Crystallization of Super-Earths' core:

a first principles study of entropy and melting curve of iron

Felipe González & Burkhard Militzer

EOS

T: 3000 K – 30000 K

P: 300 GPa – 5000 GPa

AGU23

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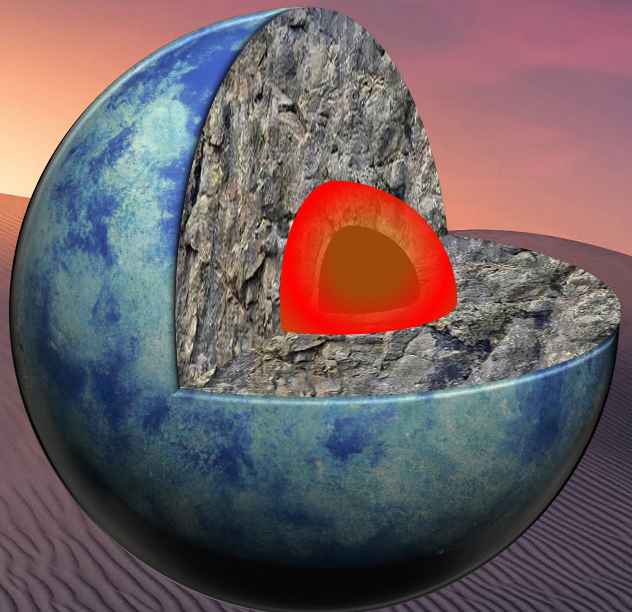
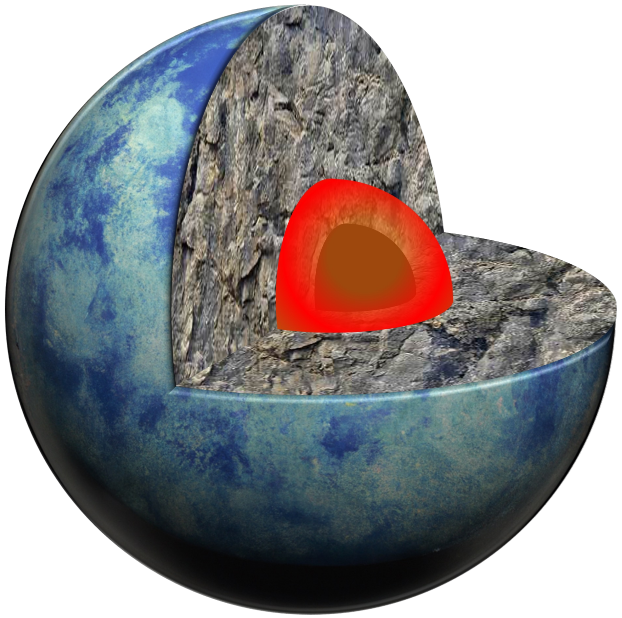
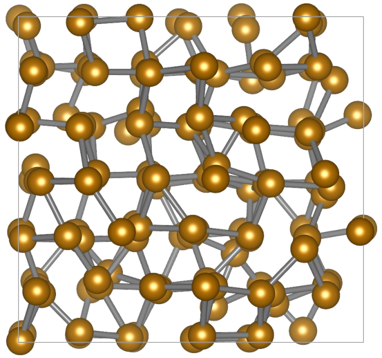


AGU23 Equation of state for iron





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Ab initio determination of iron melting at terapascal pressures and Super-Earths core crystallization

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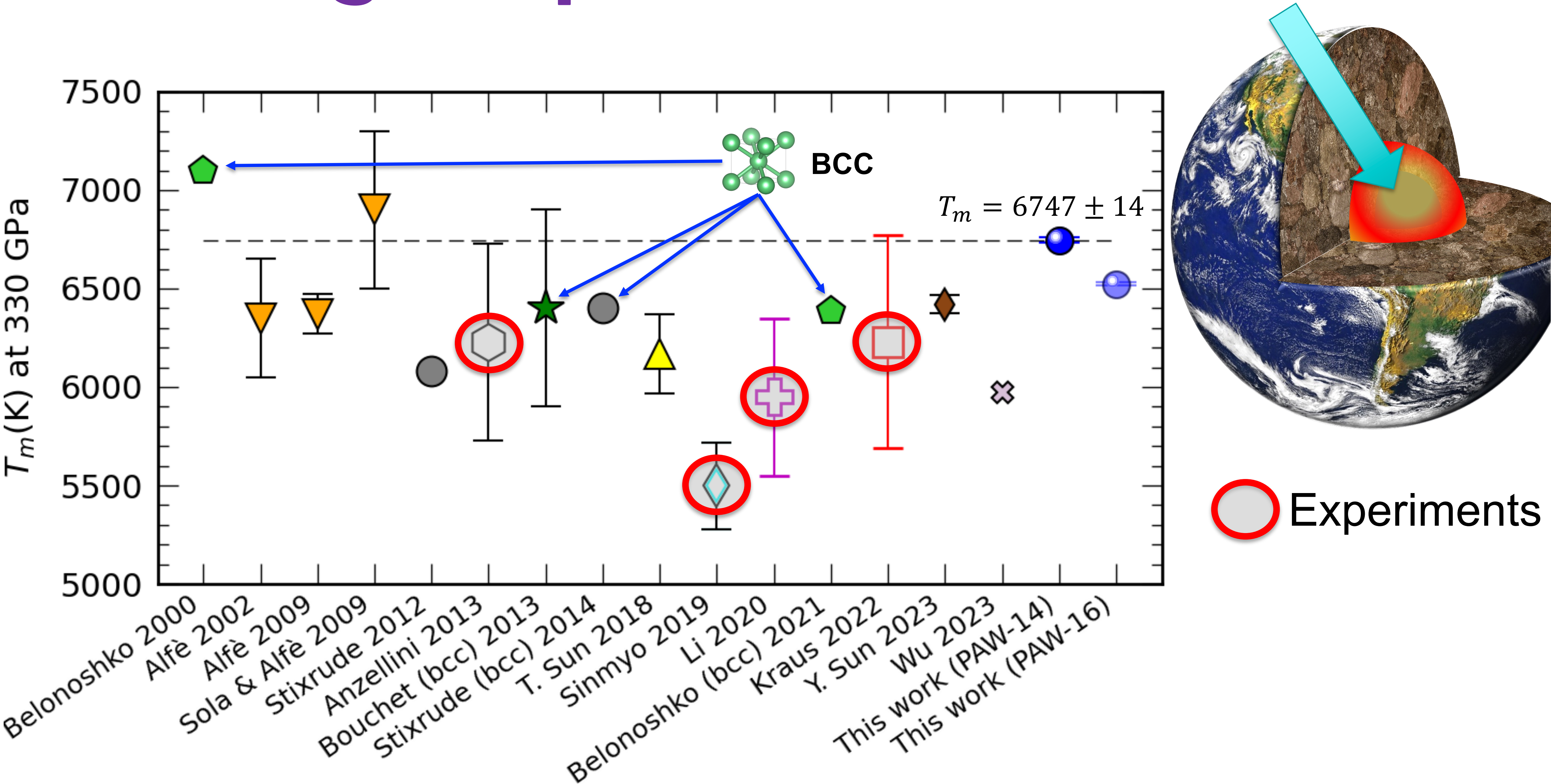
- EOS solid iron
- EOS liquid iron
- www.gnm.cl/fgonzalez

TABLE IV. Free energies of solid iron obtained from thermodynamic integration, including PAW-14, PAW-8, and PAW-16 calculations. No Frenkel correction included.

Sim. ID	Size	V (Å^3/Fe)	ρ (g/cc)	T (K)	P (GPa)	E (Ha/Fe)	F_{DFT} (Ha/Fe)	Pseudopotential
Fe132	144Fe	3.1220	29.7035	25000	5002.0470 ± 1.2800	1.36241449 ± 0.00053736	0.22674882 ± 0.00016832	PAW-14
Fe158	144Fe	3.3969	27.2991	24000	4004.2820 ± 1.9630	1.10375957 ± 0.00101313	−0.01069262 ± 0.00027722	PAW-14
Fe181	144Fe	3.4270	27.0598	27500	3998.6110 ± 1.8630	1.14044400 ± 0.00089354	−0.20447284 ± 0.00023952	PAW-14
Fe192	144Fe	3.7288	24.8695	18000	3000.9080 ± 0.4810	0.77143696 ± 0.00029430	−0.00576626 ± 0.00014488	PAW-14
Fe197	144Fe	3.7490	24.7352	20000	2998.8650 ± 1.0860	0.79315727 ± 0.00065187	−0.10782697 ± 0.00014370	PAW-14
Fe211	144Fe	3.4129	27.1716	26000	4000.6750 ± 1.1330	1.12366198 ± 0.00053203	−0.11916665 ± 0.00019601	PAW-14
Fe216	144Fe	3.7747	24.5670	22500	2999.6220 ± 1.6640	0.82230909 ± 0.00092247	−0.24003435 ± 0.00015664	PAW-14
Fe222	144Fe	4.2707	21.7137	15000	1999.7790 ± 0.8590	0.45548402 ± 0.00059509	−0.18243960 ± 0.00009119	PAW-14
Fe228	144Fe	5.2509	17.6603	10000	1002.2180 ± 0.2520	0.09743111 ± 0.00019527	−0.29959525 ± 0.00006325	PAW-14
Fe238	144Fe	3.4062	27.2247	25000	3998.2490 ± 1.0710	1.11256370 ± 0.00054860	−0.06493623 ± 0.00018534	PAW-14
Fe258	144Fe	5.3234	17.4198	12500	1000.2380 ± 0.6510	0.12551121 ± 0.00051435	−0.42066479 ± 0.00011793	PAW-14
Fe292	108Fe	3.1392	29.5400	27500	5002.3540 ± 1.9610	1.38950296 ± 0.00074986	0.09236150 ± 0.00025881	PAW-14
Fe297	180Fe	3.1388	29.5439	27500	5000.5090 ± 2.4170	1.38682803 ± 0.00096903	0.09124313 ± 0.00018293	PAW-14
Fe302	144Fe	3.1570	29.3740	30000	5007.0660 ± 3.3620	1.41703321 ± 0.00137374	−0.04816252 ± 0.00029513	PAW-14

Melting temperature iron at 330 GPa



Ramp-compressed iron: 1000 GPa

Kraus et al, Science 2022

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REPORT | PLANETARY SCIENCE

Measuring the melting curve of iron at super-Earth core conditions

RICHARD G. KRAUS, RUSSELL J. HEMLEY, SUZANNE J. ALI, JONATHAN L. BELOF, LORIN X. BENEDICT, JOEL BERNIER, DAVE BRAUN, R. E. COHEN, GILBERT W. COLLINS, [...], AND JON H. EGGERT +16 authors Authors Info & Affili

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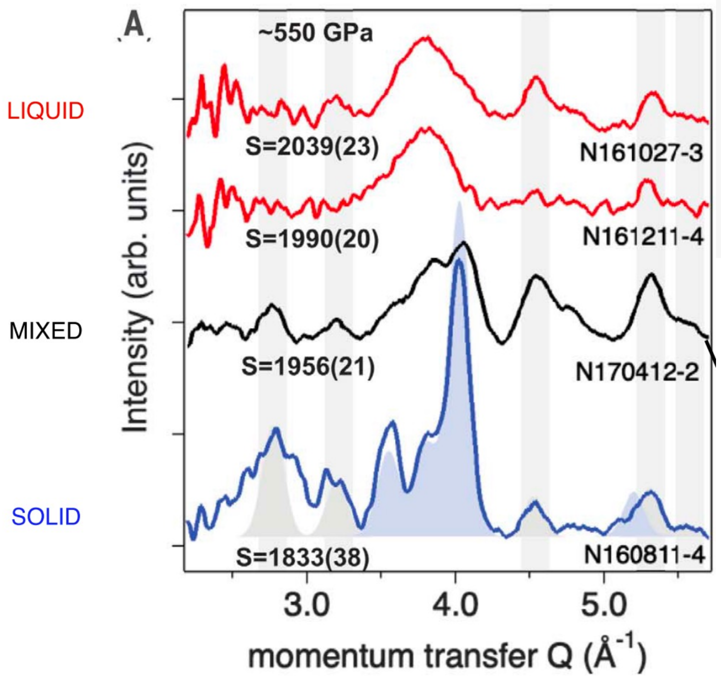
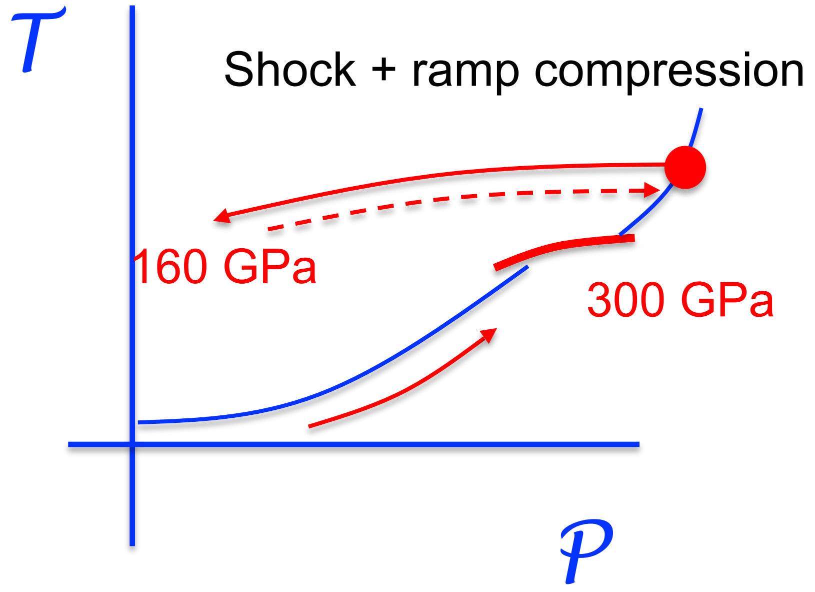




In situ crystallization of hcp

300 – 1000 GPa

$T_m = 6230 \pm 540$

at 330 GPa

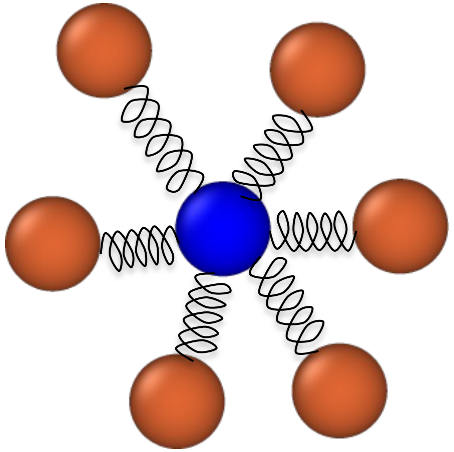
Our approach:

Melting temperature T_m:

$$G_{liquid}(P_0, T_m) = G_{solid}(P_0, T_m)$$

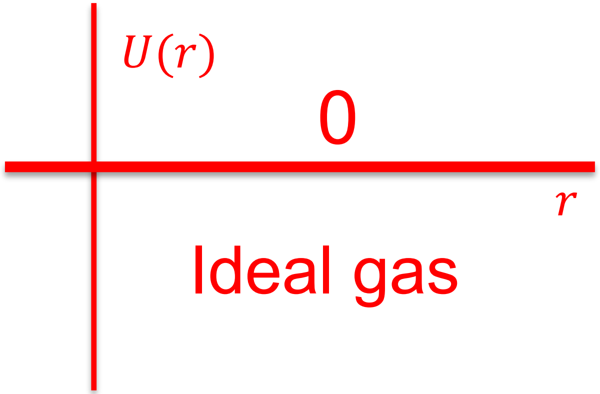
$$F_1 = F_0 + \int_0^1 d\lambda \, \langle U_1(\boldsymbol{r}) - U_0(\boldsymbol{r}) \rangle_\lambda$$

known

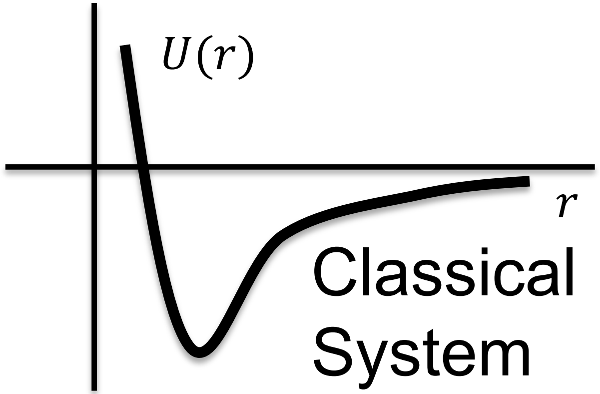


λ

Thermodynamic Integration



Ideal gas



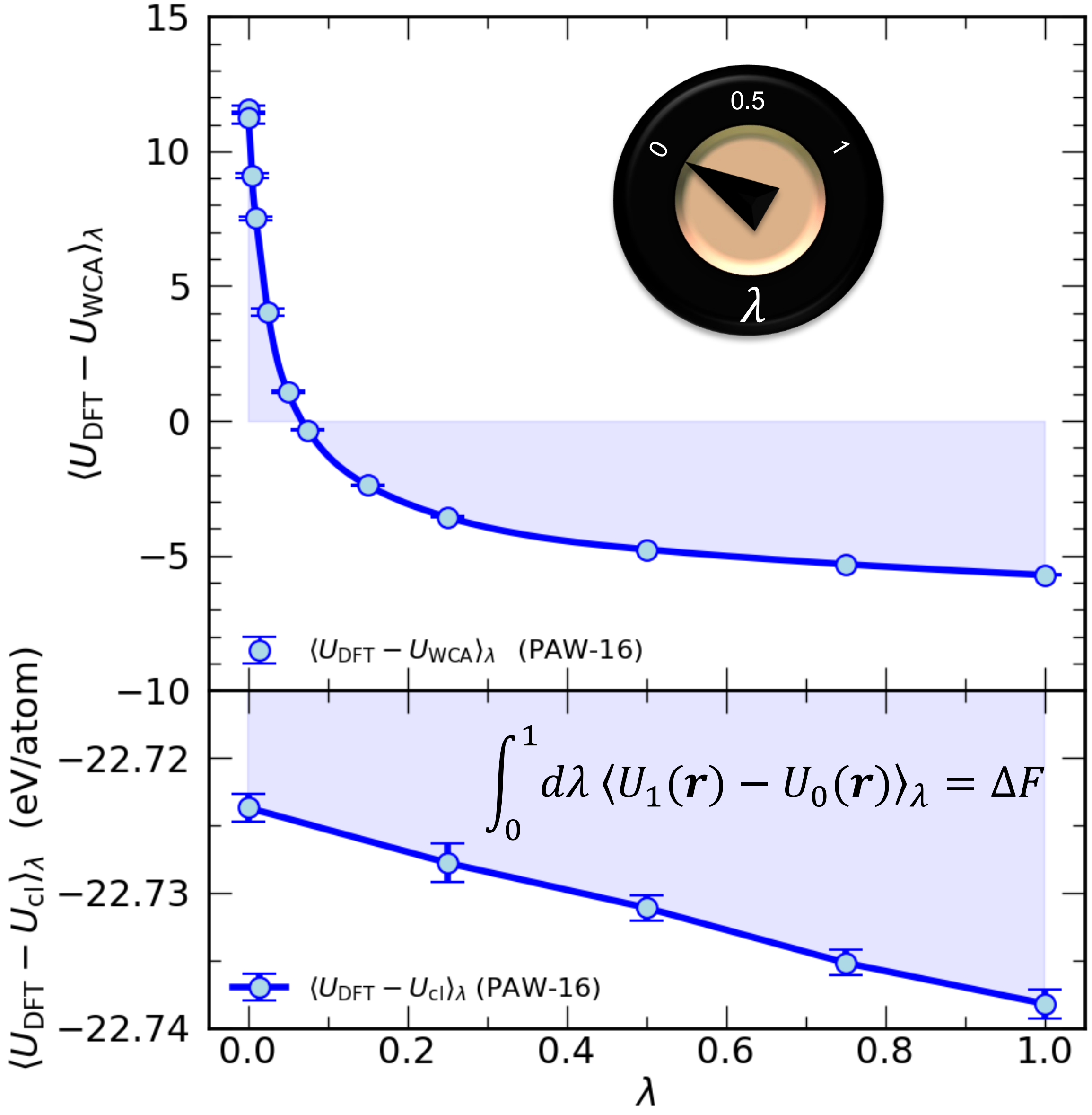
Classical System

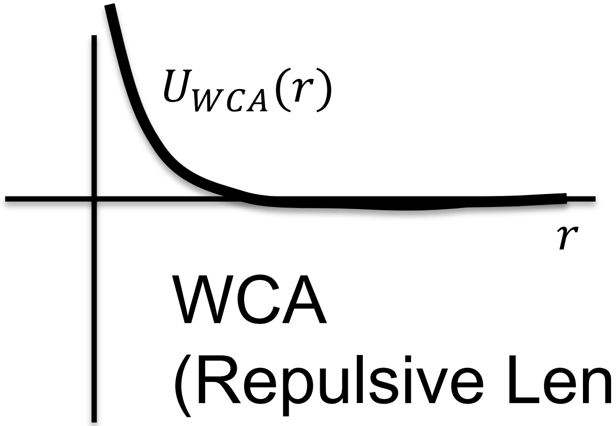
$$\hat{H}|\psi\rangle = E|\psi\rangle$$

DFT

Free energies liquid iron 330 GPa, 6400 K

class. → DFT





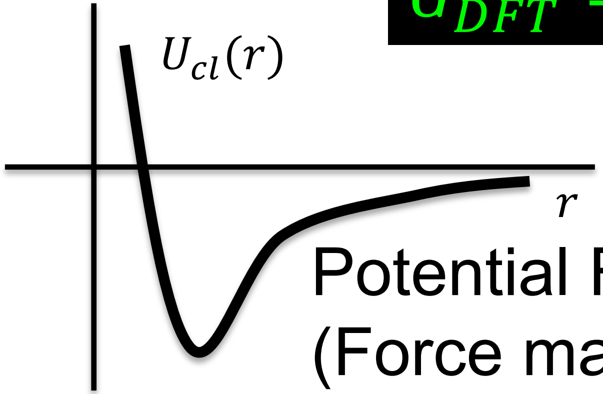
WCA
(Repulsive Lennard-Jones)

$G_{DFT} = 3.4788 \pm 0.0069$ eV

$F_{DFT} = F_0 + \Delta F$

Diff: ~ 2 meV/atom

$G_{DFT} = 3.4808 \pm 0.0006$ eV



Potential Fitted to P,T
(Force matching)

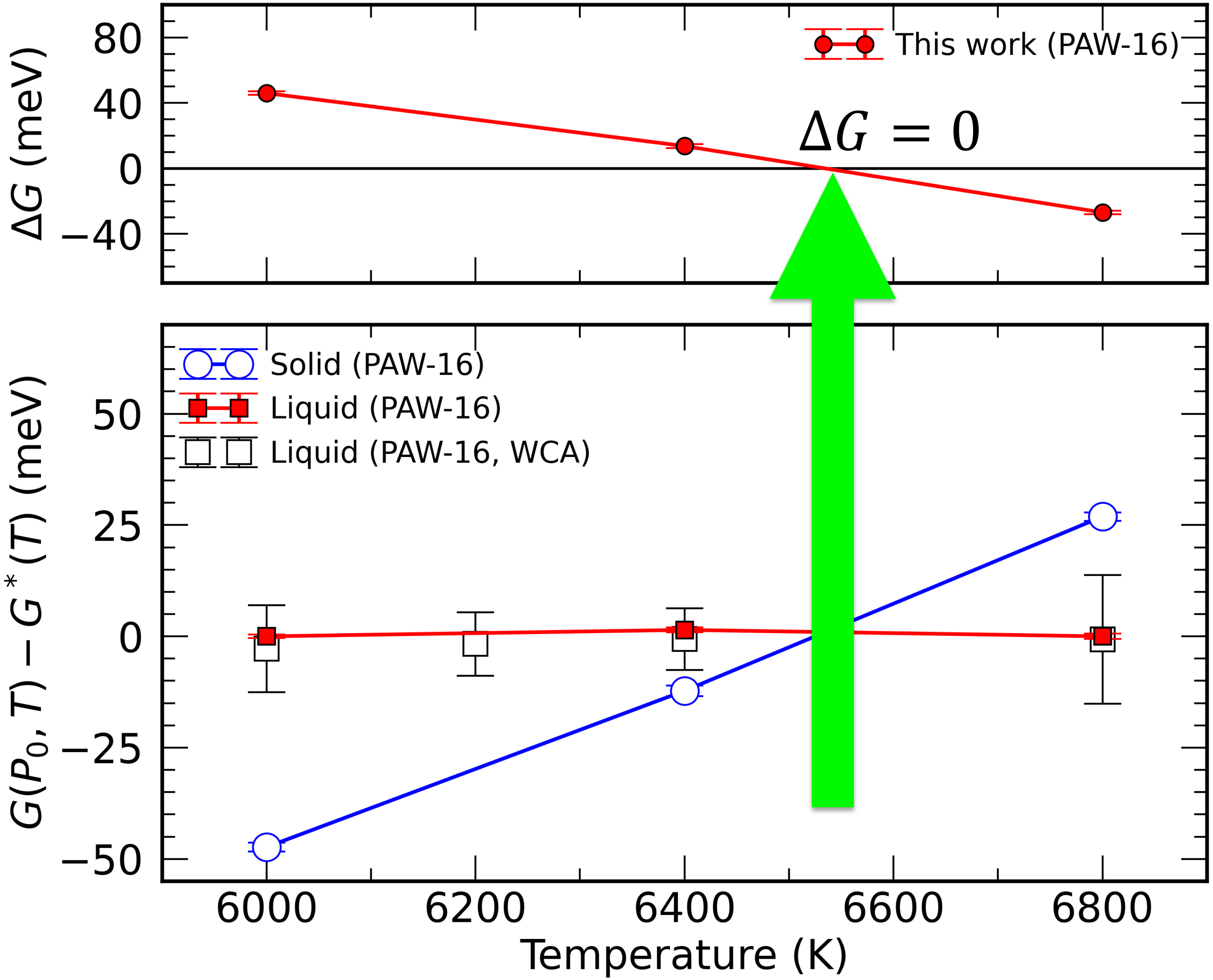
Free energies liquid iron 330 GPa

Fixed pressure:

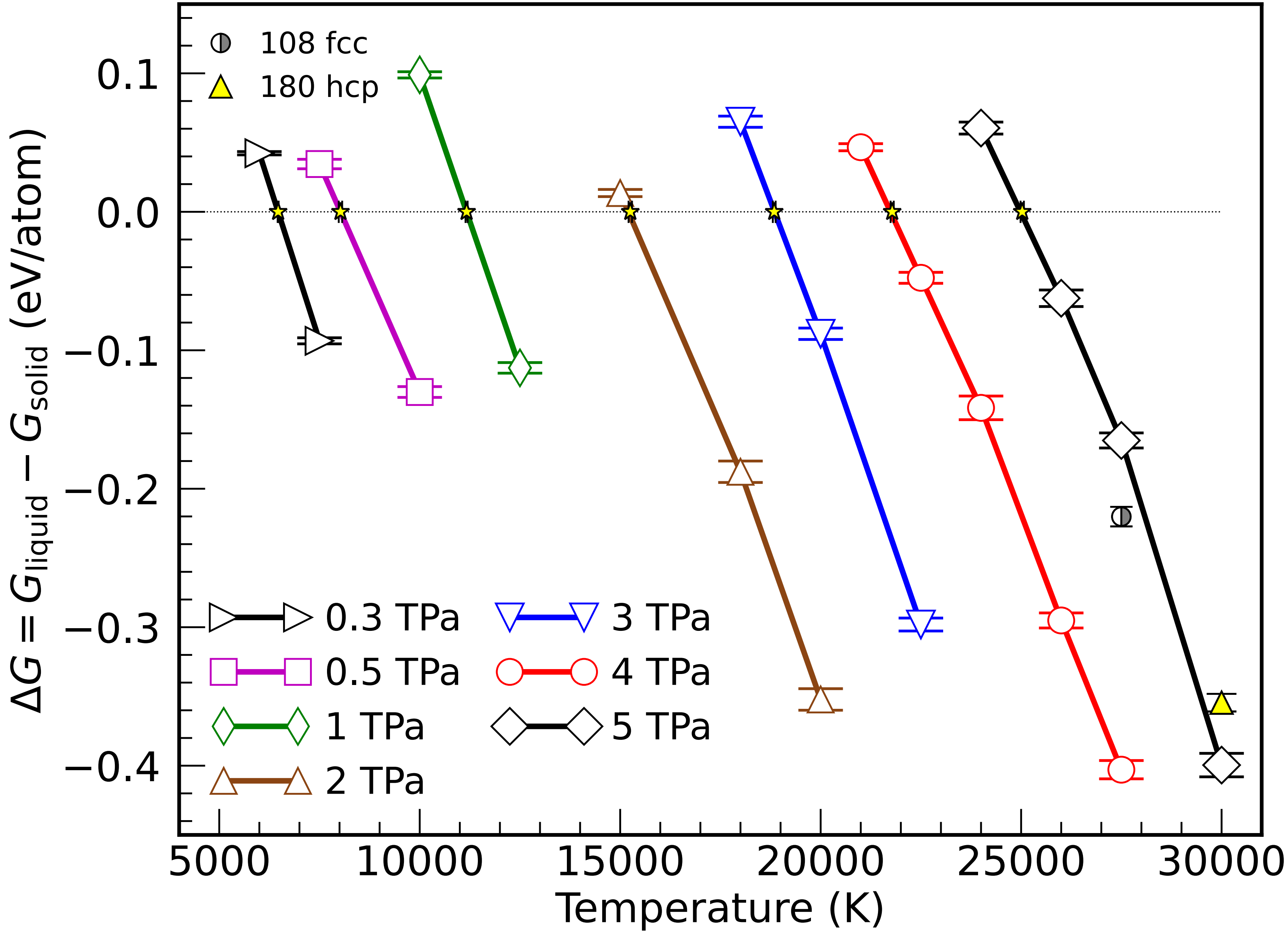
$P_0 = 330$ GPa

$\Downarrow$

$T_m = 6534 \pm 10\ K$

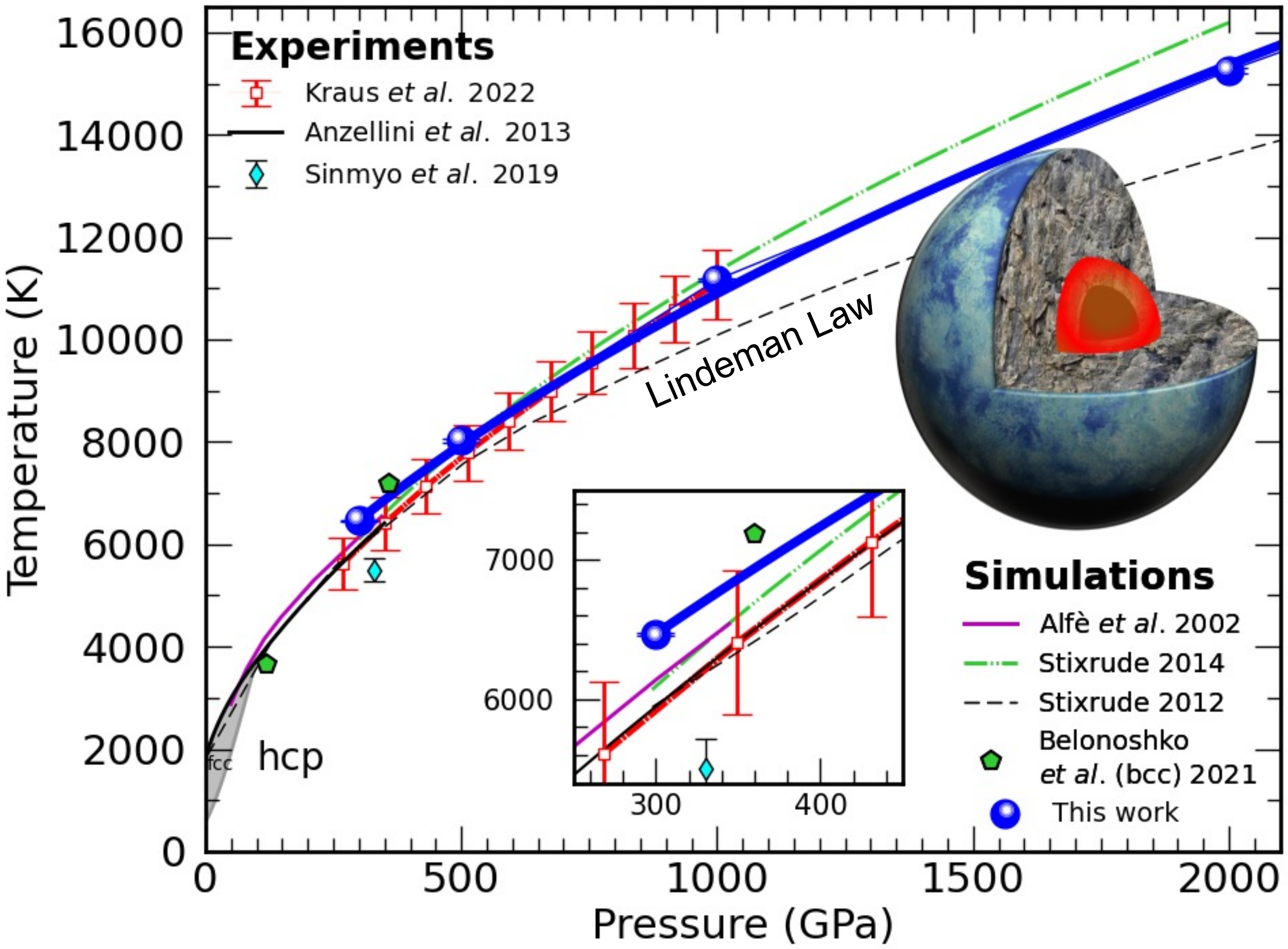


ΔG at different pressures



$$\Delta G = G_{liq} - G_{sol}$$

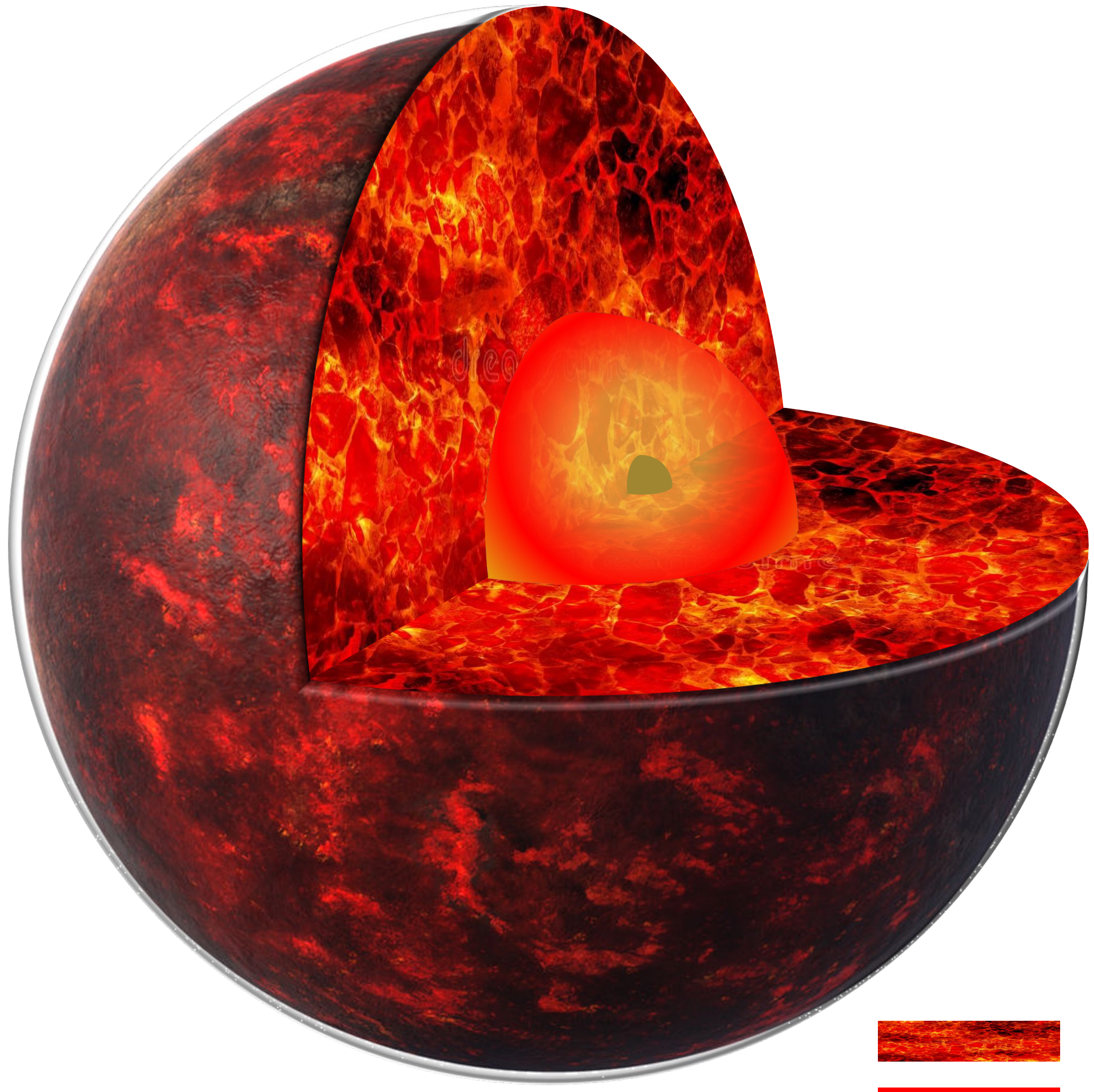
New melting curve for iron

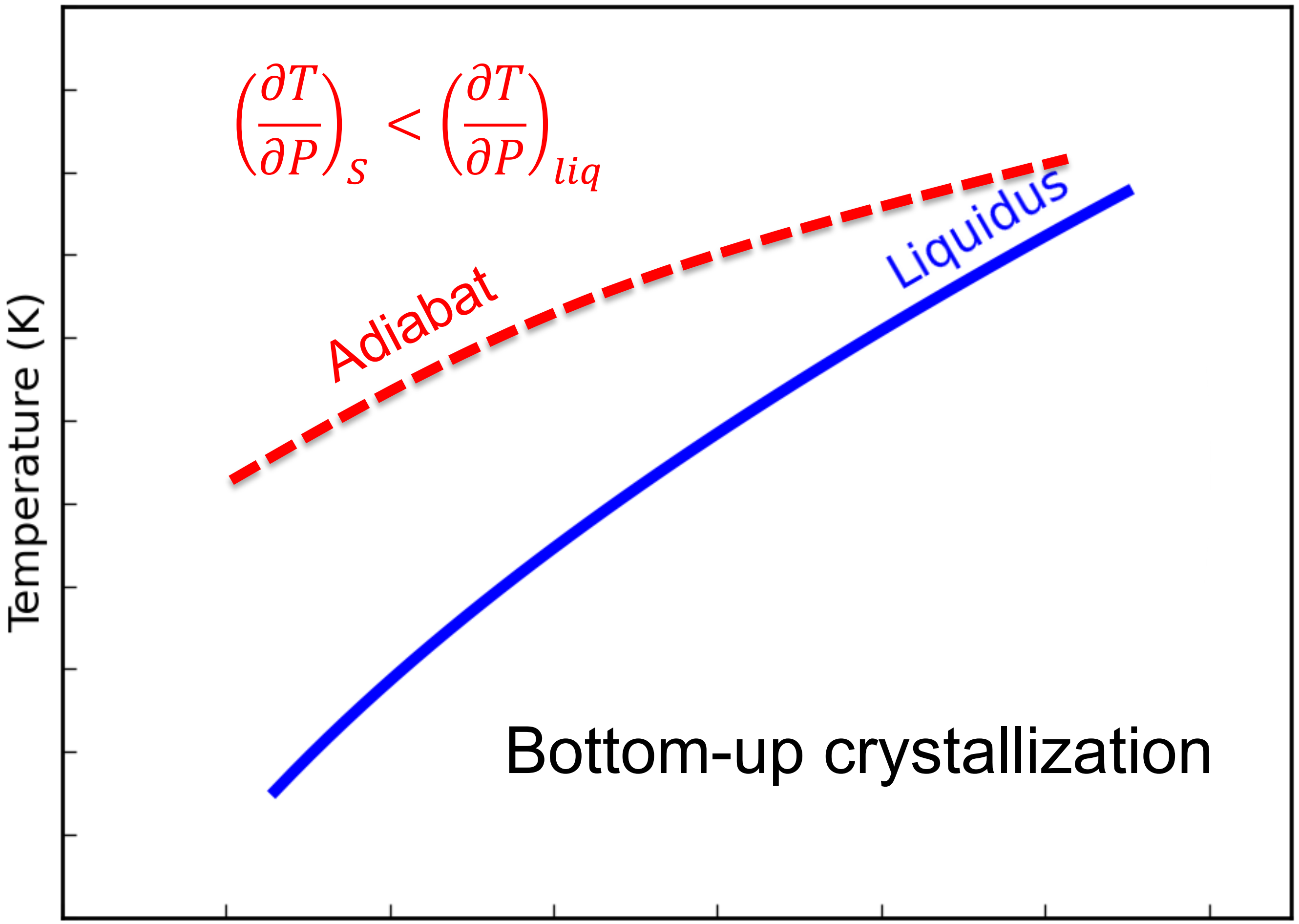


$$T_m(P) = 6469\ K\left(1 + \frac{(P - P_0)}{a}\right)^{1/c}$$

$P_0 = 300$ GPa
$a = 434.822$ GPa
$c = 1.839$

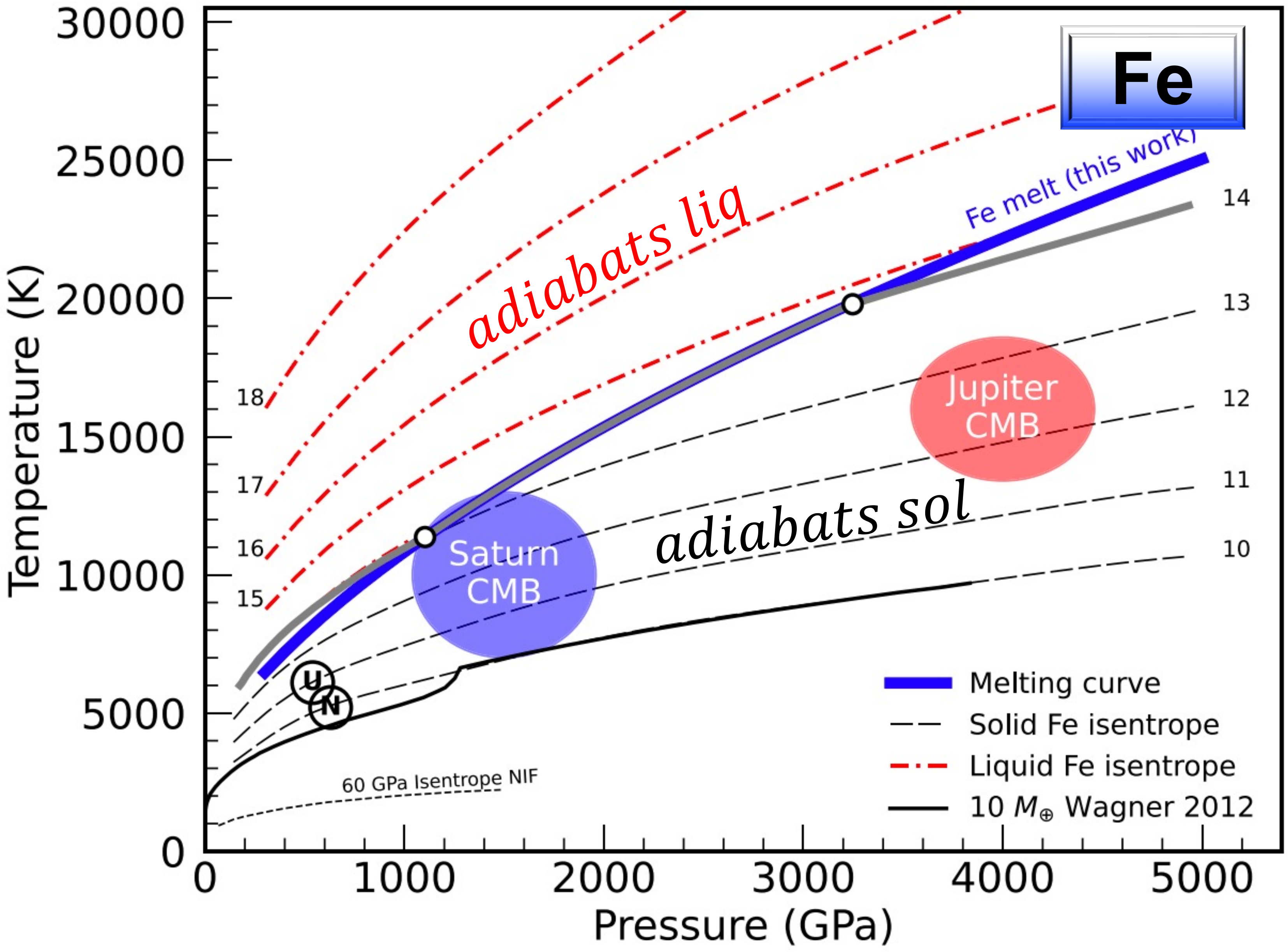
Super Earths crystallize bottom-up





- Silicate magma ocean
- Outer core (liquid Fe)
- Inner core (solid Fe)

Super Earths Crystallization



$$G_{DFT} \rightarrow S_{DFT}$$

$$(G = U - TS + PV)$$

$$\left(\frac{\partial T}{\partial P}\right)_S < \left(\frac{\partial T}{\partial P}\right)_{liq}$$

Iron Core of Super-Earths:
Bottom-up crystallization

Planetary Interior Models

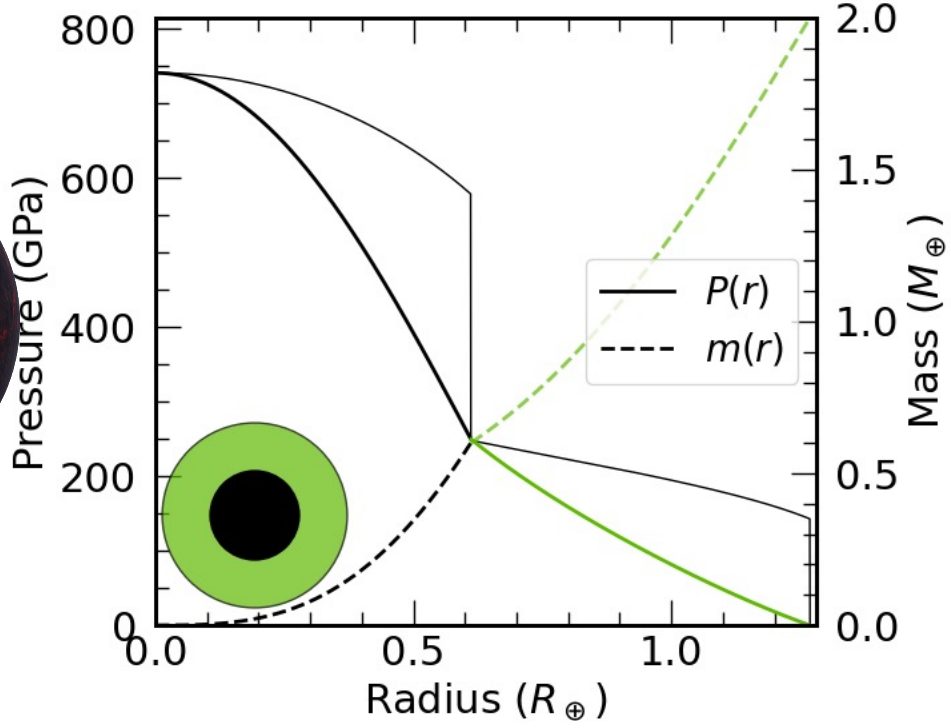
"The internal activity and thermal evolution of Earth-like planets,"
A. M. Papuc and G. F. Davies, Icarus 195, 447 (2008).

	$\langle T \rangle$ 2 ME	$\langle T \rangle$ 5 ME
Start	4300 K	5100 K
Drops to	3300 K	4300 K

Our melting line and planet model

Core crystall.	$\langle T \rangle$ 2 ME	$\langle T \rangle$ 5 ME
starts at	8070 K	12500 K
ends at	7410 K	10650 K

2-layer planet: iron + silicates



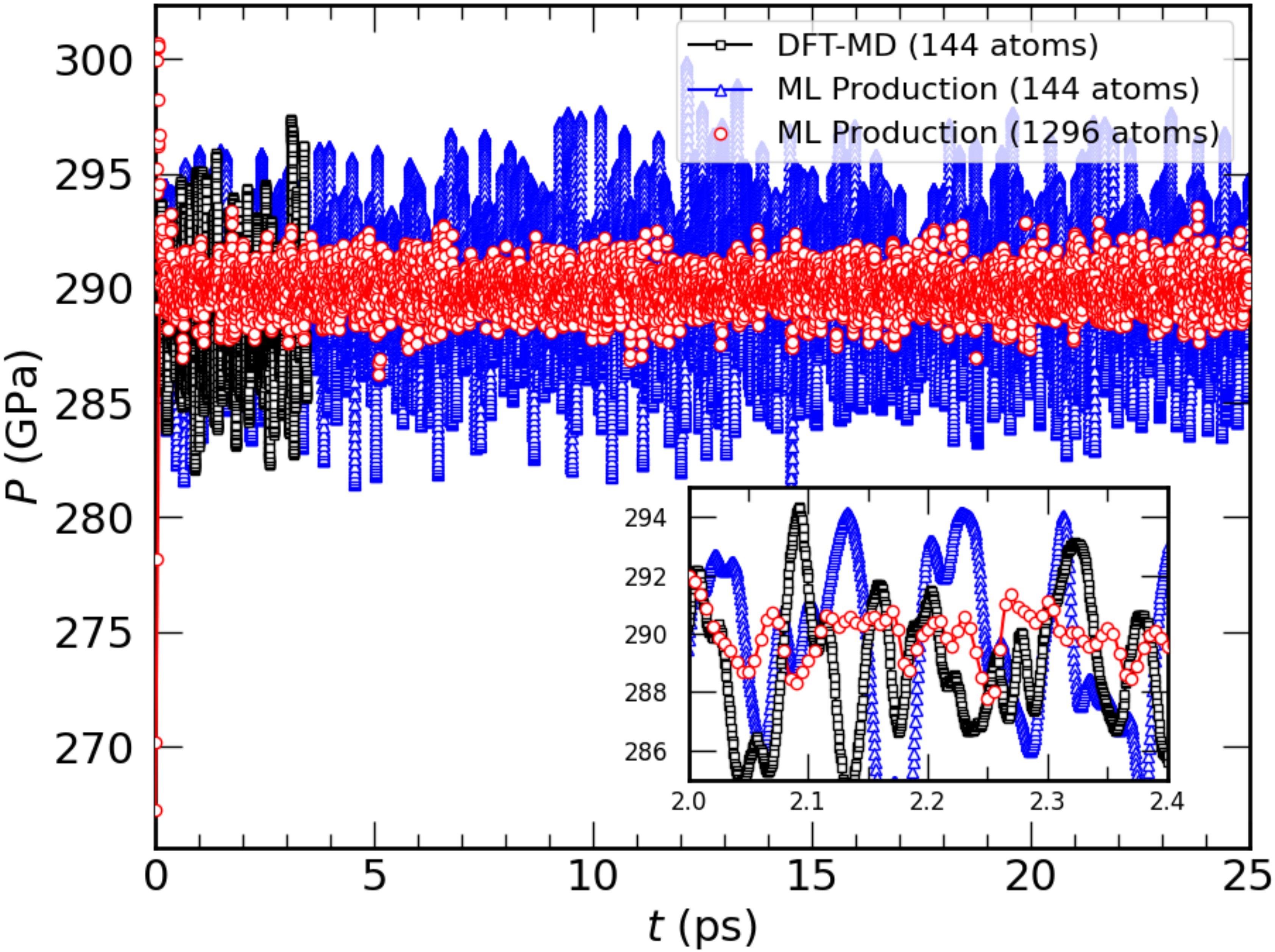
EOS &

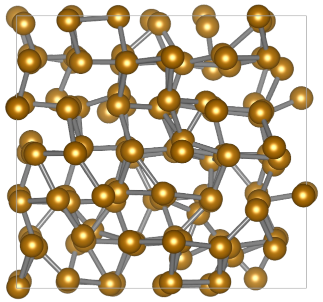
$$\frac{dP}{dr} = -\frac{Gm\rho}{r^2},$$

$$\frac{dm}{dr} = 4\pi r^2 \rho.$$

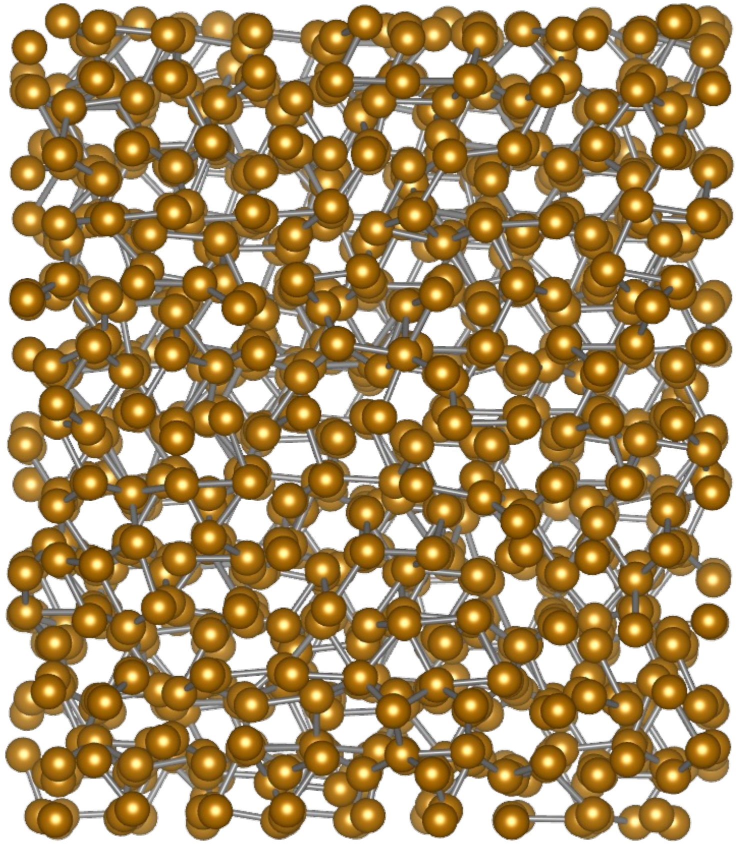
Most models with low T profiles → frozen cores

Machine Learning



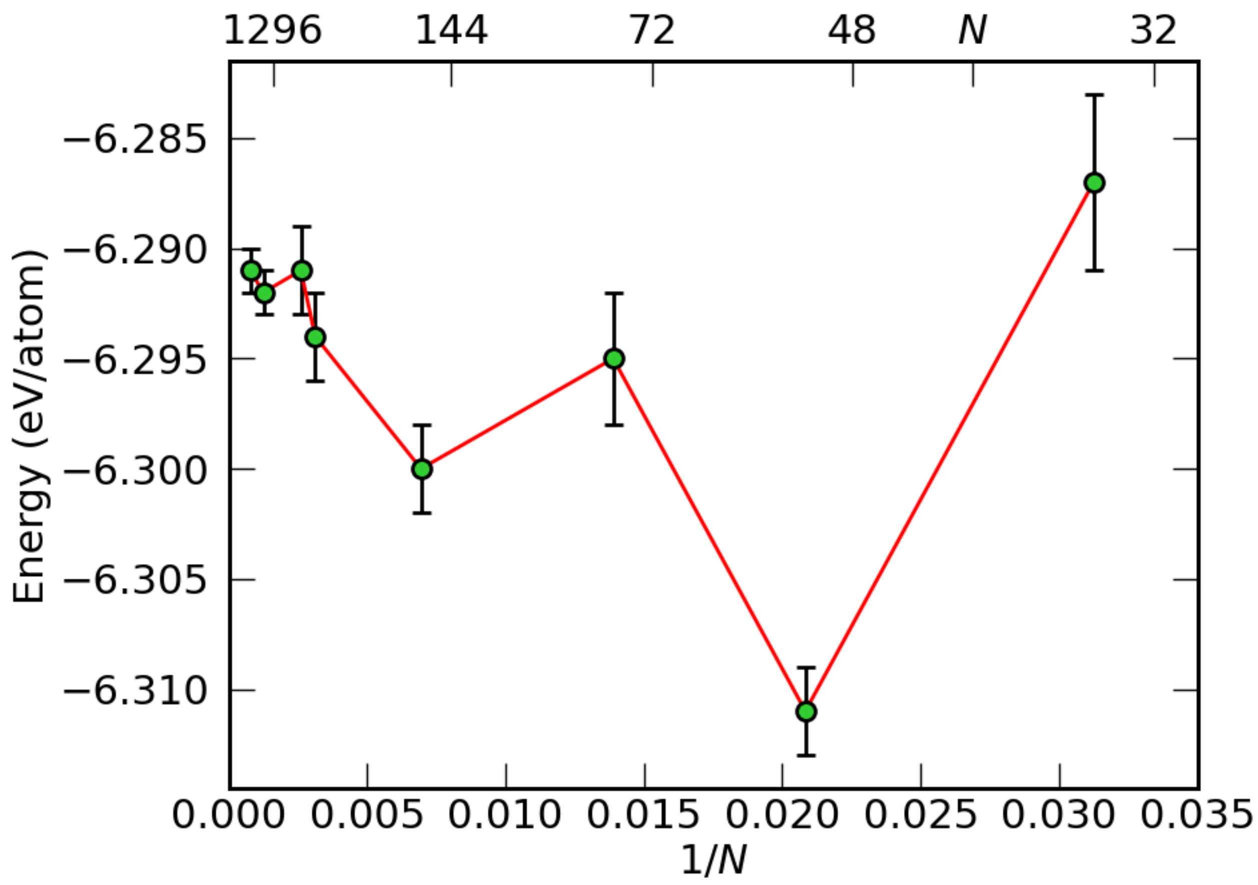


~1300 atoms ML-MD

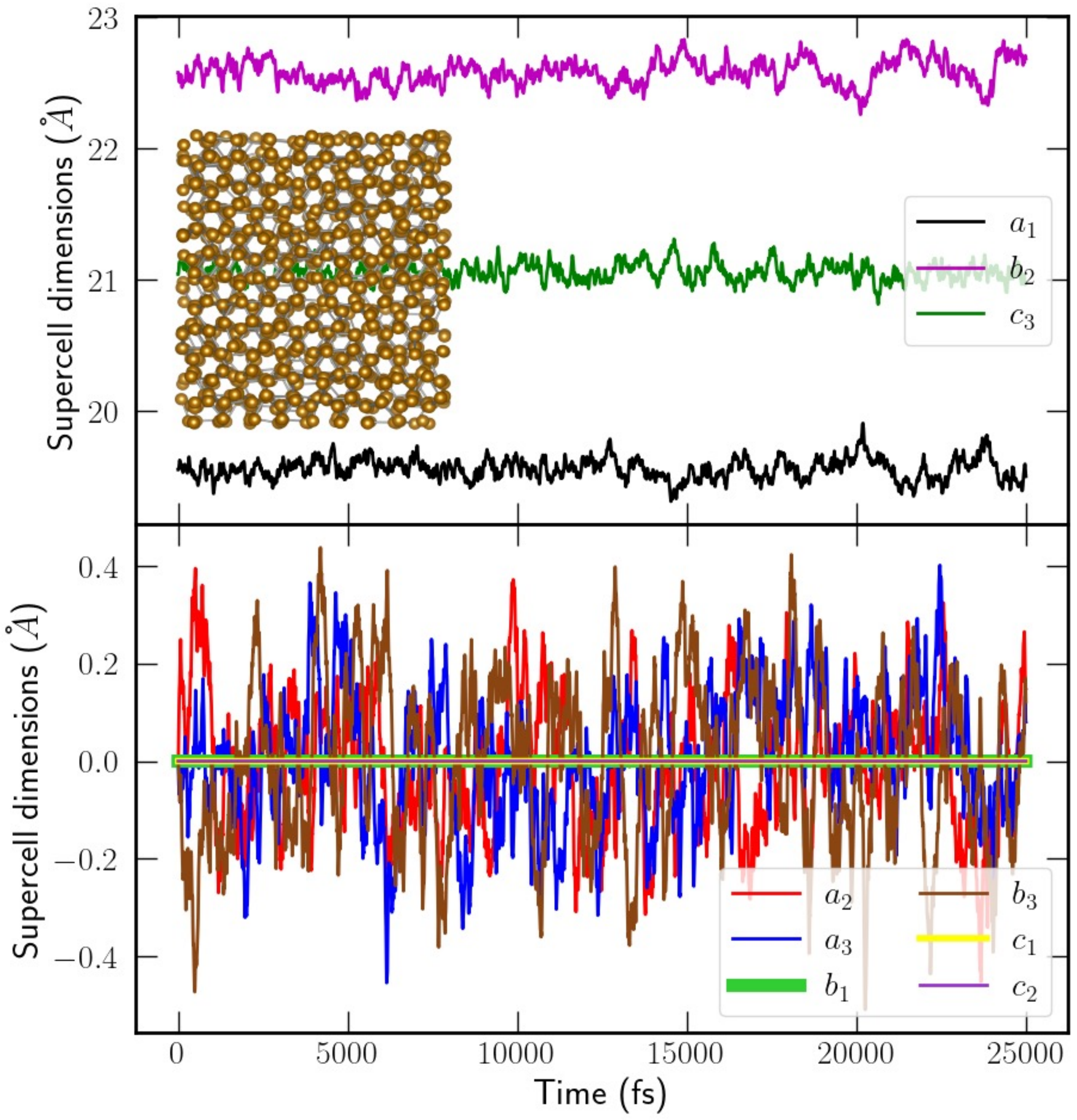


Machine Learning

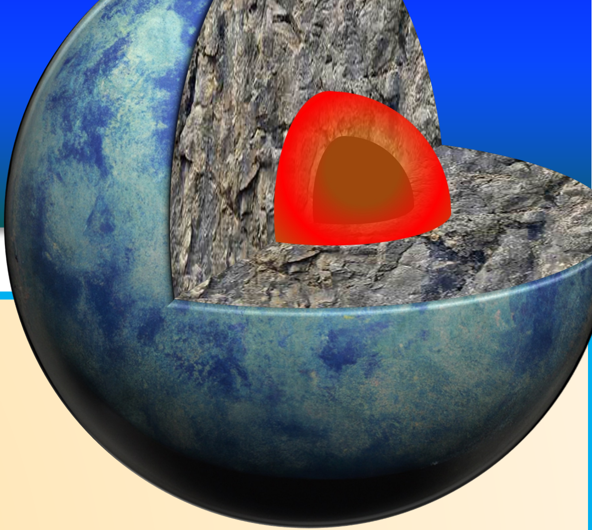
Size effects (144 atoms is enough)



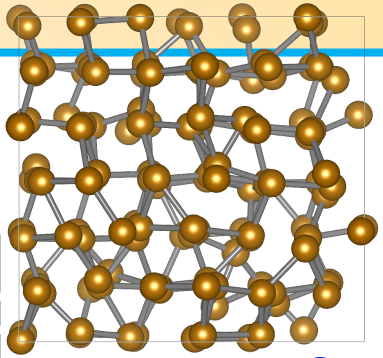
Stability: Constant Pressure



CONCLUSIONS



1. Tm(330 GPa) = 6534 ± 10 K (PAW-16)
2. Super Earths:
   - Bottom-up crystallization (300 – 5000 GPa)
   - Possible frozen cores: pressures too high to have a liquid core.
3. Machine-learning MD validates our ab initio precision.



Thanks

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