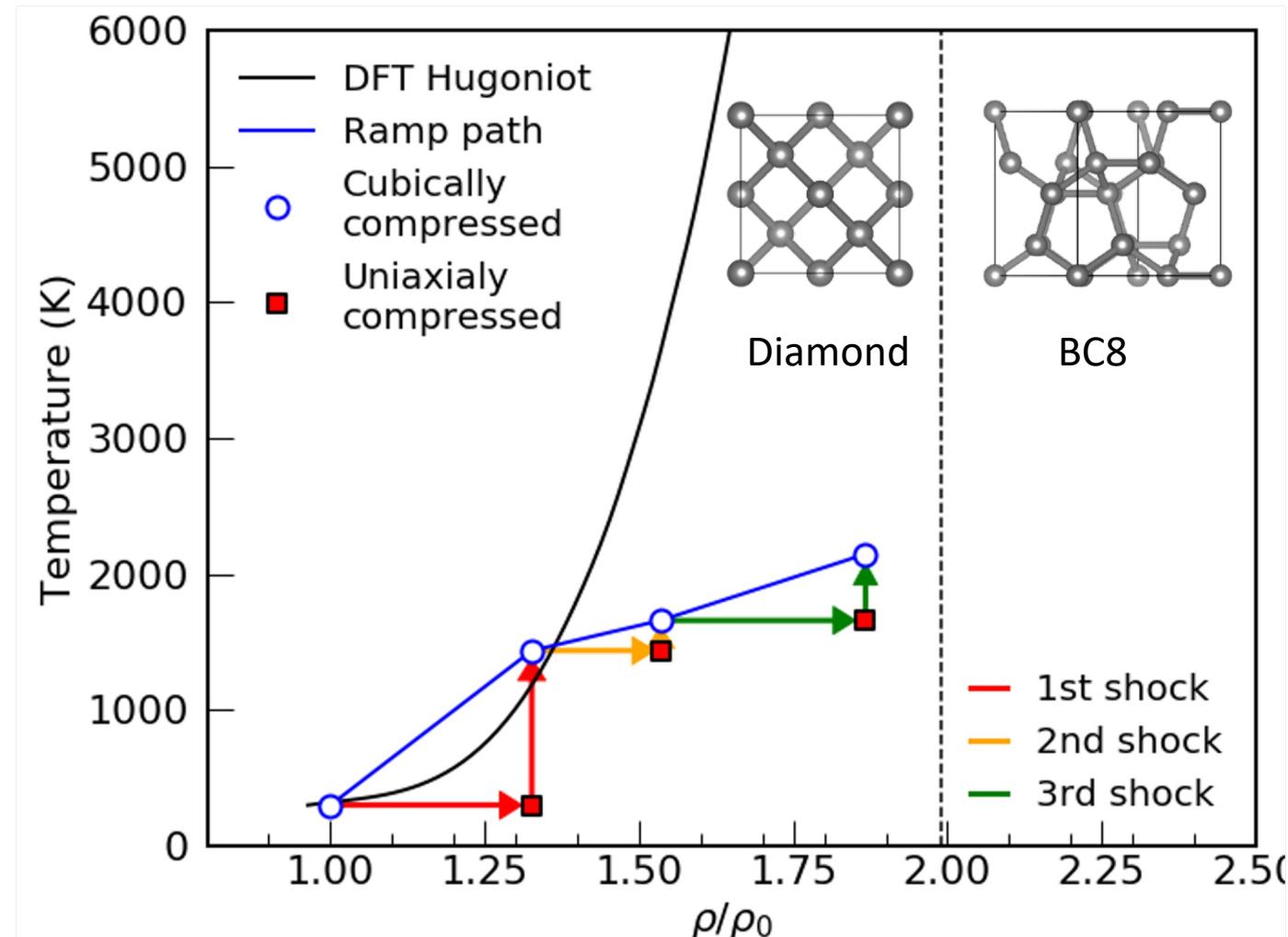
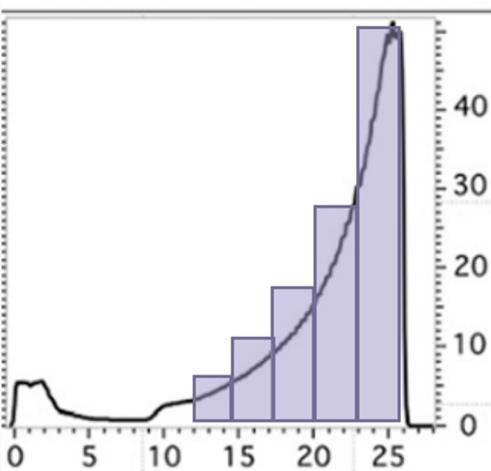
3 shocks:

- 0 GPa
- ↓  
200 GPa
- ↓  
400 GPa
- ↓  
800 GPa



# OUR MODEL

3 steps

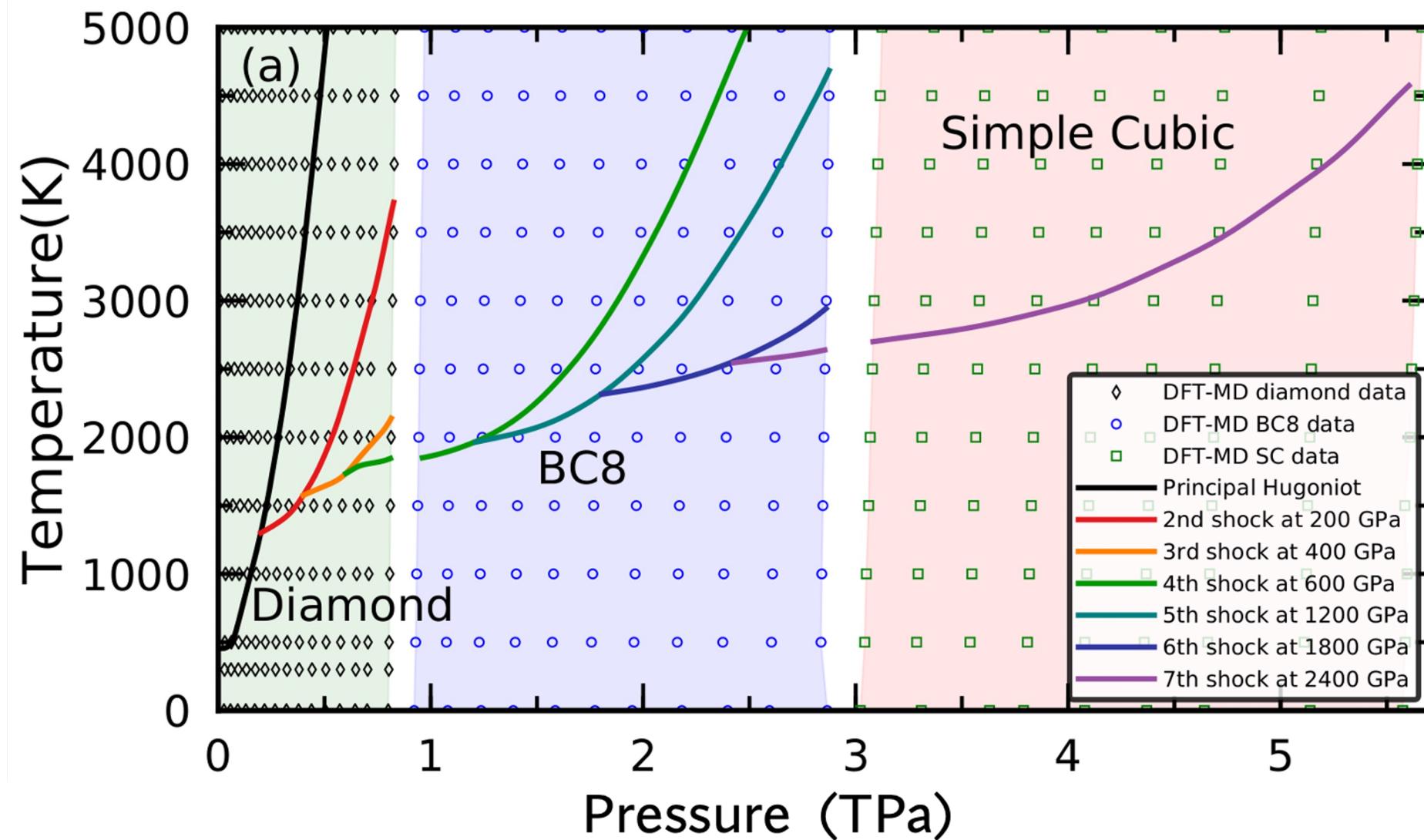


3 shocks:

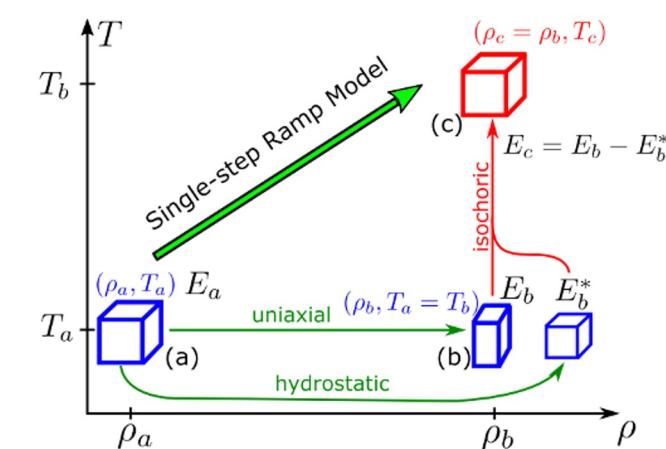
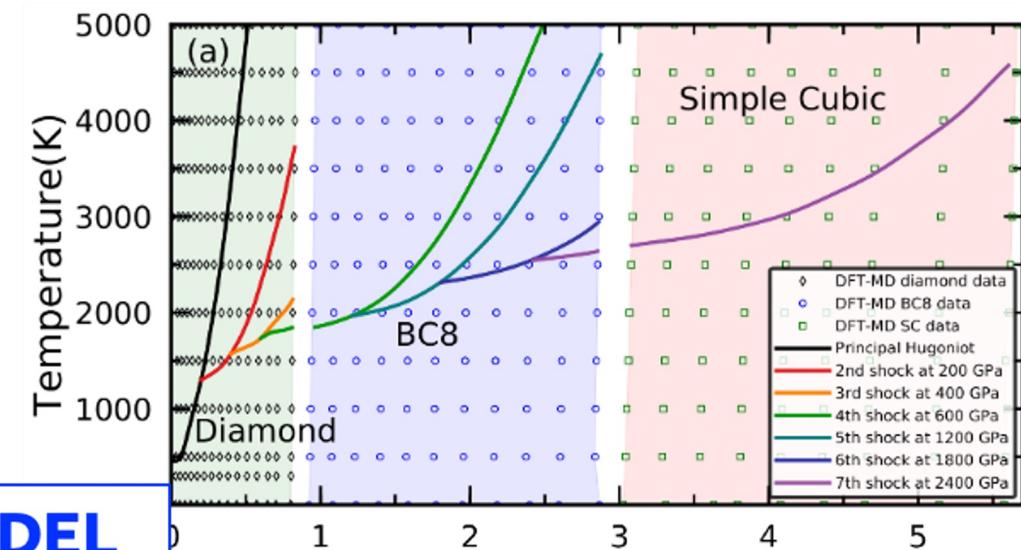
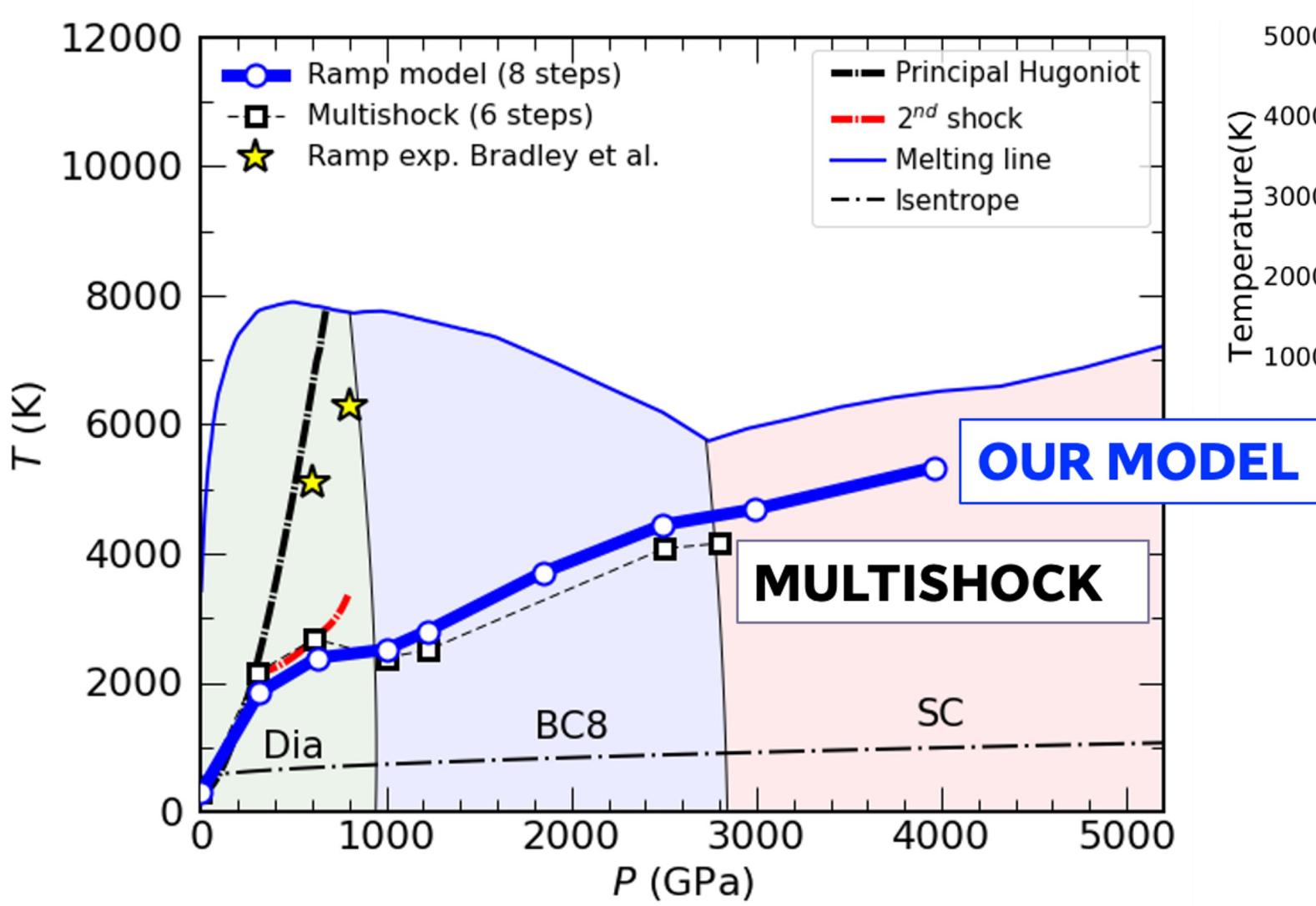
- 0 GPa
- 200 GPa
- 400 GPa
- 800 GPa

# MULTISHOCKS

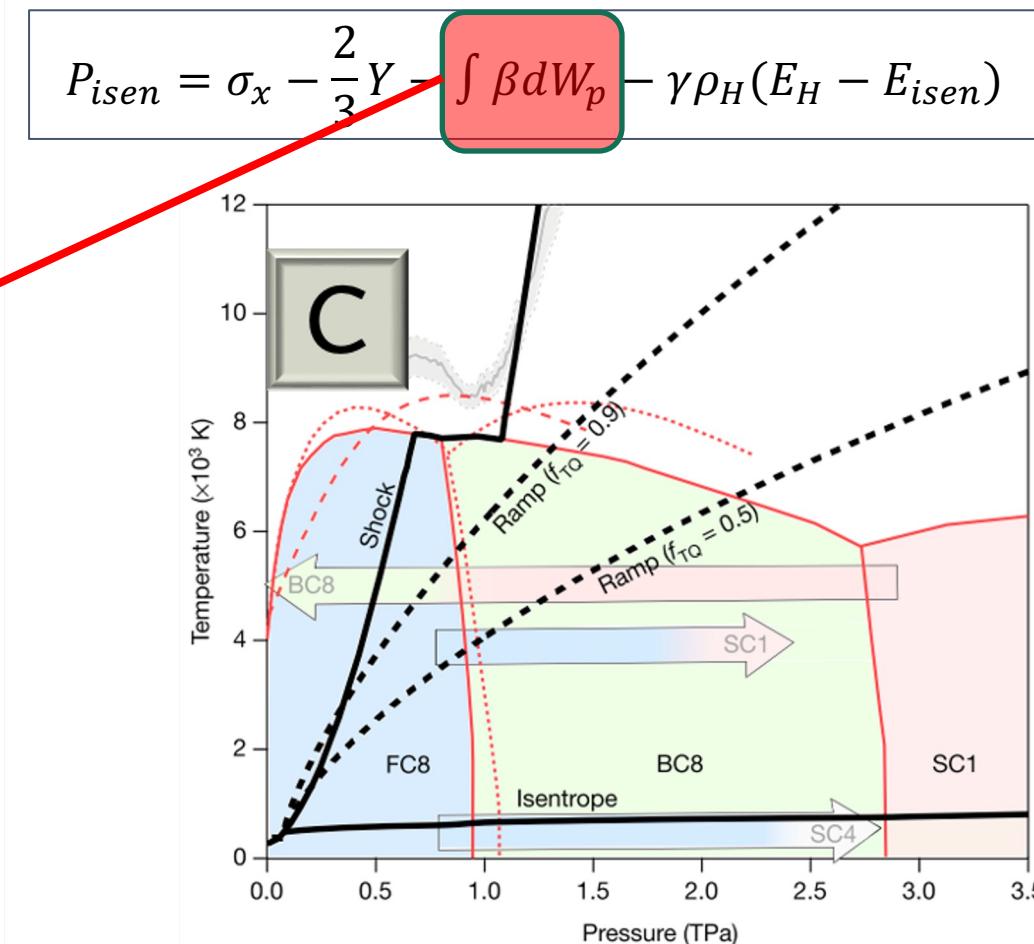
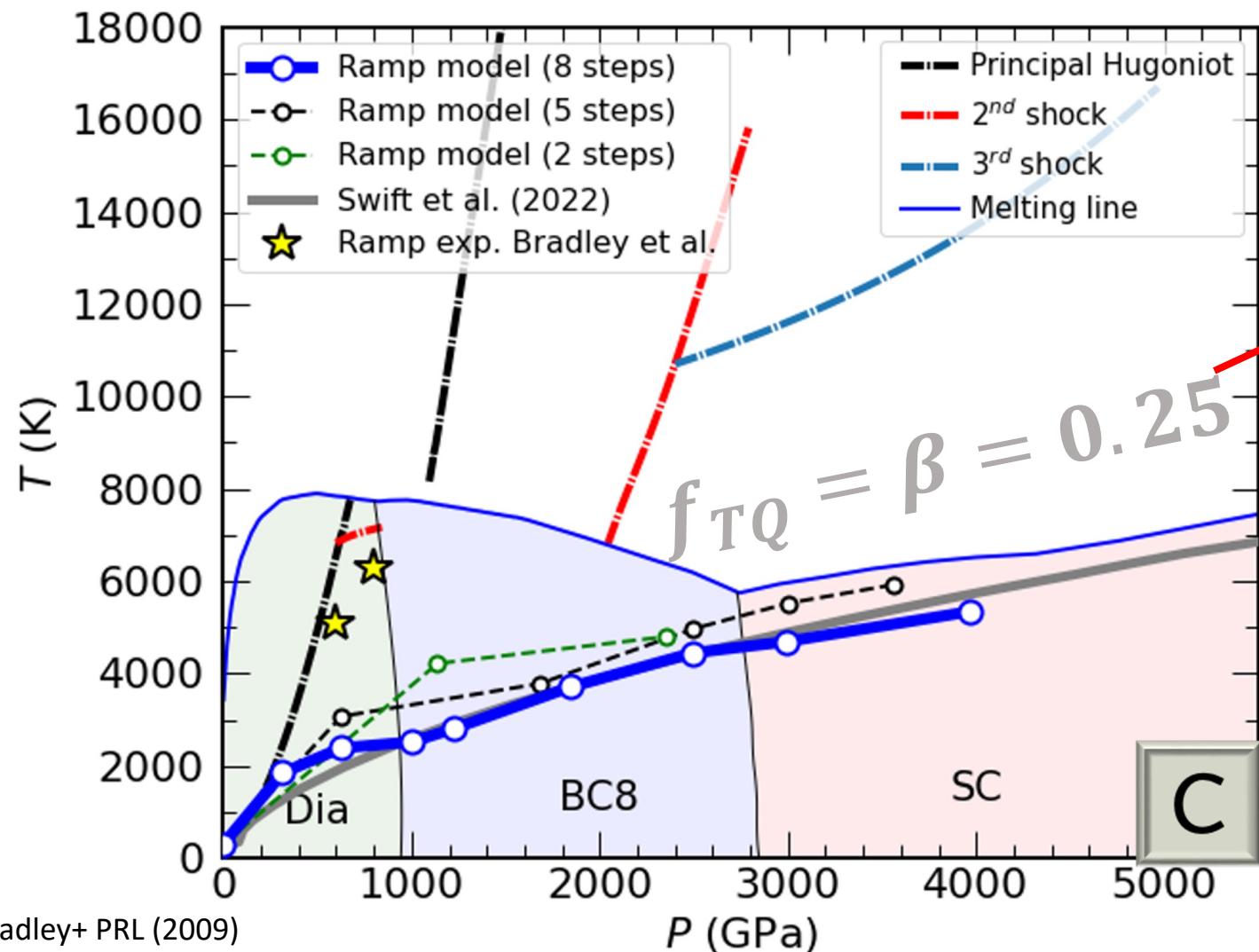
Testing  
our  
model



# MULTISHOCKS / OUR MODEL



# MULTISHOCKS / OUR MODEL



\* Diamond is weaker than expected  
\* 3/4 plastic work absorbed by defects!

# CONCLUSIONS

1. Our model & Multishock Hugoniots &  $f_{TQ}$  are consistent.
2. Experiment/EOS discrepancies:
  - $T \rightarrow$  liquid
  - High strain
  - Porosity
3. Plastic work energies ~ Our model (uniax. vs. hydro.)



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## Special Issue “First Principles Simulations of Minerals”

### Keywords

- High pressure
- High temperature
- First principles
- Density Functional Theory
- Ab initio
- Planetary interiors
- Condensed matter physics
- Phase diagrams
- Molecular dynamics
- Hugoniot curve



# THANKS!



[mdpi.com/si/119387](https://mdpi.com/si/119387)

## Special Issue

Guest Editor:

**Dr. Felipe González Cataldo**

Department of Earth and  
Planetary Science, University of  
California, Berkeley, CA 941720,  
USA

f\_gonzalez@berkeley.edu

Deadline for manuscript  
submissions:

**18 November 2022**

### Message from the Guest Editor

Dear Colleagues,

The purpose of this Special Issue is to highlight recent advances and examine future directions in the study of minerals relevant to geophysics and planetary science using first principles techniques. Examples include high pressure transitions, melting curves, equations of state, phase diagrams, elastic, and transport properties. As these properties remain largely unconstrained at high pressure and temperature, particular emphasis will be sought in this regime, as they can unfold the physics of planetary interiors.

The combination of different approaches (e.g., Density Functional Theory, Path Integral Monte Carlo, Quantum Monte Carlo, etc.) and comparison with available experimental results are critical to assess the validity of predictions from first principles. Therefore, benchmarking predictions of density functionals with more sophisticated theories is encouraged. This Special Issue covers all aspects of first principles calculations applied to minerals, with an emphasis in applications to planetary science, understanding basic physics at high pressure, numerical methods, and novel approaches.