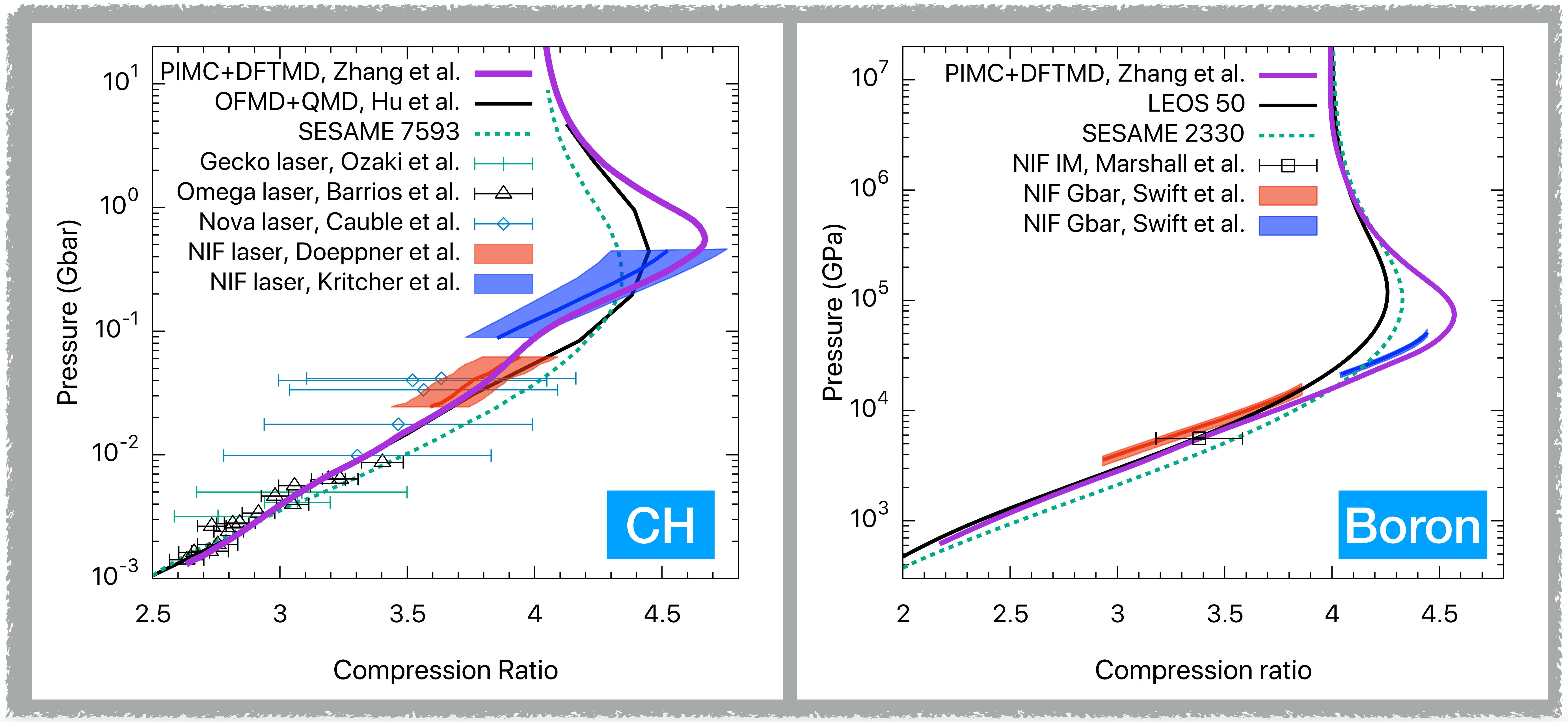
WIDE-RANGE EOS OF C- AND B- MATERIALS FROM FIRST PRINCIPLES



1 Gbar=10^3 Mbar=100 TPa=10^5 GPa

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Laboratory for Laser Energetics

APS DPP Meeting
Fort Lauderdale, FL
October 22, 2019

COLLABORATORS

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Suxing Hu *(University of Rochester)*

Walter Johnson *(University of Notre Dame)*

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We have used first-principles methods (PIMC, DFT-MD, etc) that fully capture the microscopic physics (e.g., ion thermal interaction and atomic shell effects) to calculate the EOS

- We have obtained self-consistent EOS data for ablator materials (CH, B, BN, B_4C) over wide T (10^3—10^8 K), ρ (0.1—100 g/cm^3) regimes
- Our predicted Hugoniots agree very well with experiments, and have compression maxima (due to K shell ionization) that are significantly sharper than Thomas-Fermi/orbital-free predictions
- Our computed EOS, together with experimental data, set constraints for the construction of EOS tables and clarification of their roles in ICF/HED experiments via hydro simulations

References:

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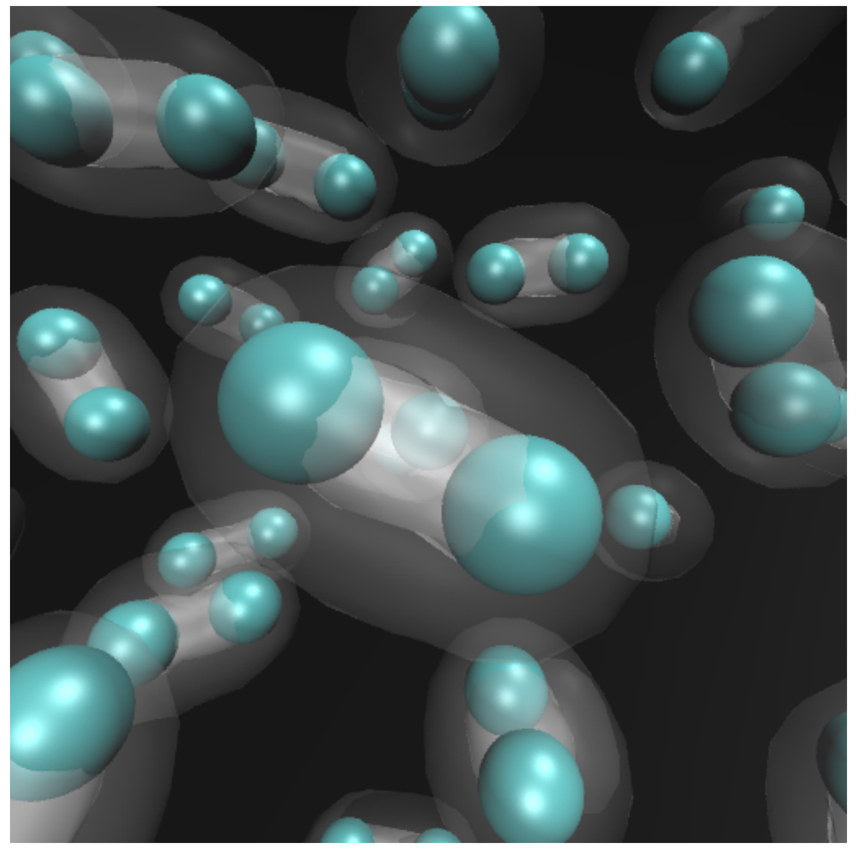
B: Zhang et al., Phys. Rev. E **98**, 023205 (2018)
BN: Zhang et al., Phys. Rev. B **99**, 165103 (2019)
B_4C: Zhang et al., to be published.

WE COMBINE QUANTUM-MECHANICAL METHODS TO CALCULATE THE EOS



DFT-MD: for low-T

$$M_I \ddot{\boldsymbol{R}}_I = -\frac{\partial E}{\partial \boldsymbol{R}_I} = \boldsymbol{F}_I\left[\{\boldsymbol{R}_J\}\right]$$

$$\hat{H}\psi_i(\boldsymbol{r}) = \varepsilon\psi_i(\boldsymbol{r})$$

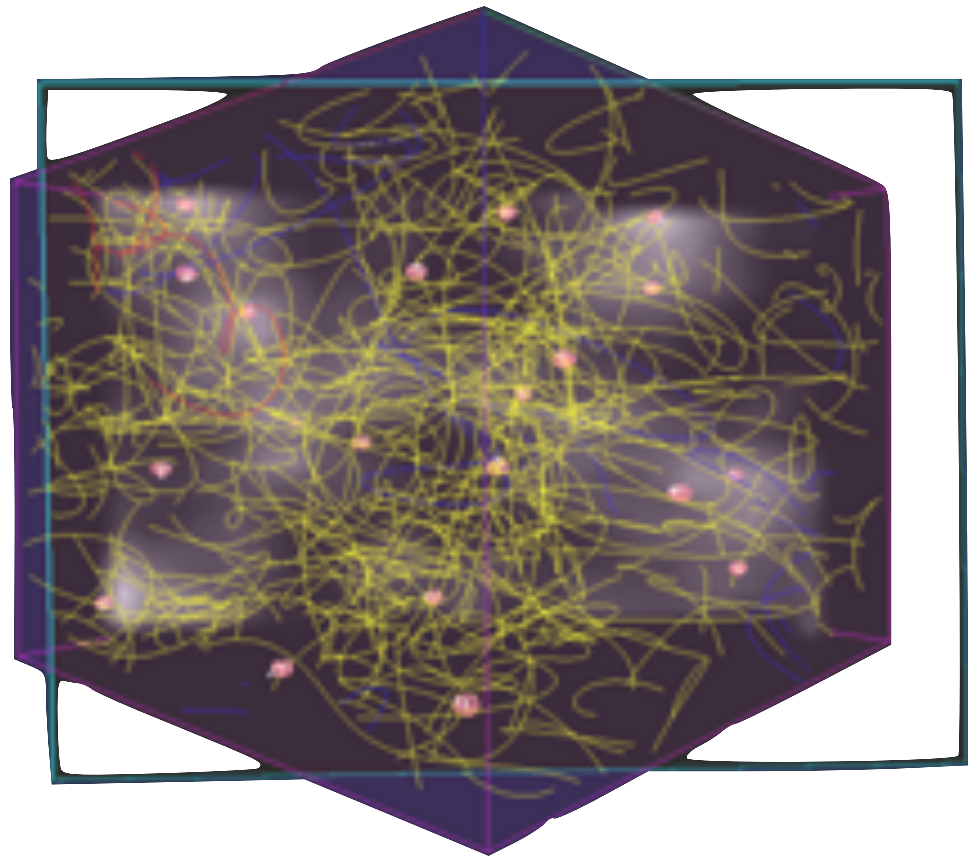
PIMC: for high-T

$$\langle O \rangle = Z^{-1}\int d\mathbf{R}d\mathbf{R}'\rho\left(\mathbf{R},\mathbf{R}';\beta\right)\left\langle \mathbf{R}\,|\,\hat{O}\,|\,\mathbf{R}'\right\rangle$$

$$\rho\left(\mathrm{R},\mathrm{R}';\beta\right) = \left\langle \mathrm{R}\left|e^{-\beta\hat{H}}\right|\mathrm{R}'\right\rangle \quad e^{-\beta\hat{H}} = \left(e^{-\tau\hat{H}}\right)^M, \tau = \beta/M$$

$$\Downarrow$$

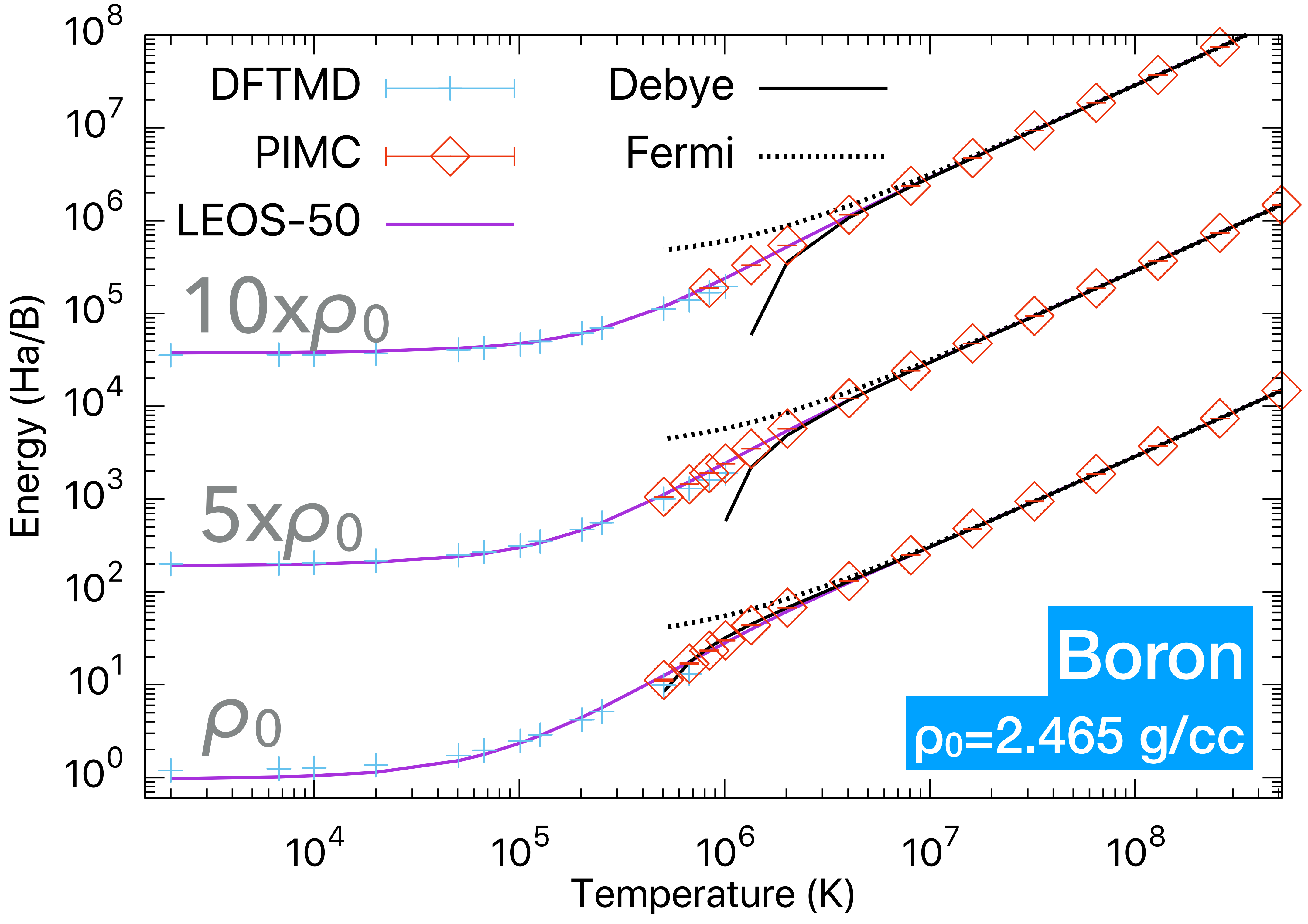
$$\rho\left(\mathrm{R},\mathrm{R}';\beta\right) = \int d\mathrm{R}_1 \ldots d\mathrm{R}_{M-1} e^{-\sum_{m=1}^{M-1} S_m}$$

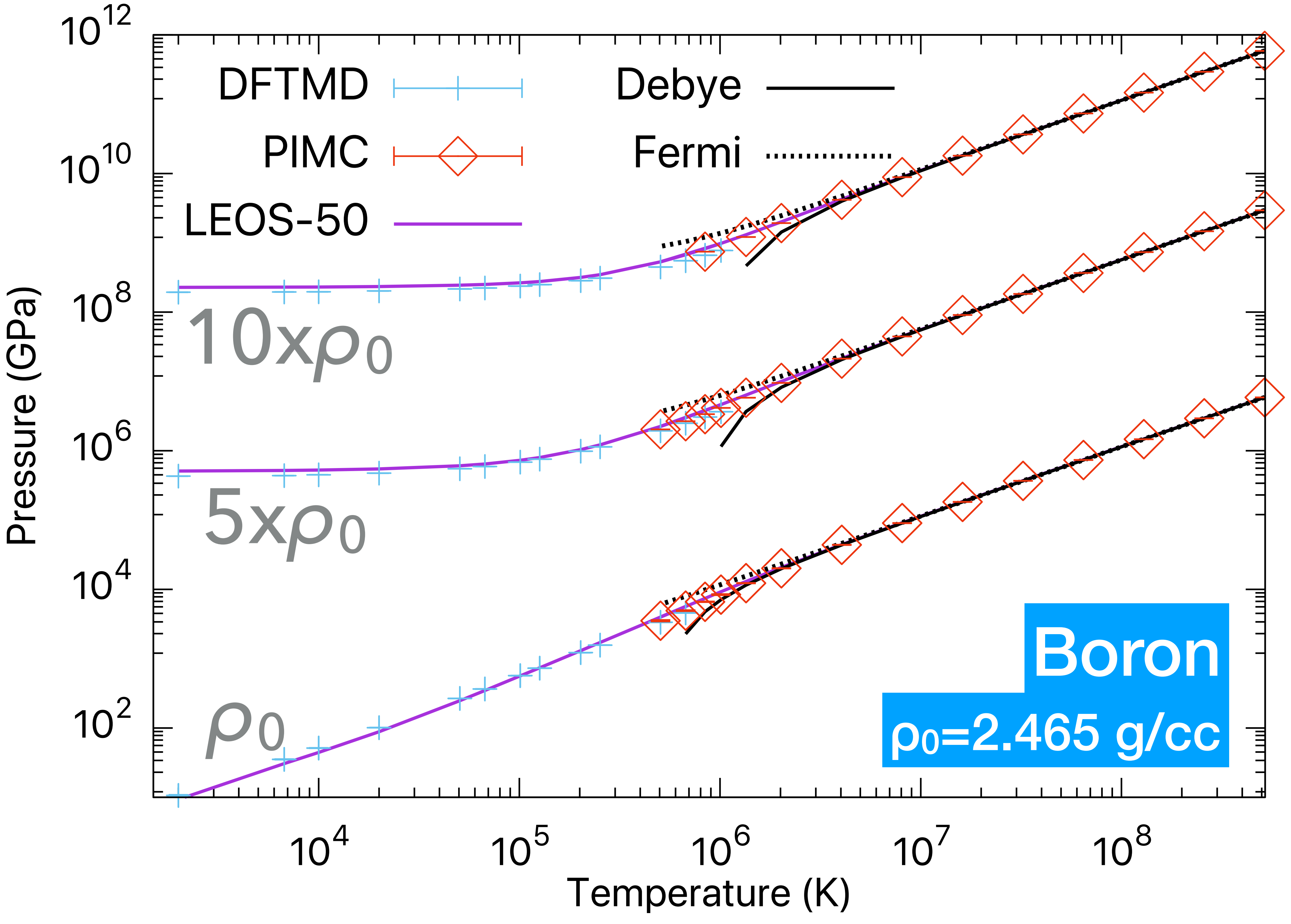


- Born-Oppenheimer Approximation – Classical Ions
- Single-Particle Mean Field Theory, XC
- Pseudopotential: rcore, Zval
- Plane Wave Basis
- **Inefficient or Not-applicable at High *T***

- All Particles Treated as Quantum Paths – Naturally Include Nuclear Quantum Effects
- All-Electron Many-Body Method
- Fermionic Sign Problem – Fixed-node Approximation
- **More Expensive and Less Accurate at Lower *T***

OUR APPROACH PRODUCES ACCURATE, SELF-CONSISTENT, WIDE-RANGING EOS





- * Isochores shifted apart for clarity
- * LEOS 50: based on Thomas-Fermi theory;
- * Debye: Debye-Hückel model; Fermi: ideal Fermi gas

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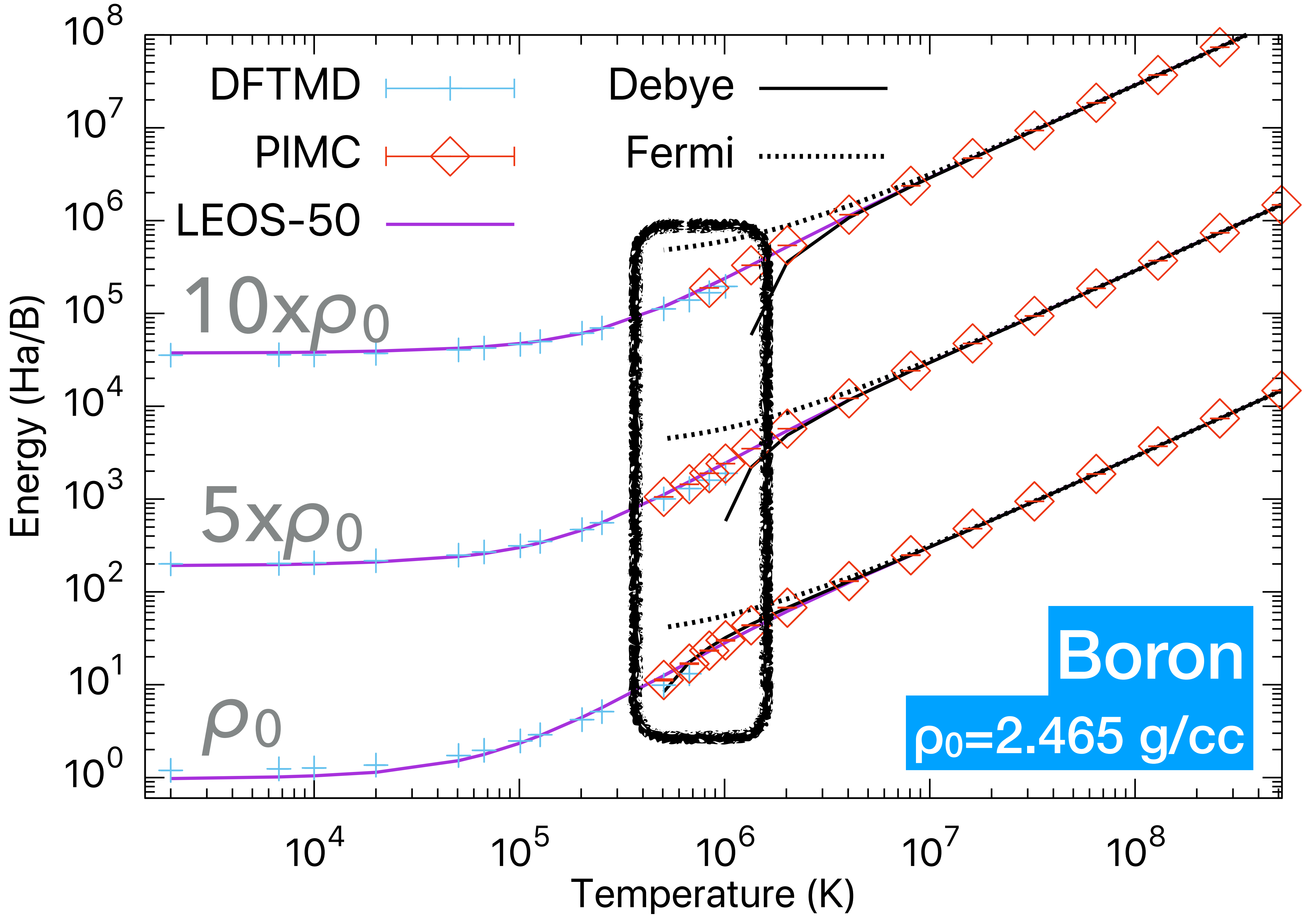

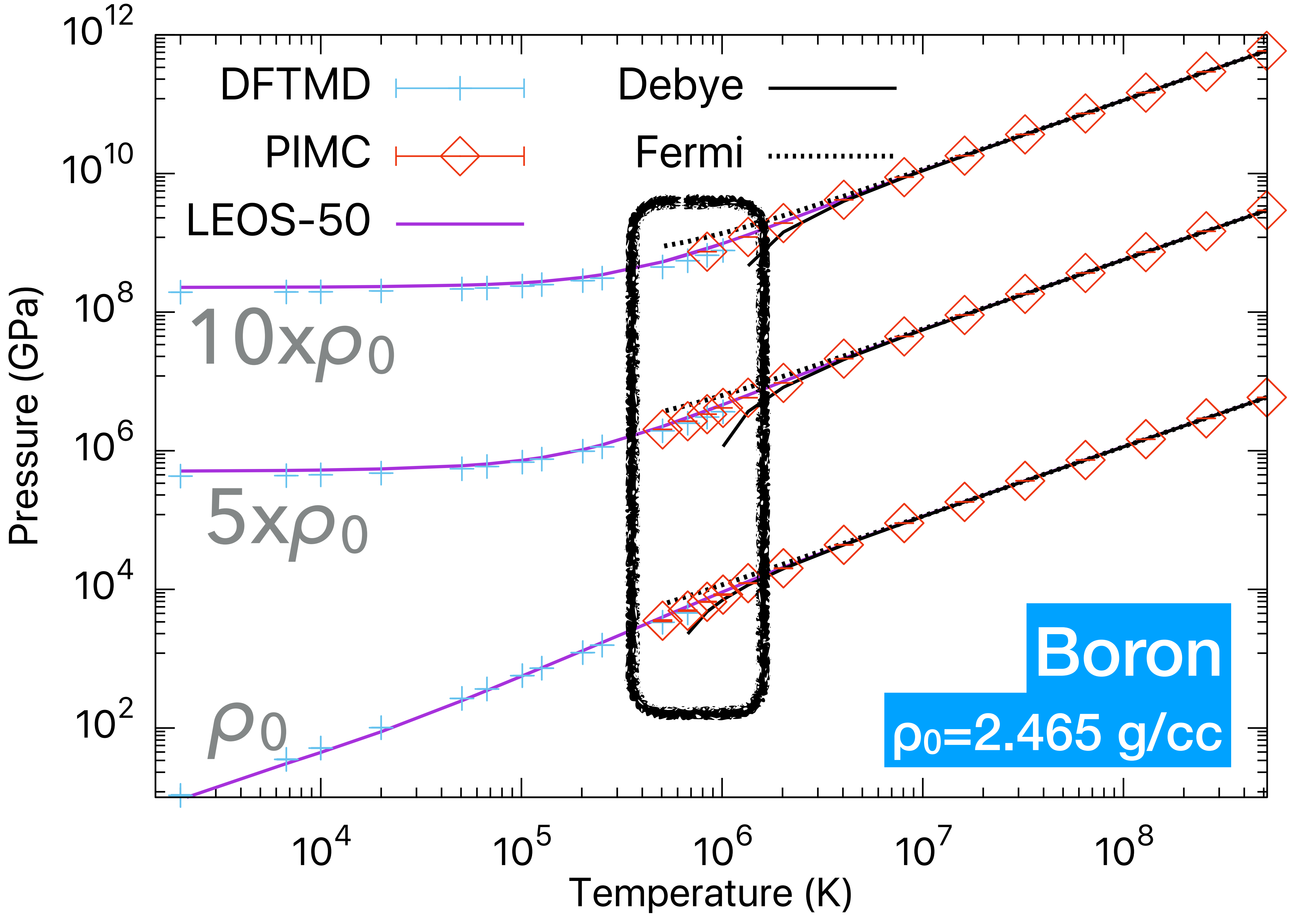

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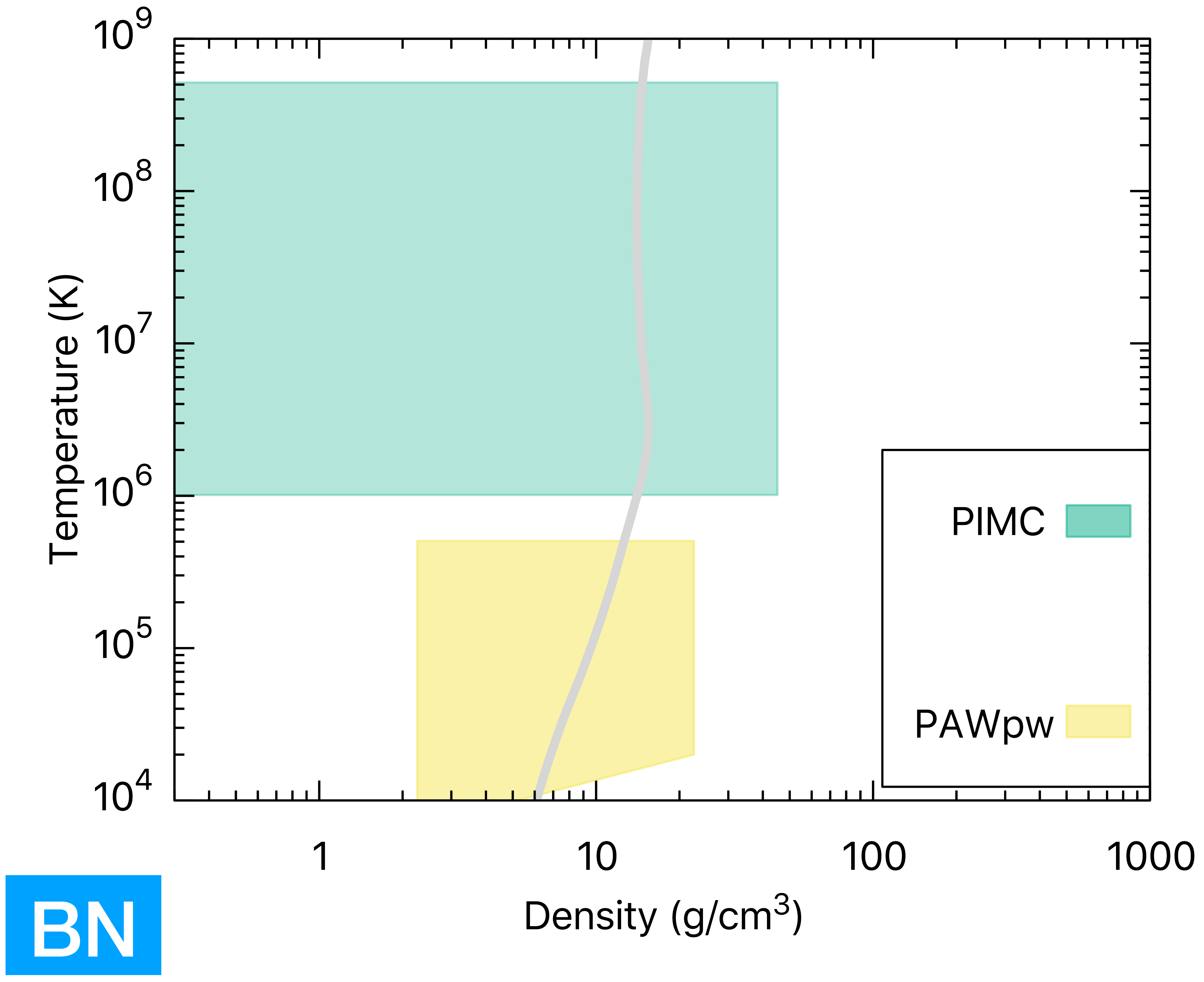
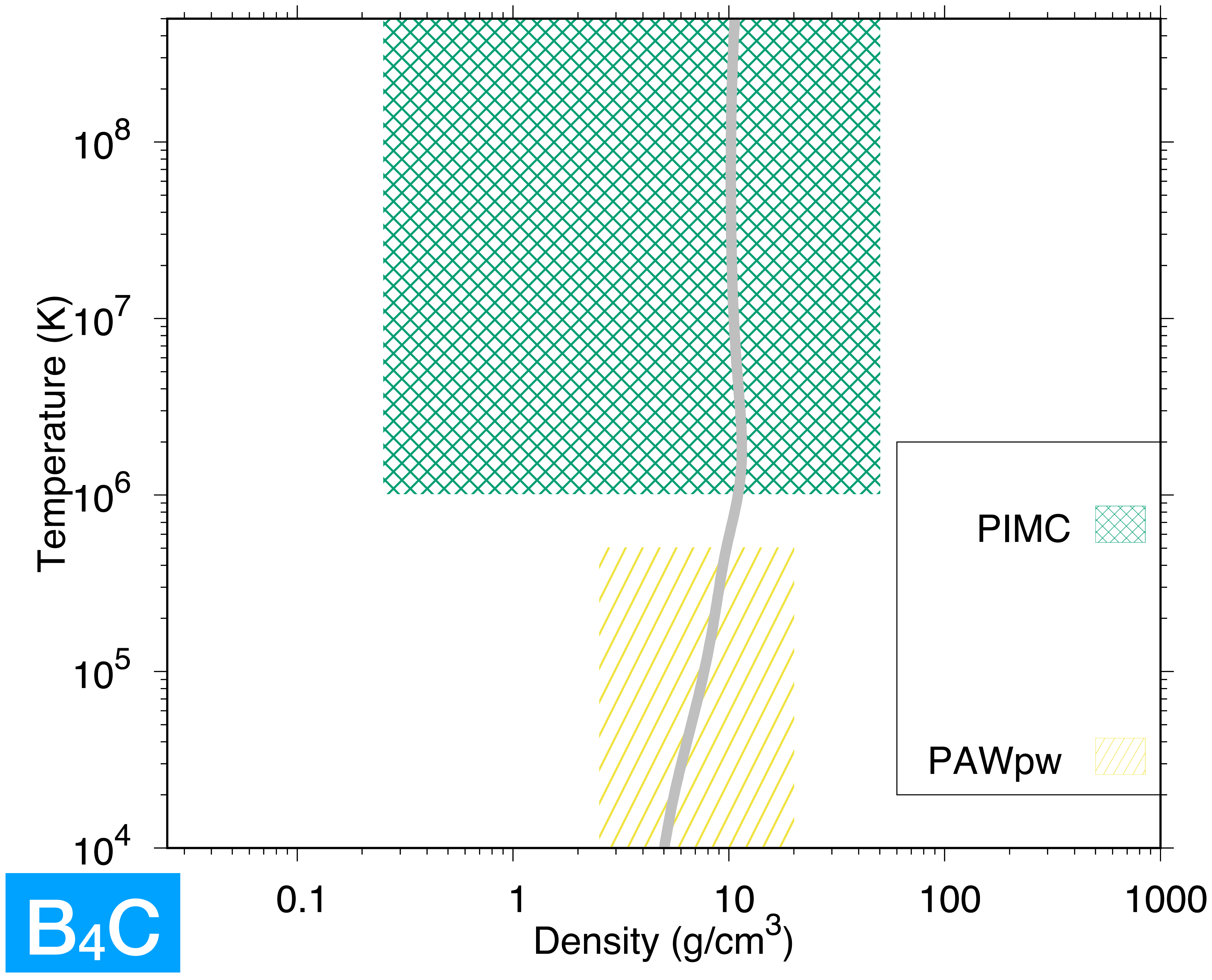
$|\Delta E| < 1.5$ Ha/B, $|\Delta P/P| < 5\%$

Note: 1.5 Hartree/B ≈ 5%*$E_{\text{ideal gas}}$

OUR RECENT DEVELOPMENTS EMPLOY ADDITIONAL METHODS FOR BN & B4C





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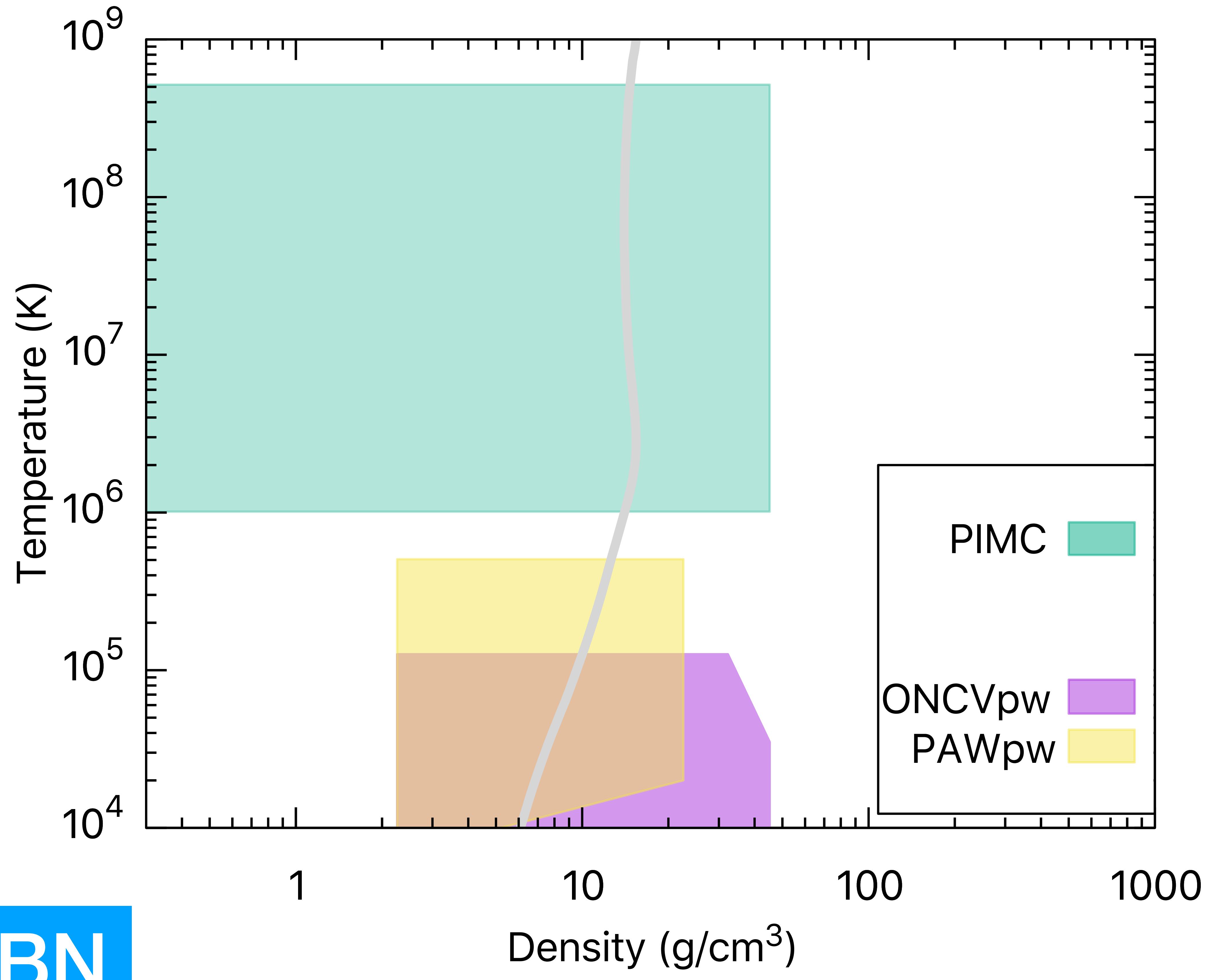
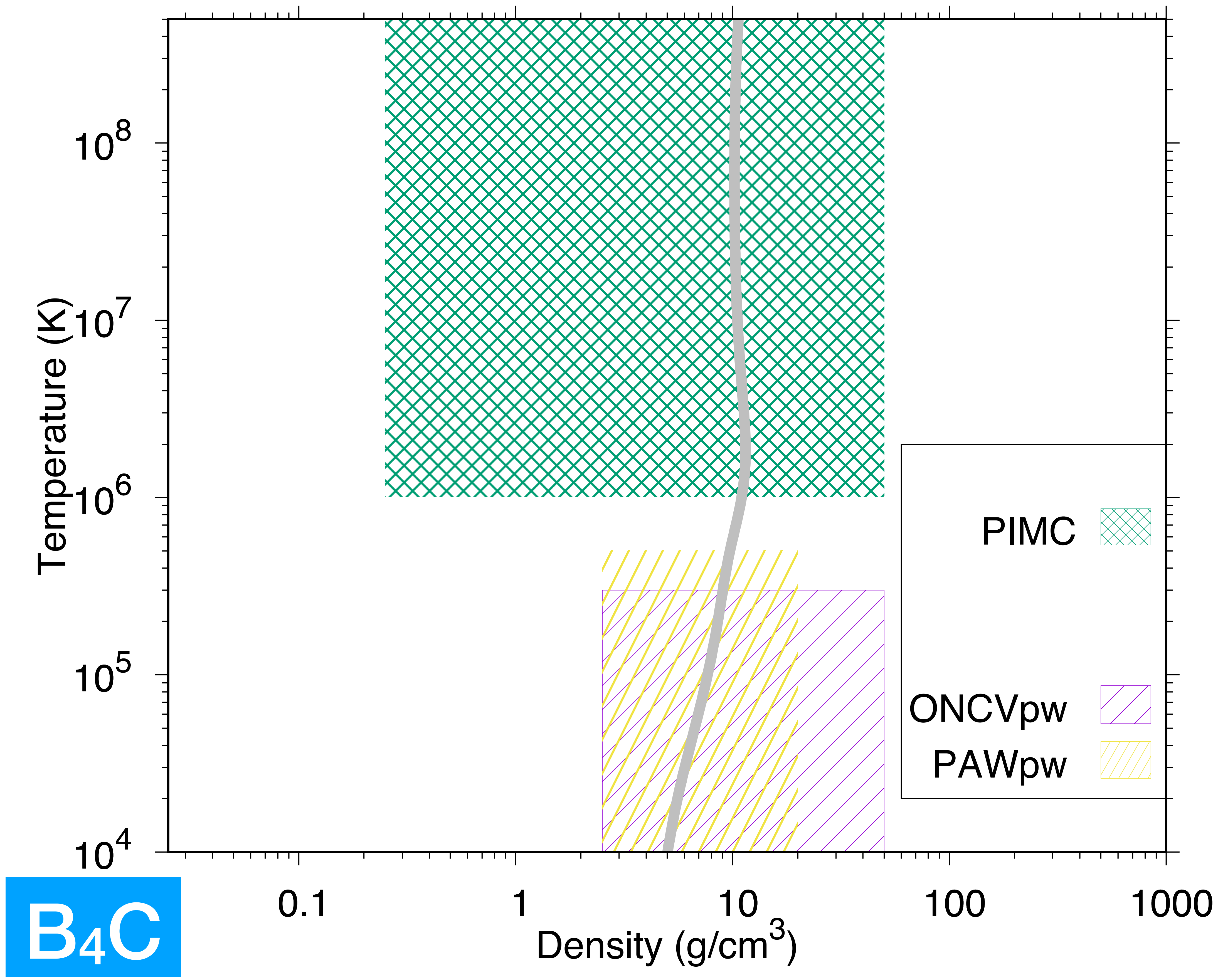


BN



B_4C

* **ONCVpw/PAWpw**: DFT-MD with ONCV/PAW potentials

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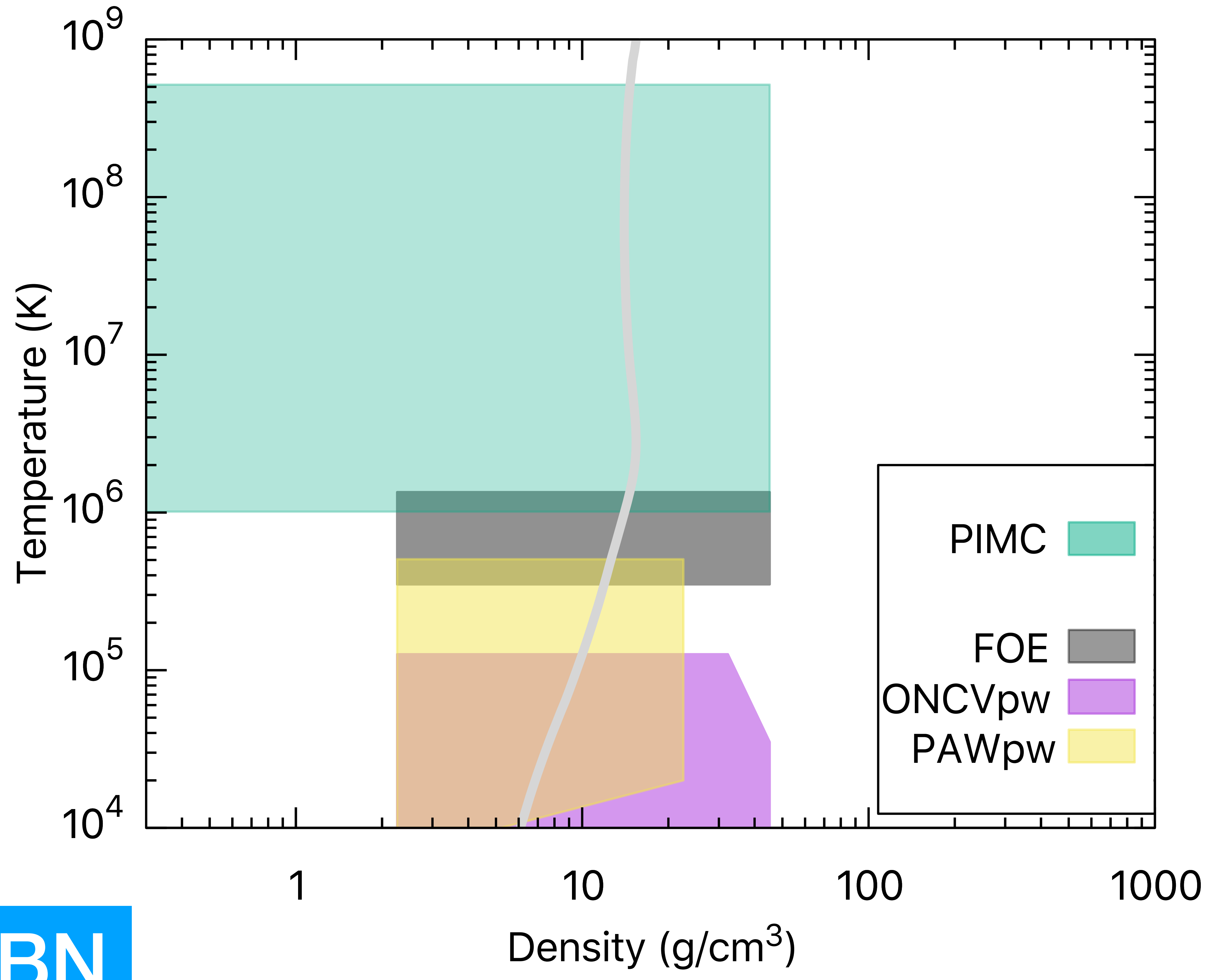

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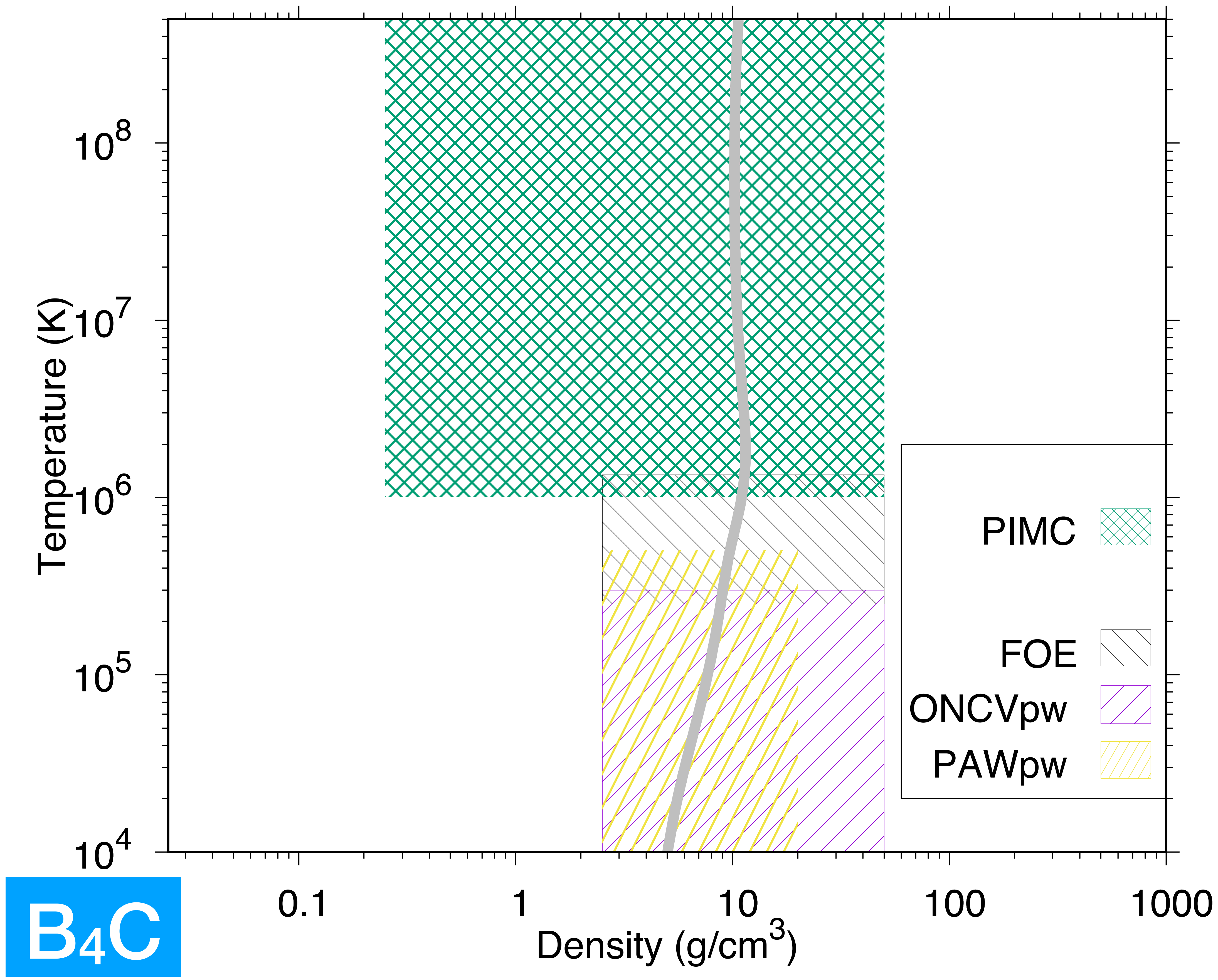

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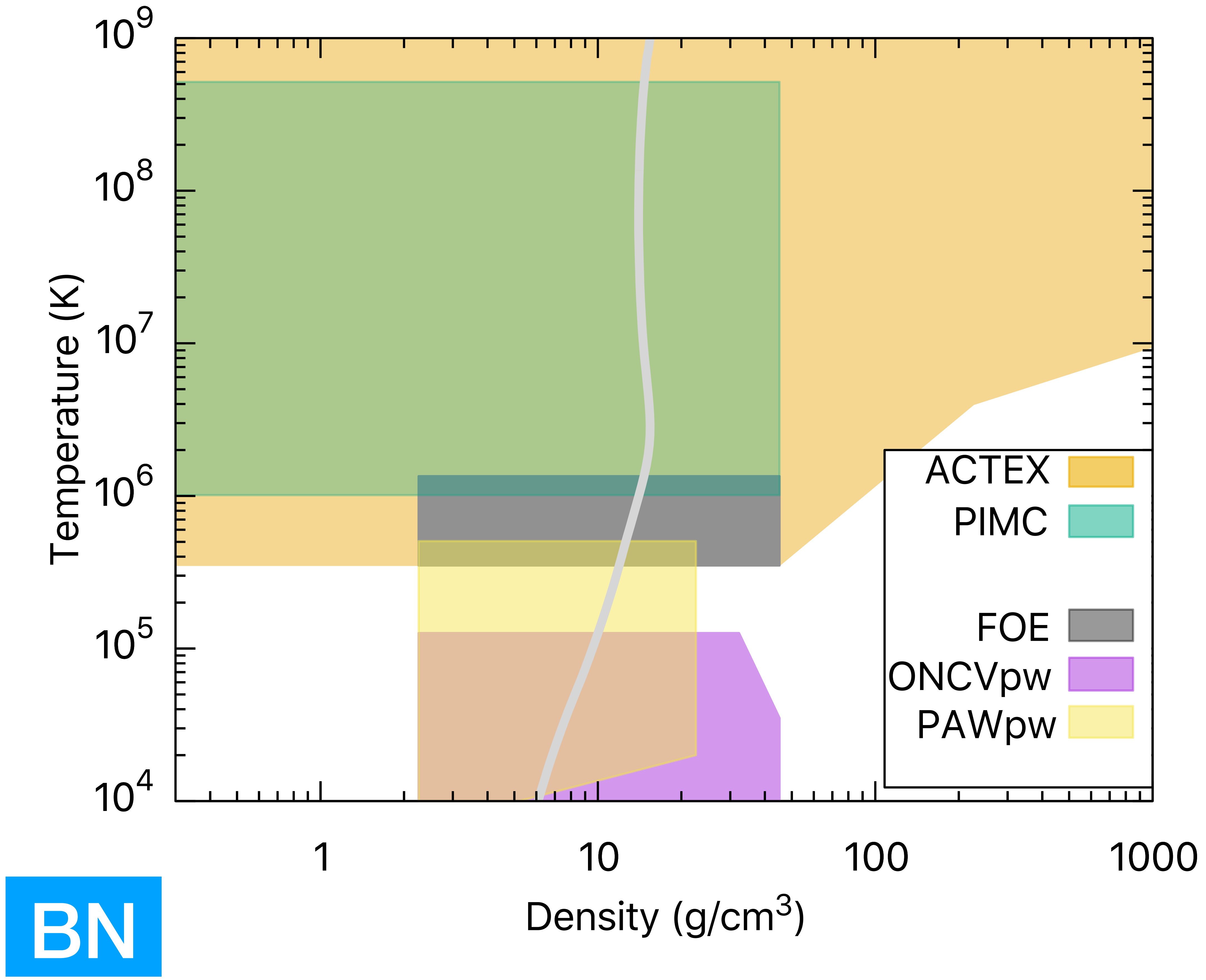

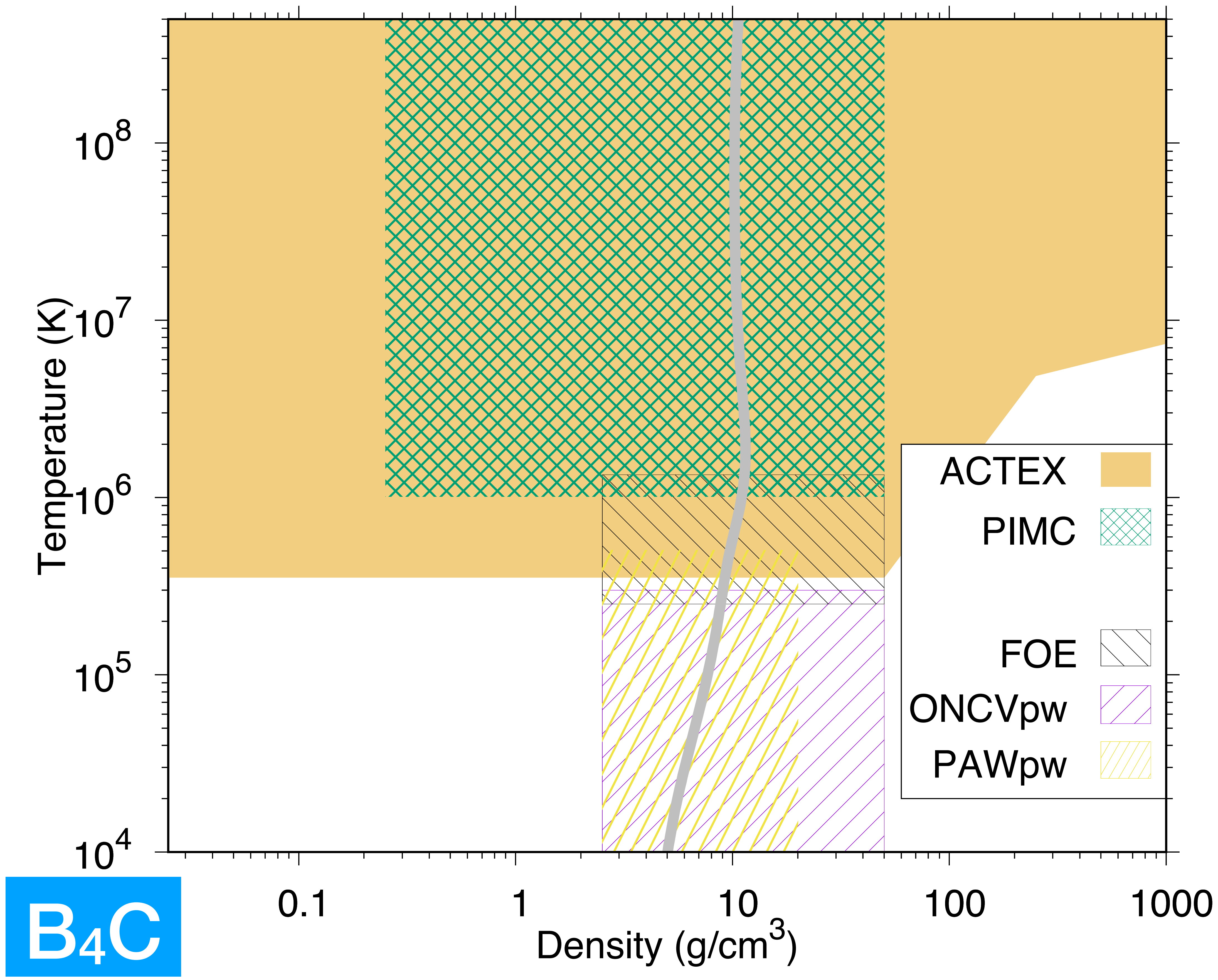

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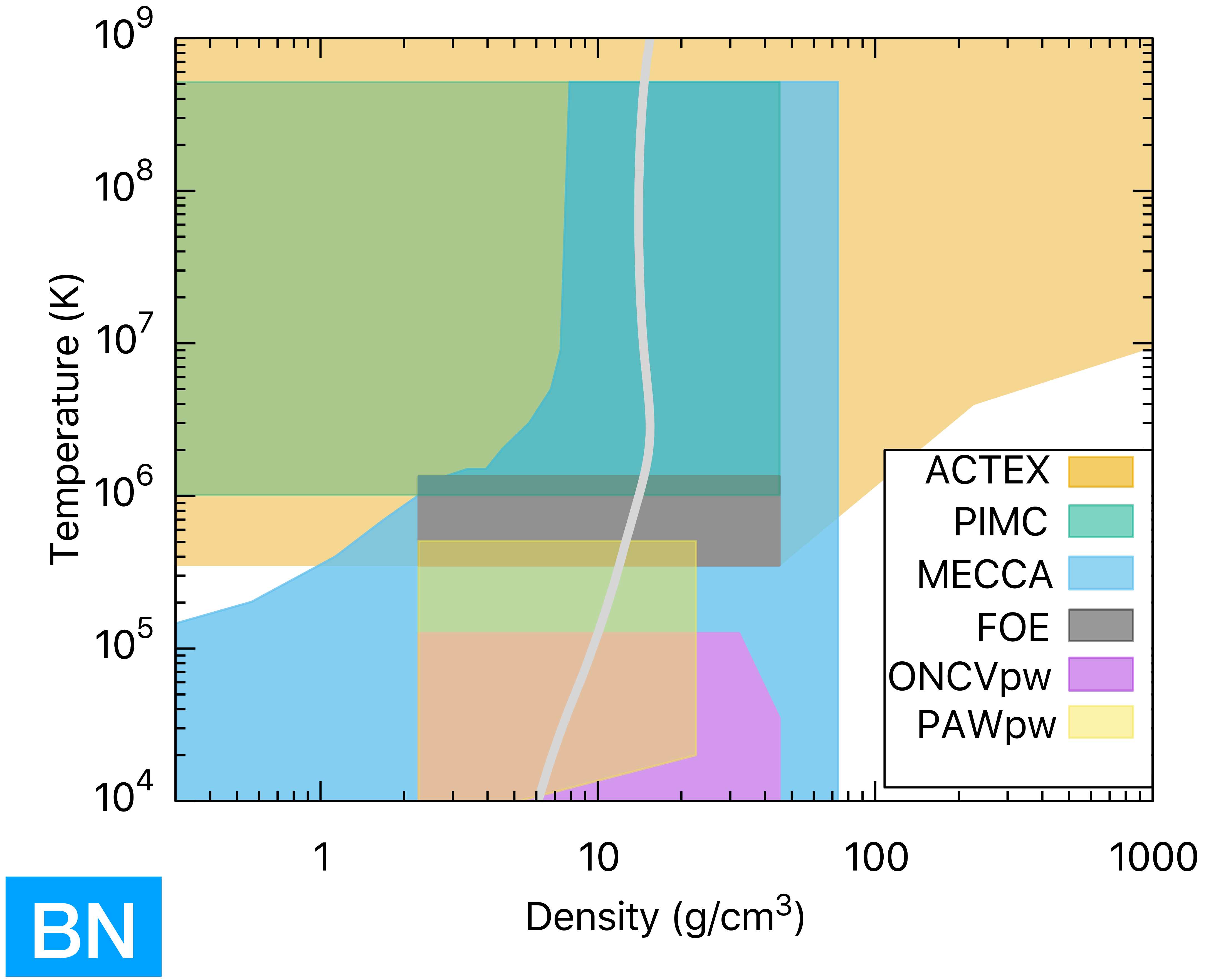

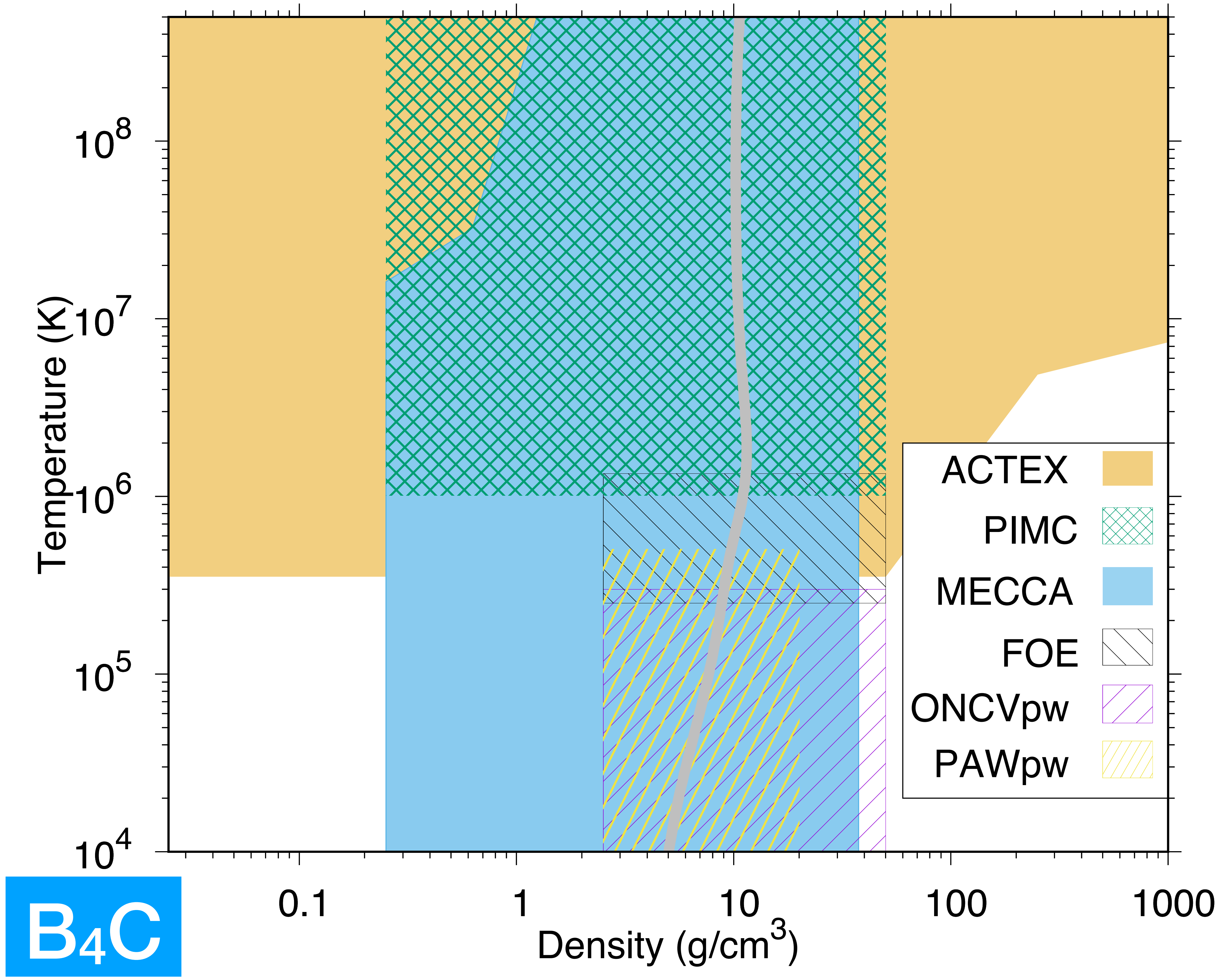

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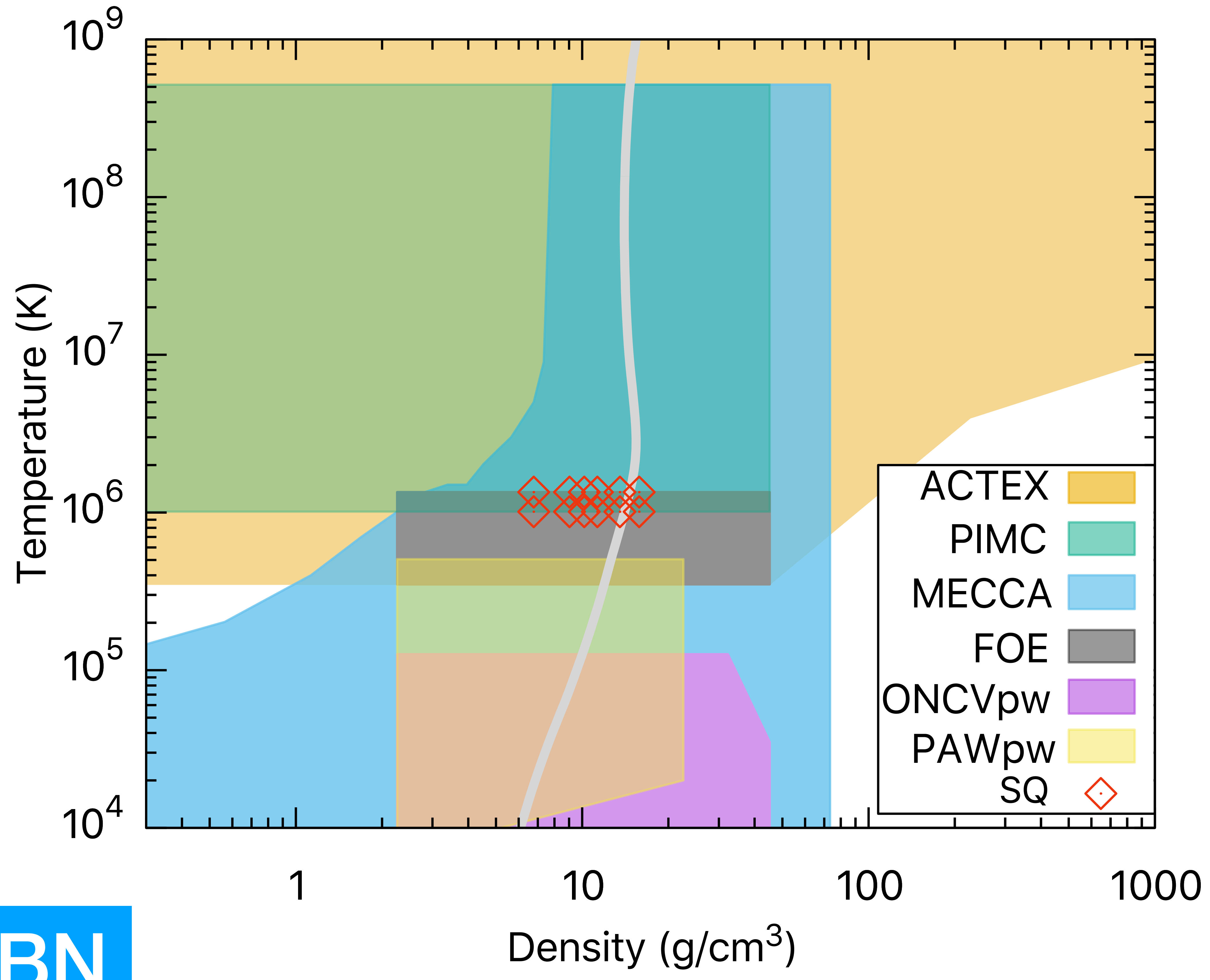

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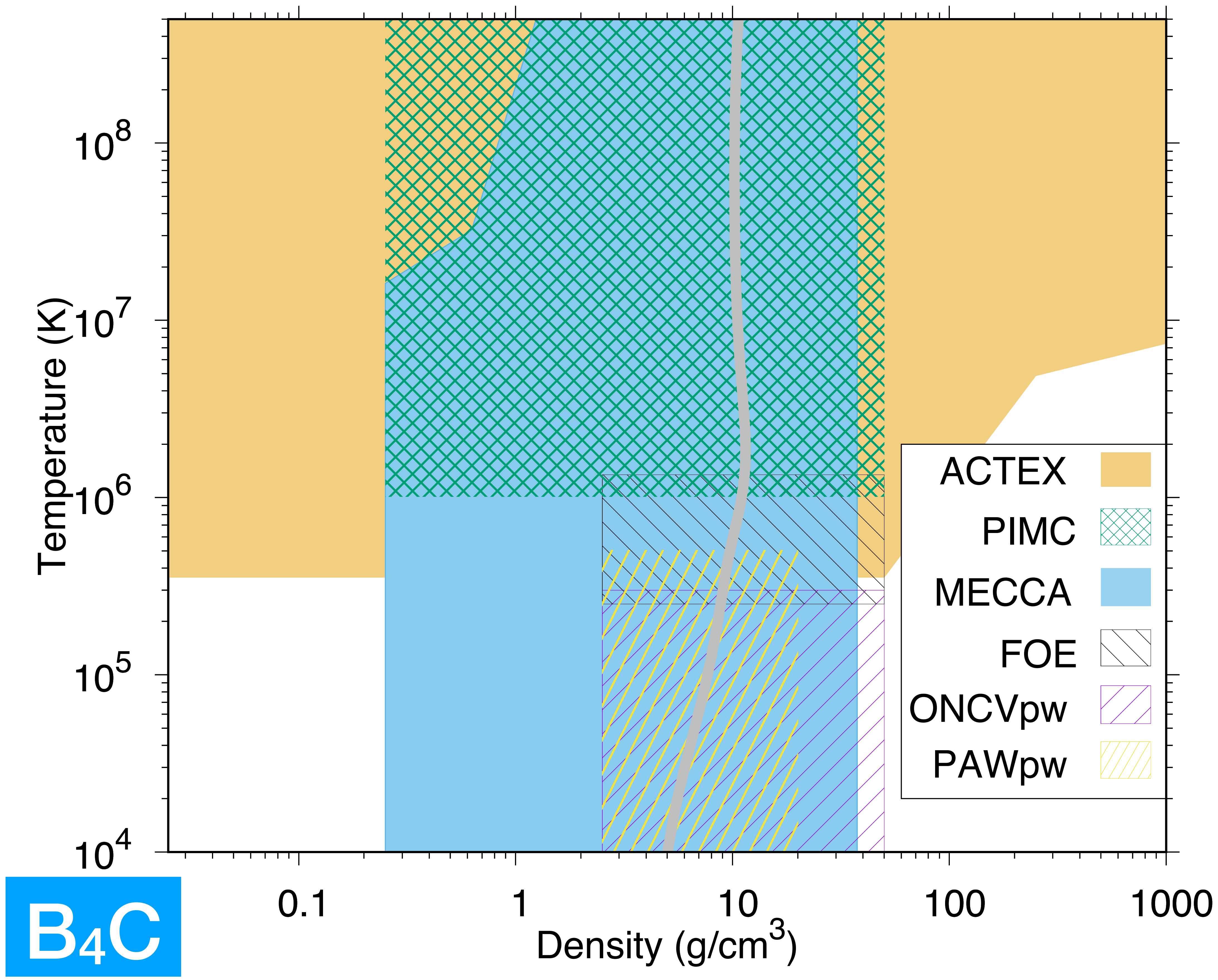

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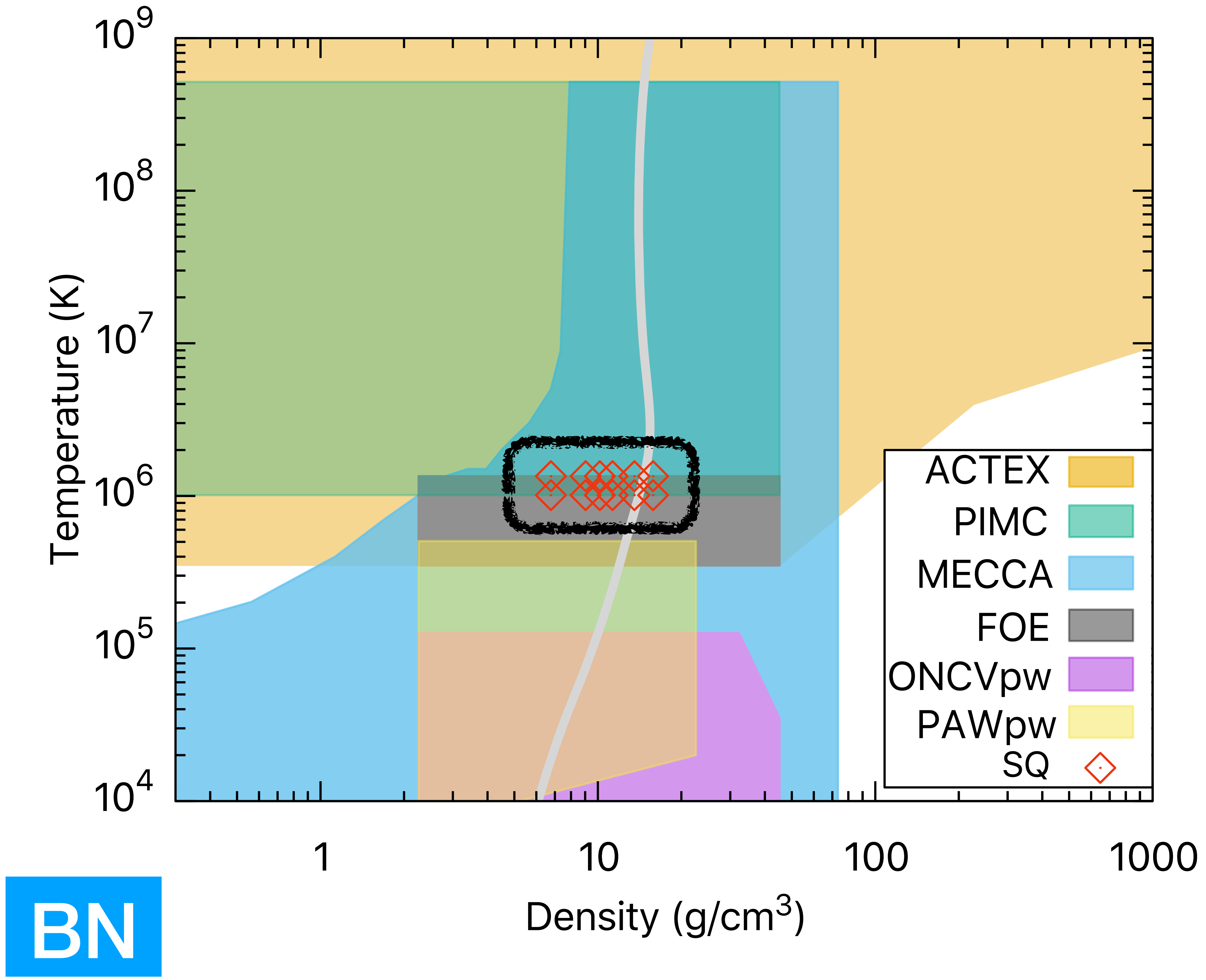

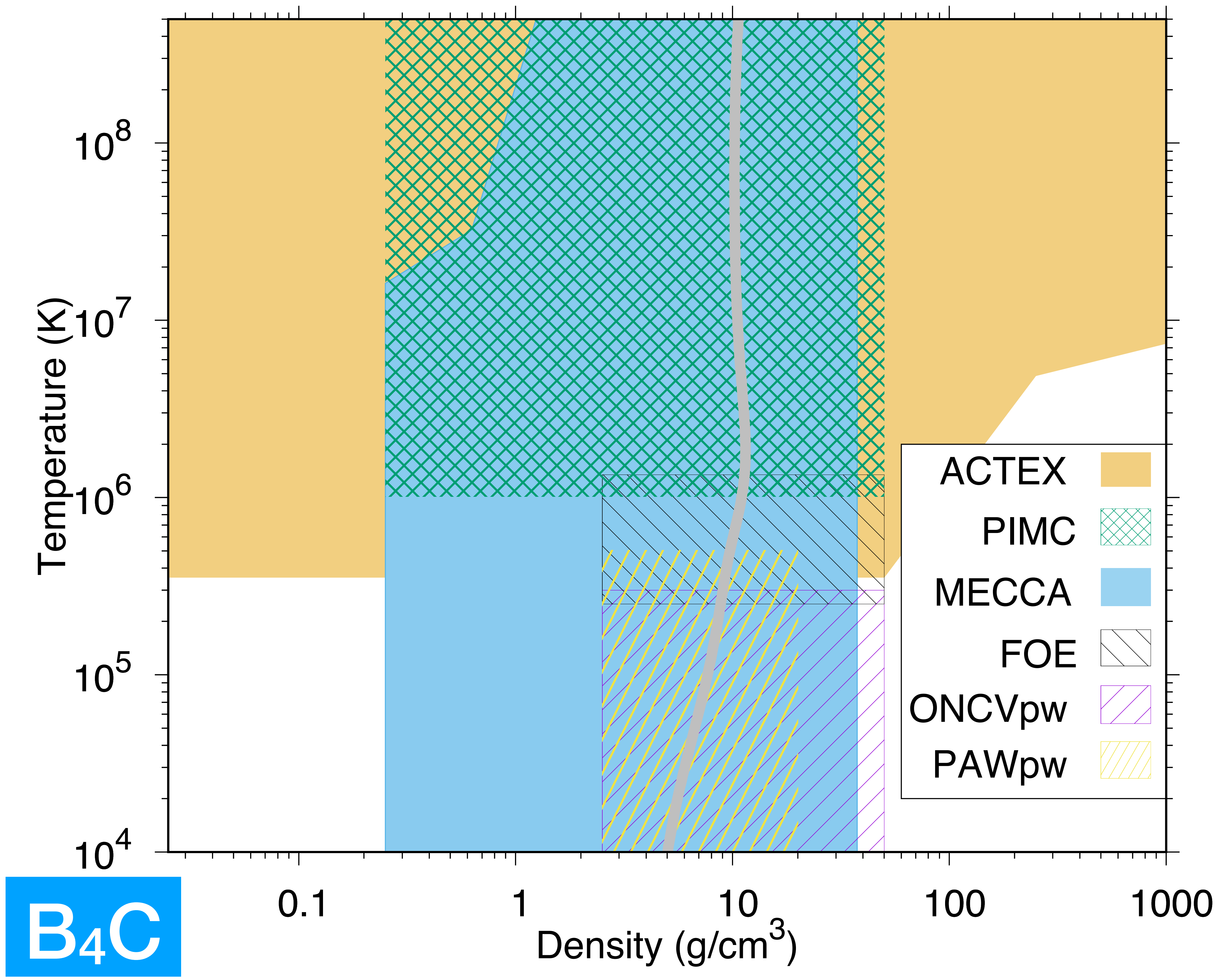

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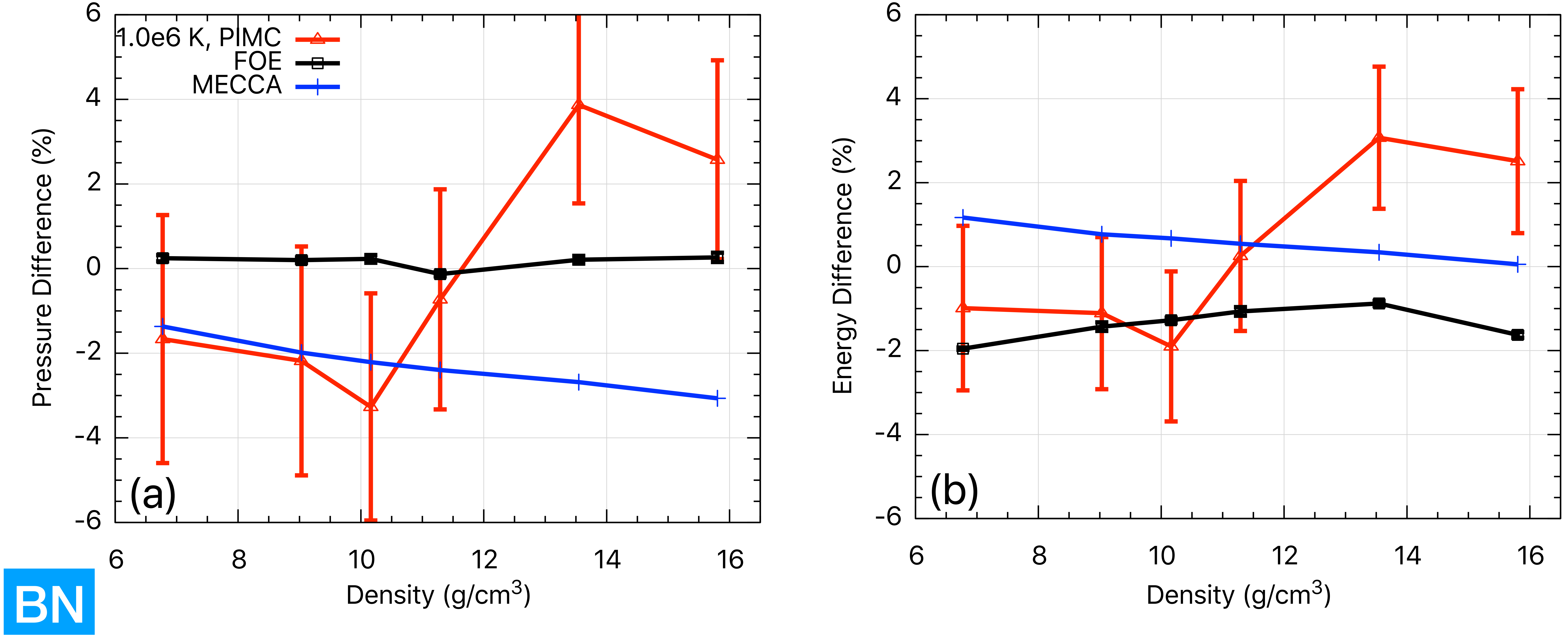
AT THE PARTIALLY IONIZED, WARM DENSE REGIME, DIFFERENT METHODS AGREE TO 3%



* Results plotted relative to the EOS values from SQ

* Energy differences normalized by the ideal gas values ($21k_BT$/BN)

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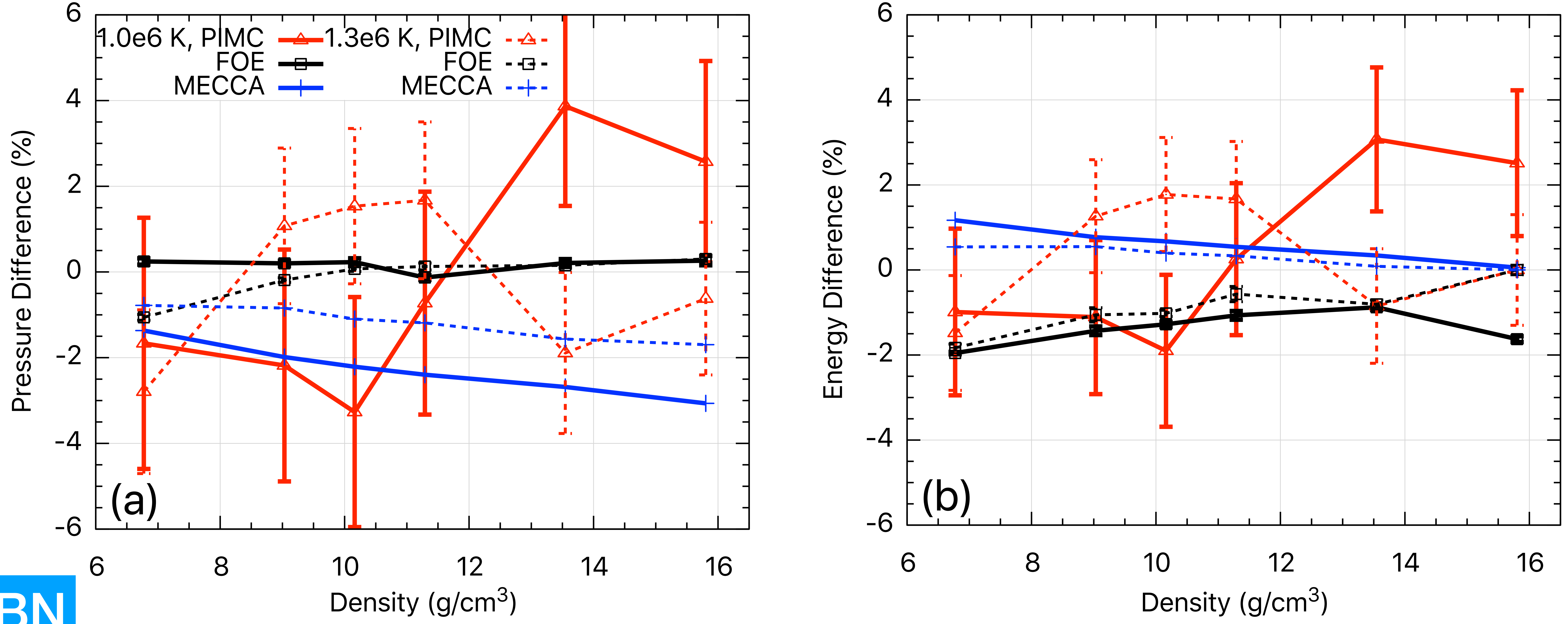

BN

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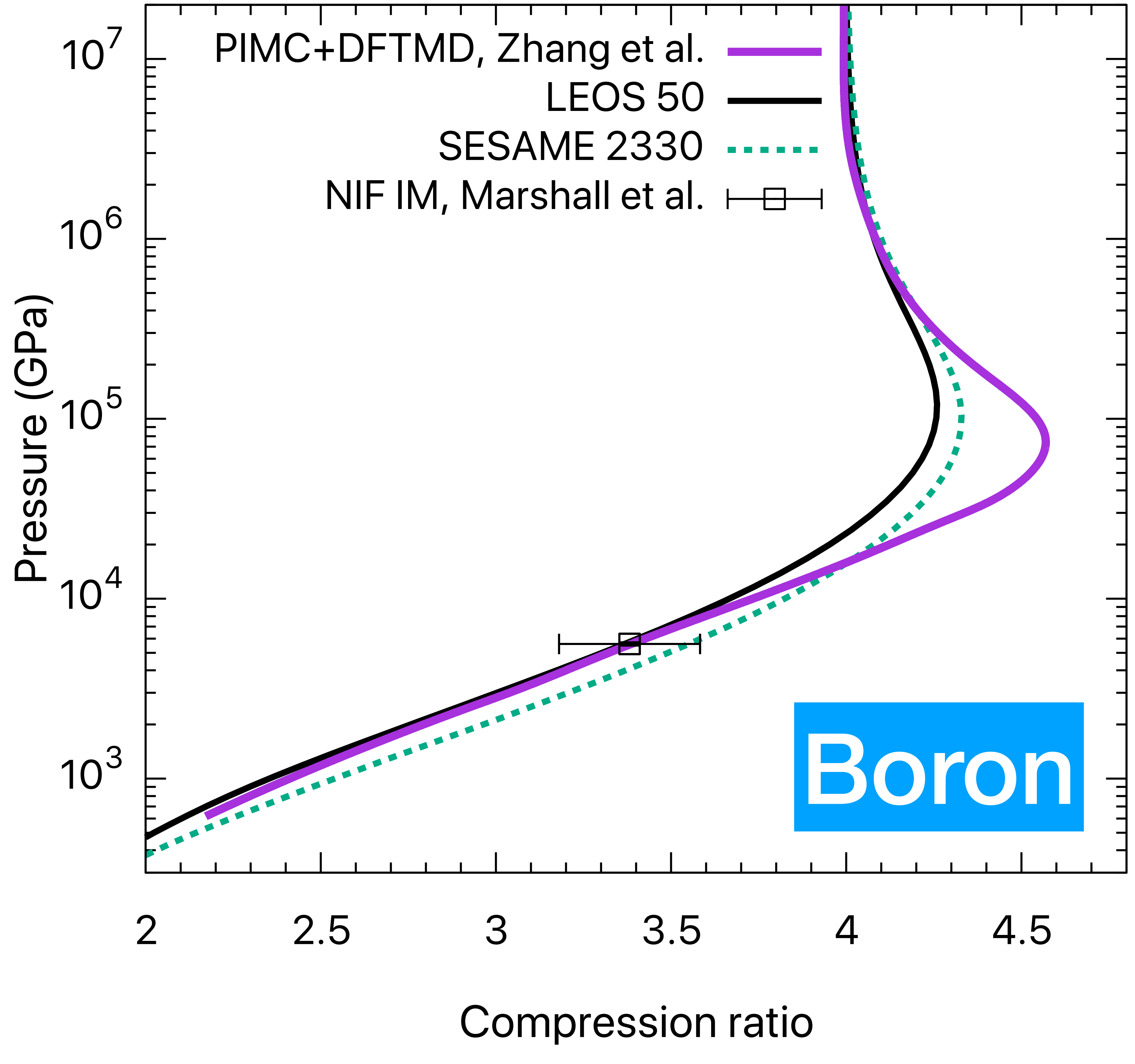
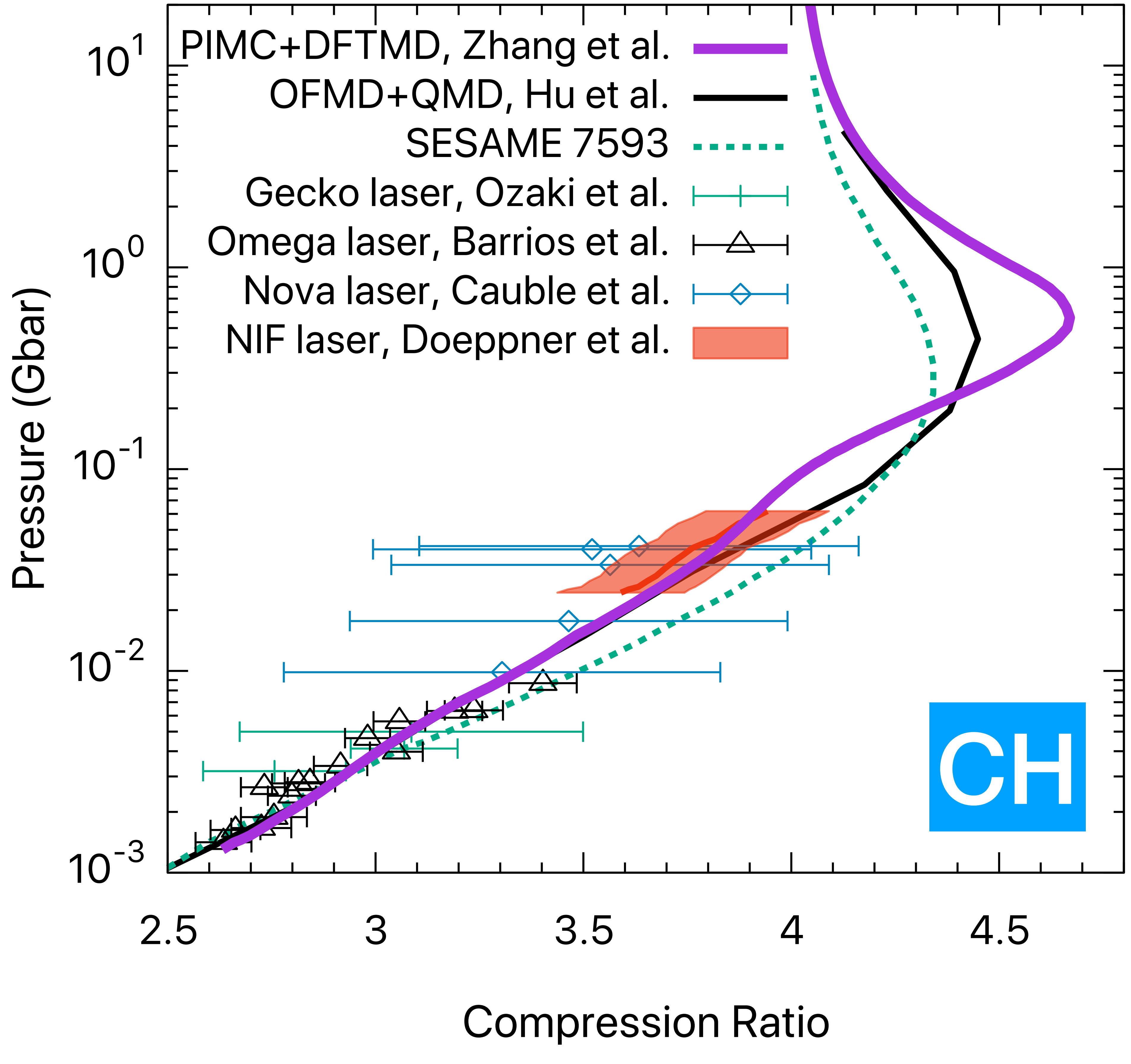
WE PREDICT HUGONIOTS THAT AGREE WITH EXPT. BUT DIFFER FROM THOMAS–FERMI





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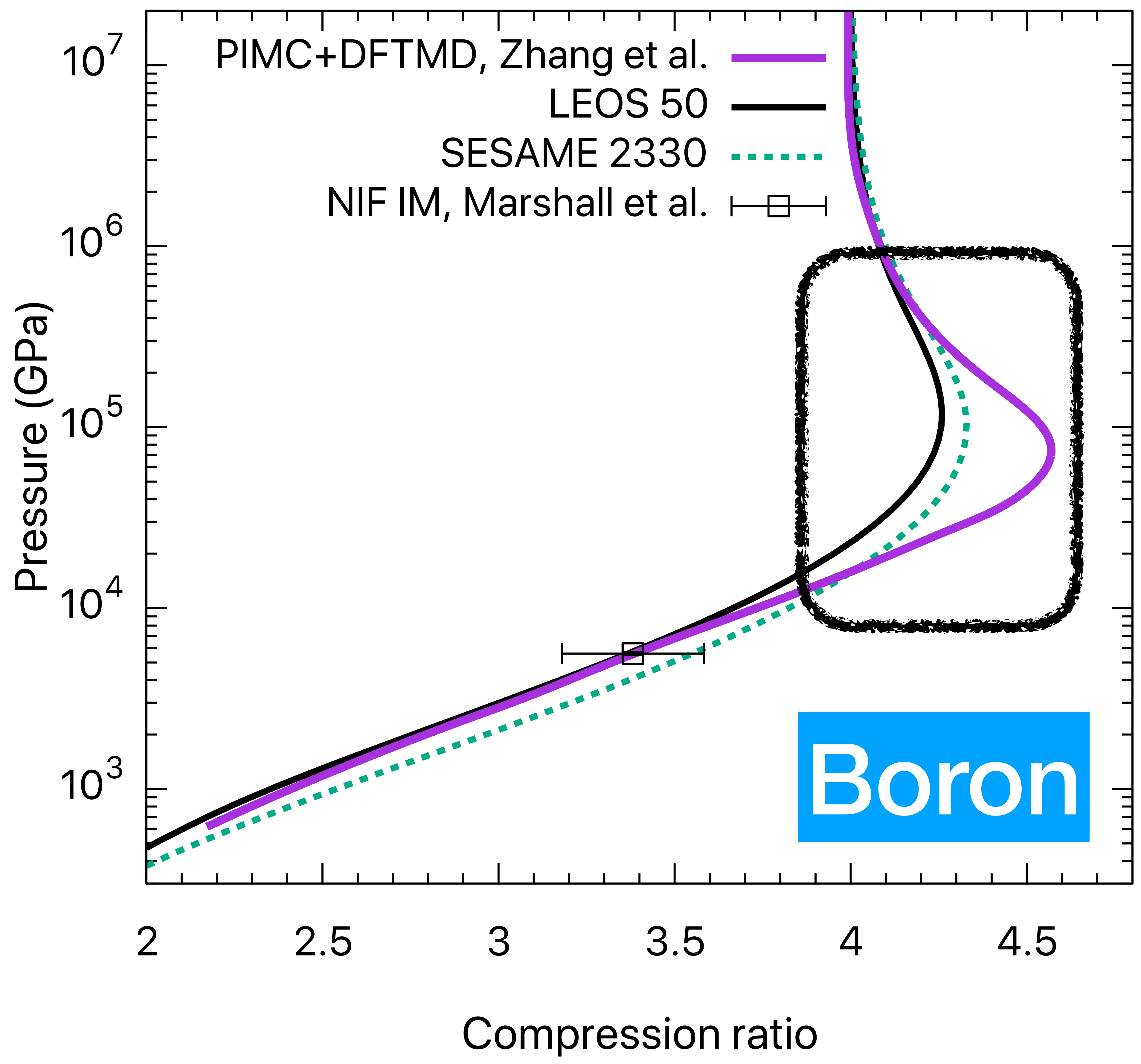

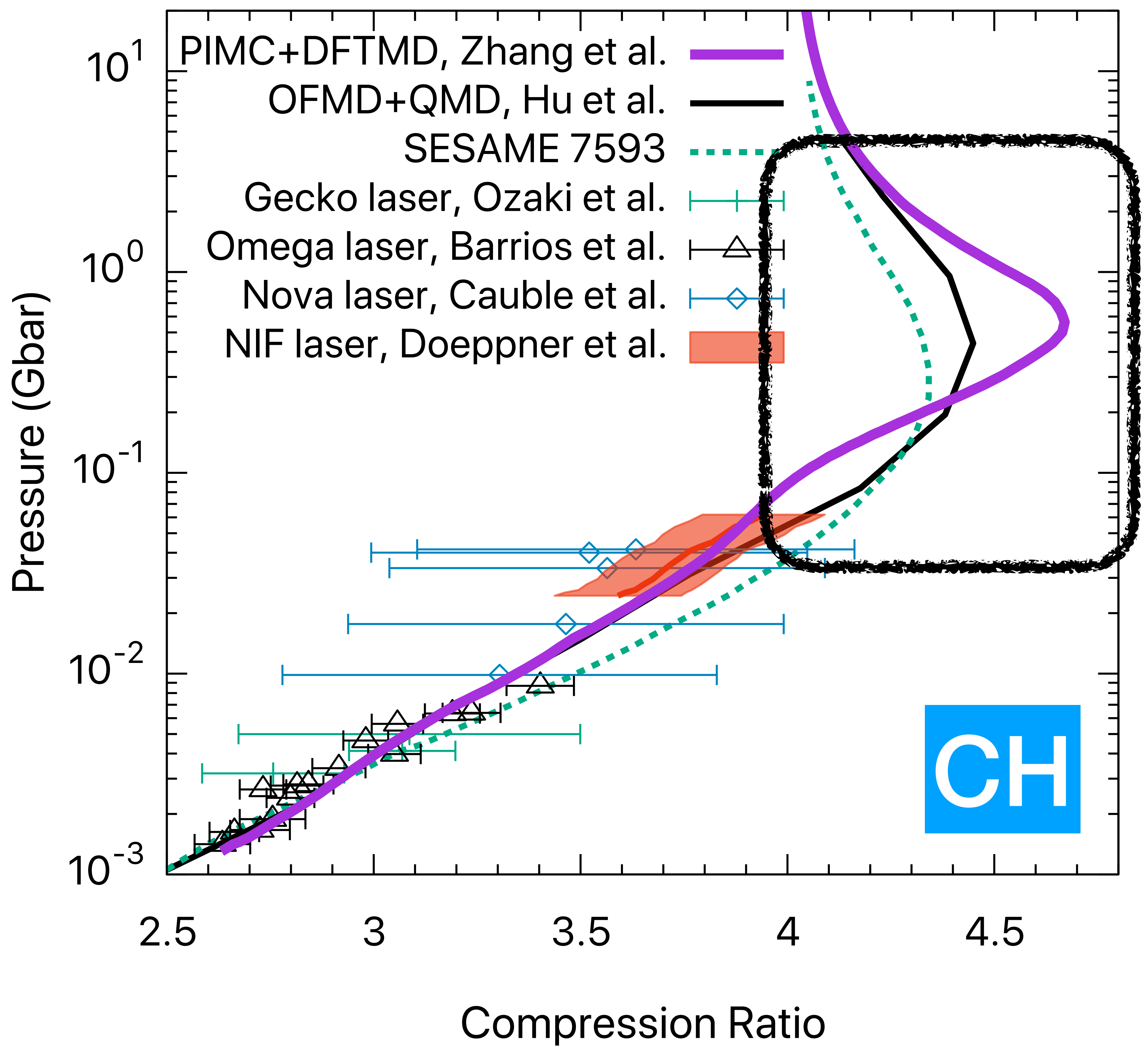

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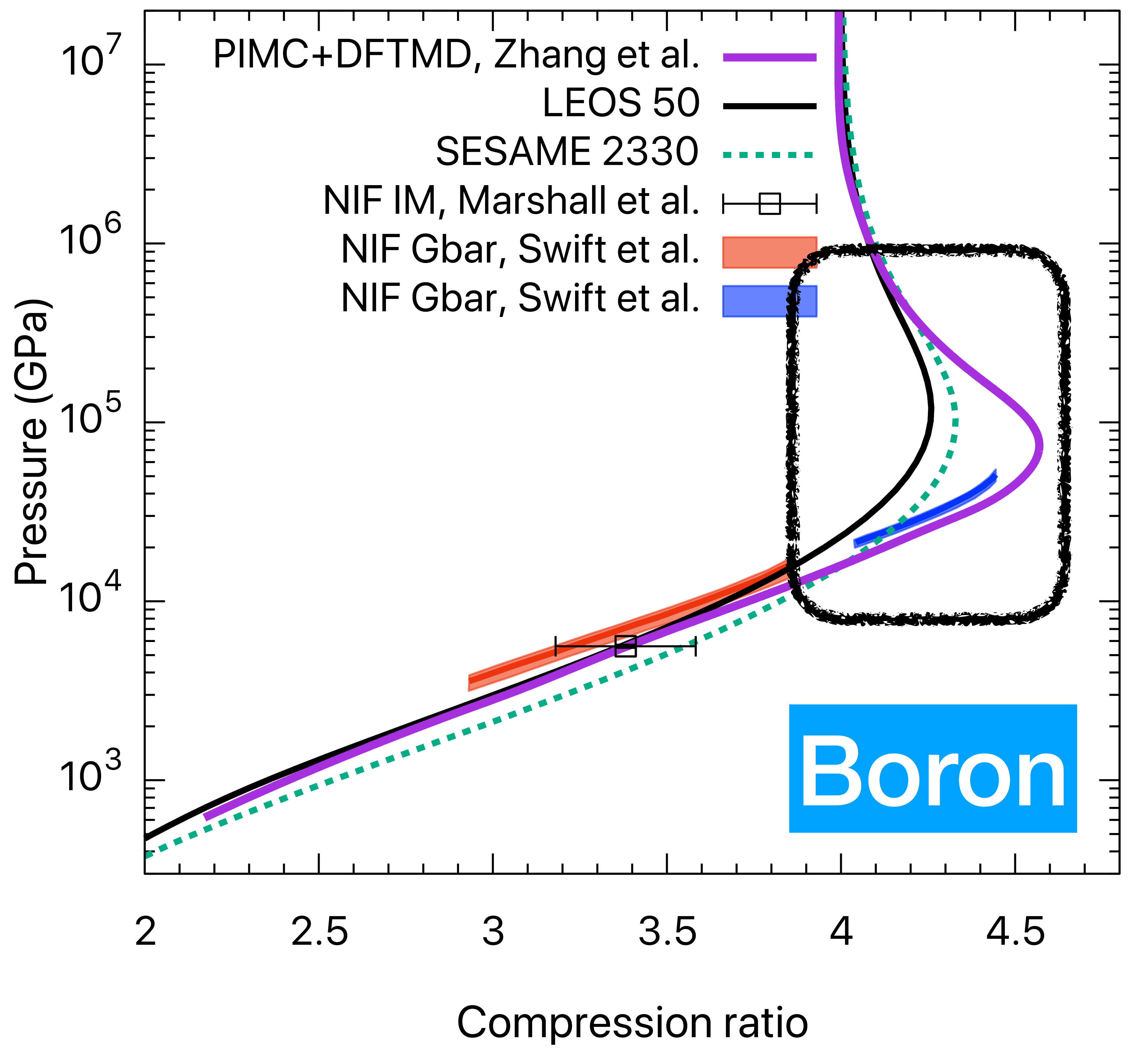

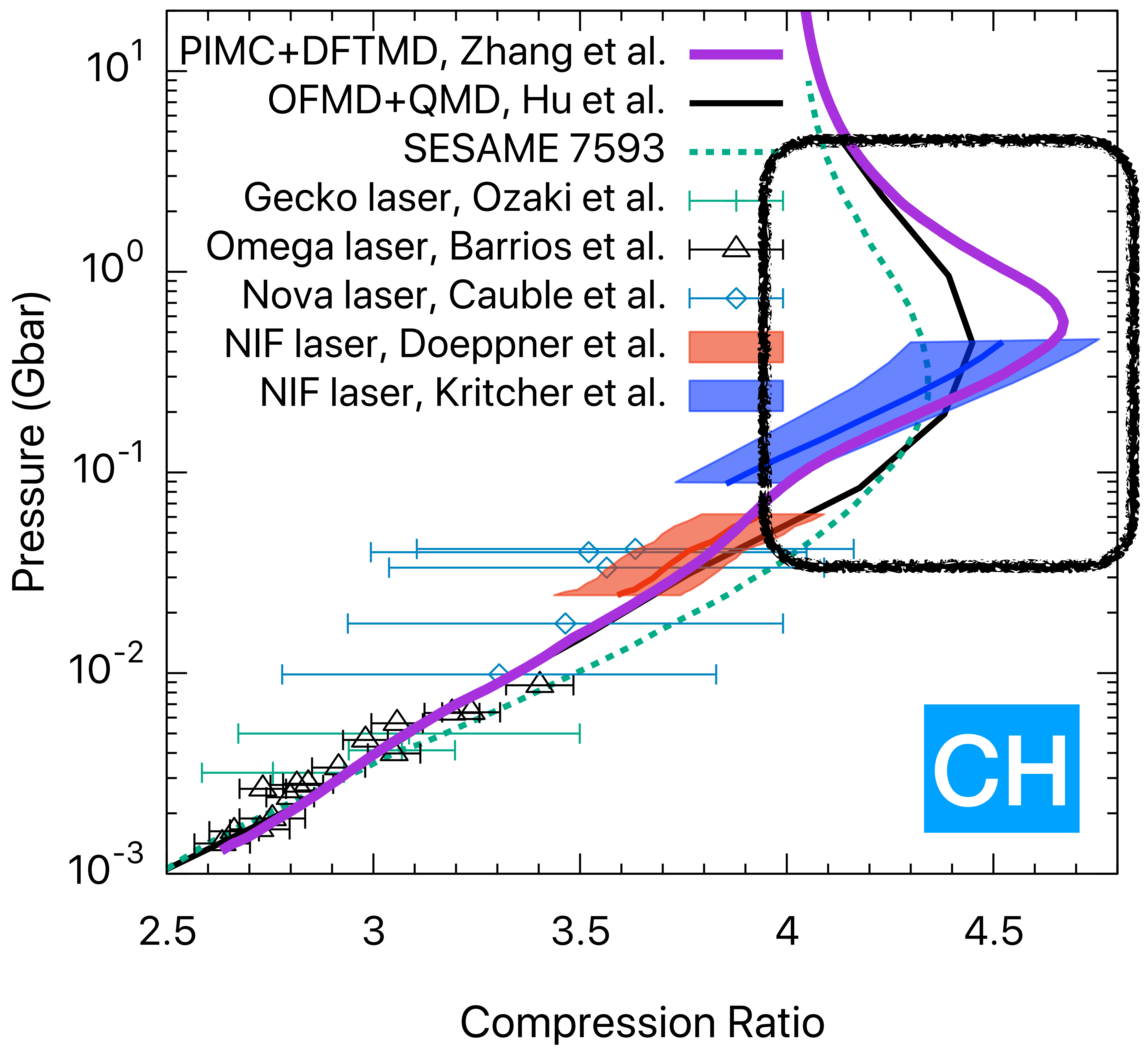

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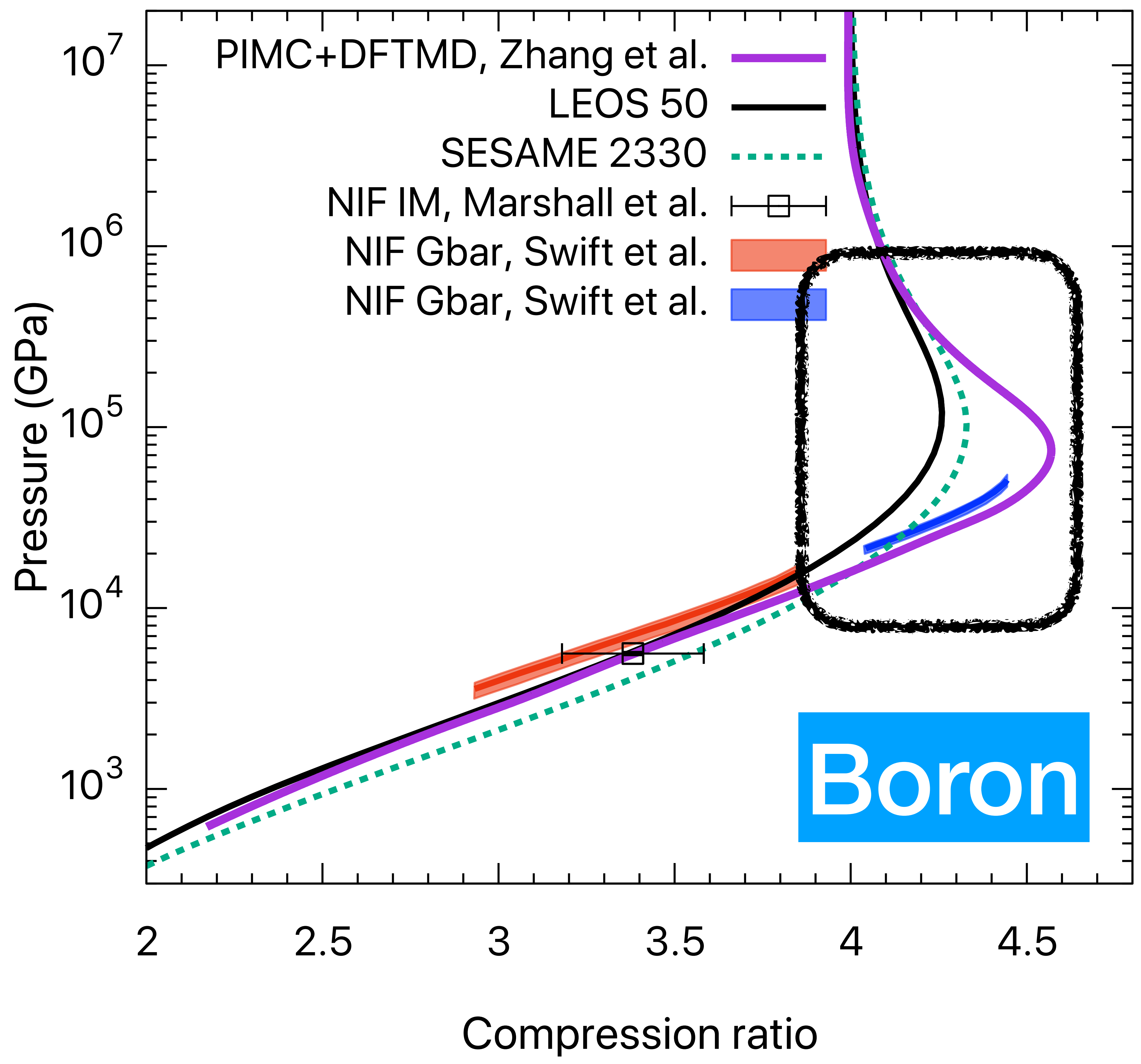
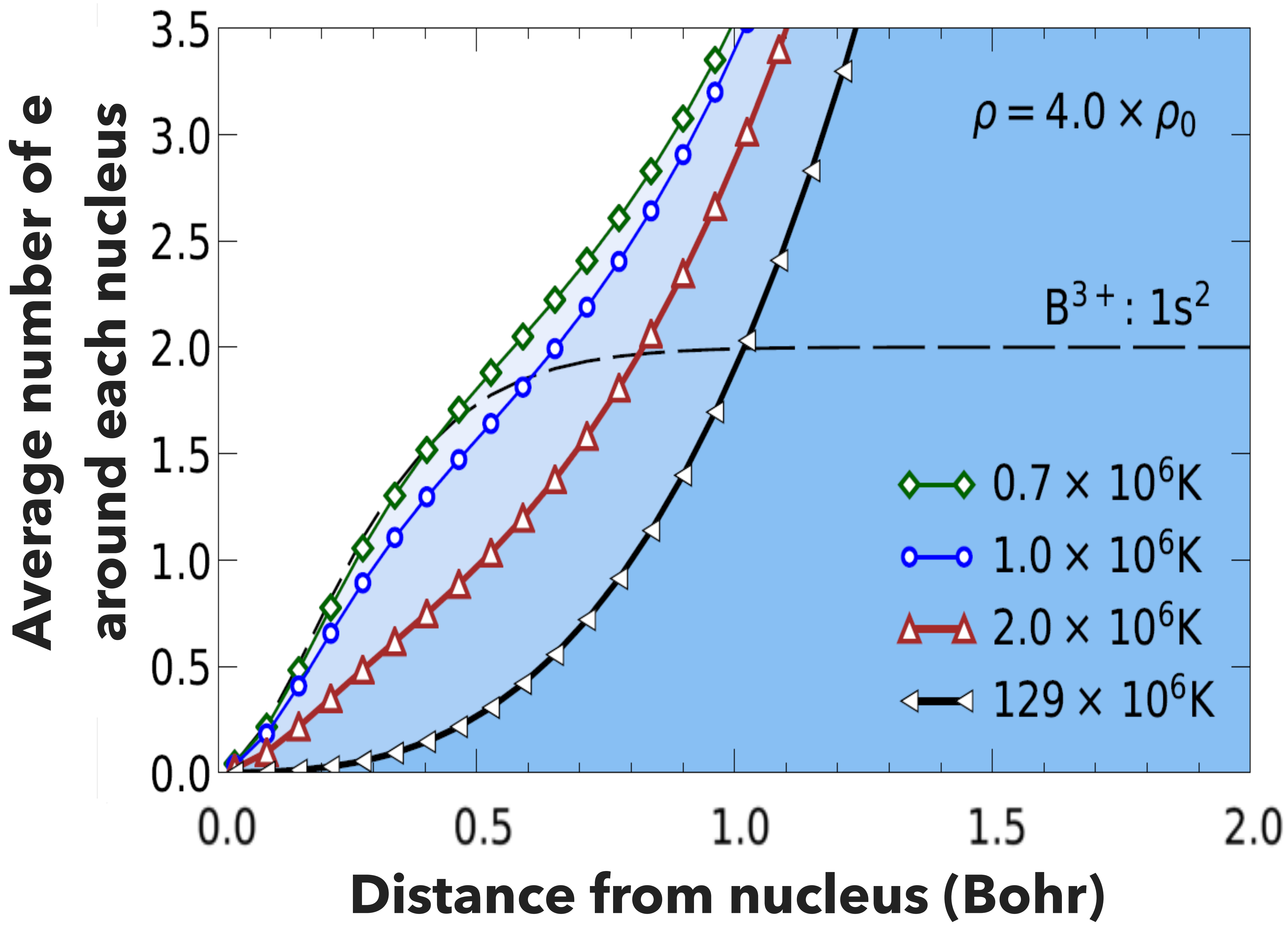
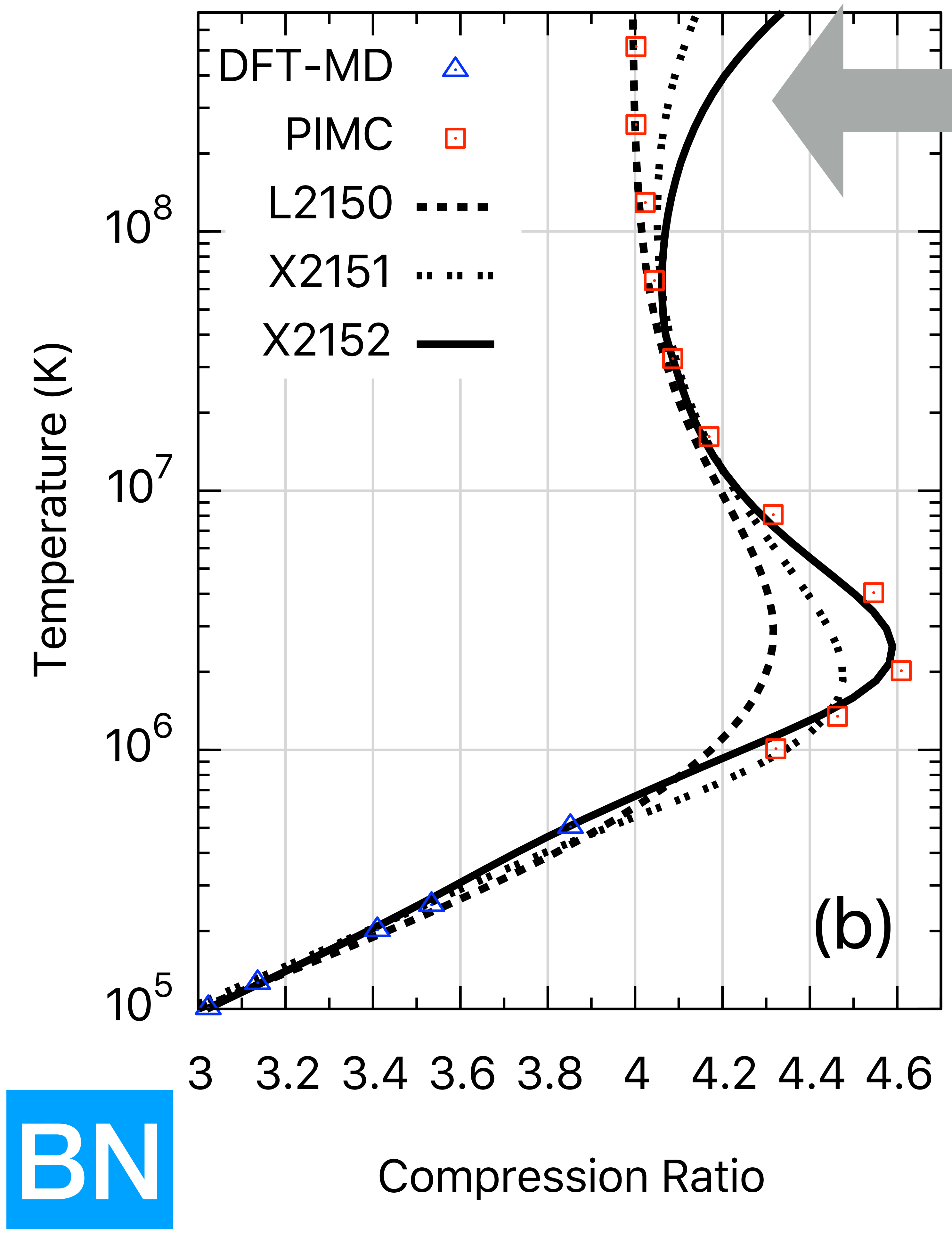
SHARPER COMPRESSION MAXIMUM IS DUE TO K SHELL IONIZATION





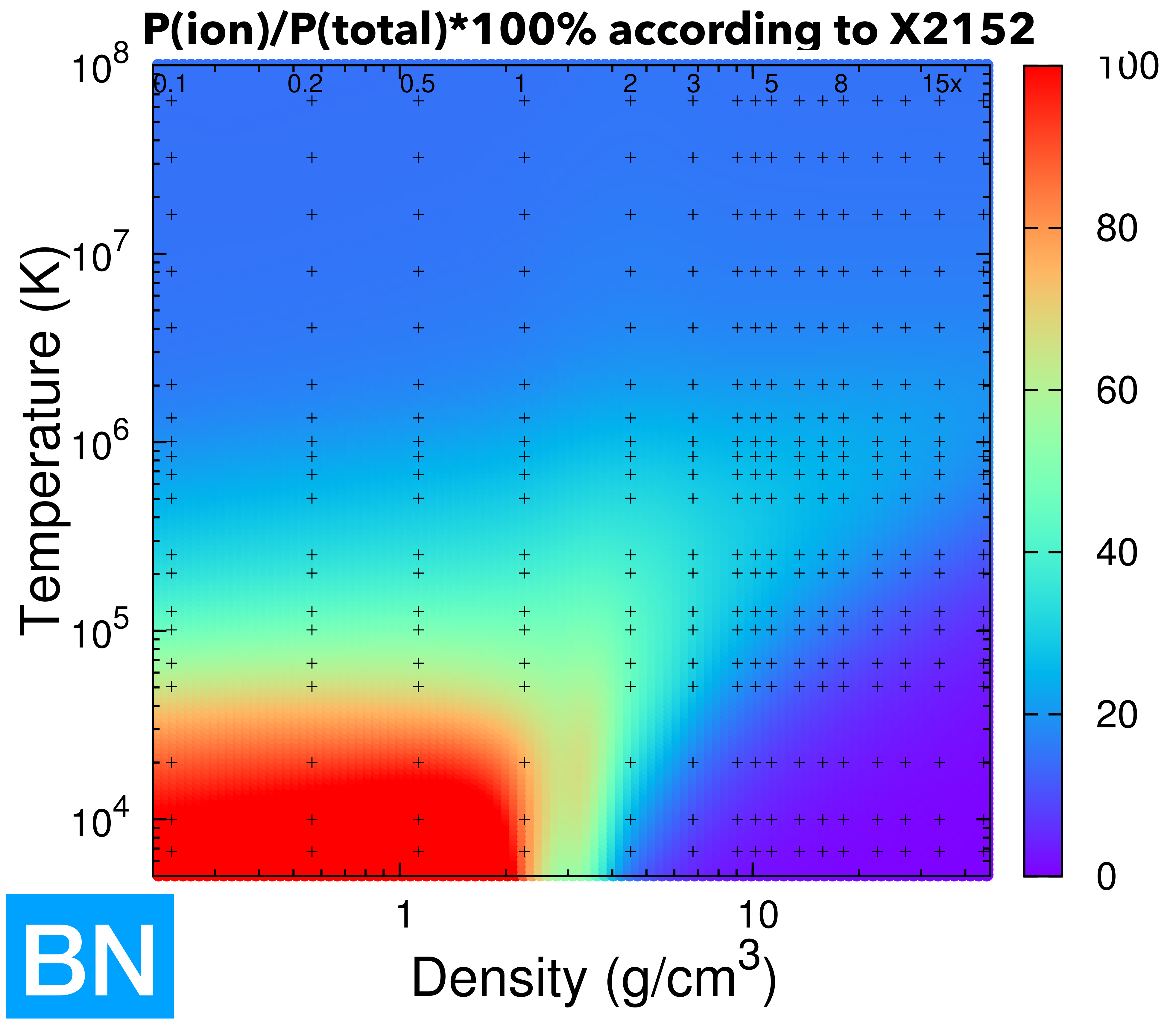
Atomic shell effects not included in Thomas-Fermi or orbital-free methods

OUR DATA SET CONSTRAINTS FOR THE CONSTRUCTION OF ACCURATE EOS TABLES



Electron relativistic effect

QEOS: $F(\rho,T) = E_{cold}(\rho) + F_{ion}(\rho,T) + F_{ele}(\rho,T)$



- LEOS 2150: legacy TF model
- X2151: TF (N) +Purgatorio (B)
- X2152: Purgatorio

WE RUN 1D SIMULATIONS TO CLARIFY THE PERFORMANCE SENSITIVITY TO EOS

EOS Model (P multiplier)	Neutron Yield
LEOS 50 (0.8)	2.15×10^{13}
LEOS 50 (1.0)	3.60×10^{13}
LEOS 50 (1.2)	5.70×10^{13}
X52 (1.0)	3.53×10^{13}
GDP	2.14×10^{13}

Polar direct-drive exploding pusher expt. simulations based on 1D Ares model*
Capsule thickness:
Boron: 6 μm
GDP: 18 μm

- Variations of L50 pressures by 20% show ~50% change in neutron yield.
- X52 gives similar results to L50, substantially narrowing the range of EOS-dependent uncertainty in capsule yield
- **Important to constrain both pressure and internal energy in EOS models**
- Using a higher tensile strength material (e.g., B) could enable the design of a thinner capsule that is more "exploding-pusher like" than plastics

* Ellison, Whitley, et al., Phys. Plasmas 25, 072710 (2018).

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ACKNOWLEDGEMENT

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Blue Waters Computing Project, Livermore Computing

Thank you!