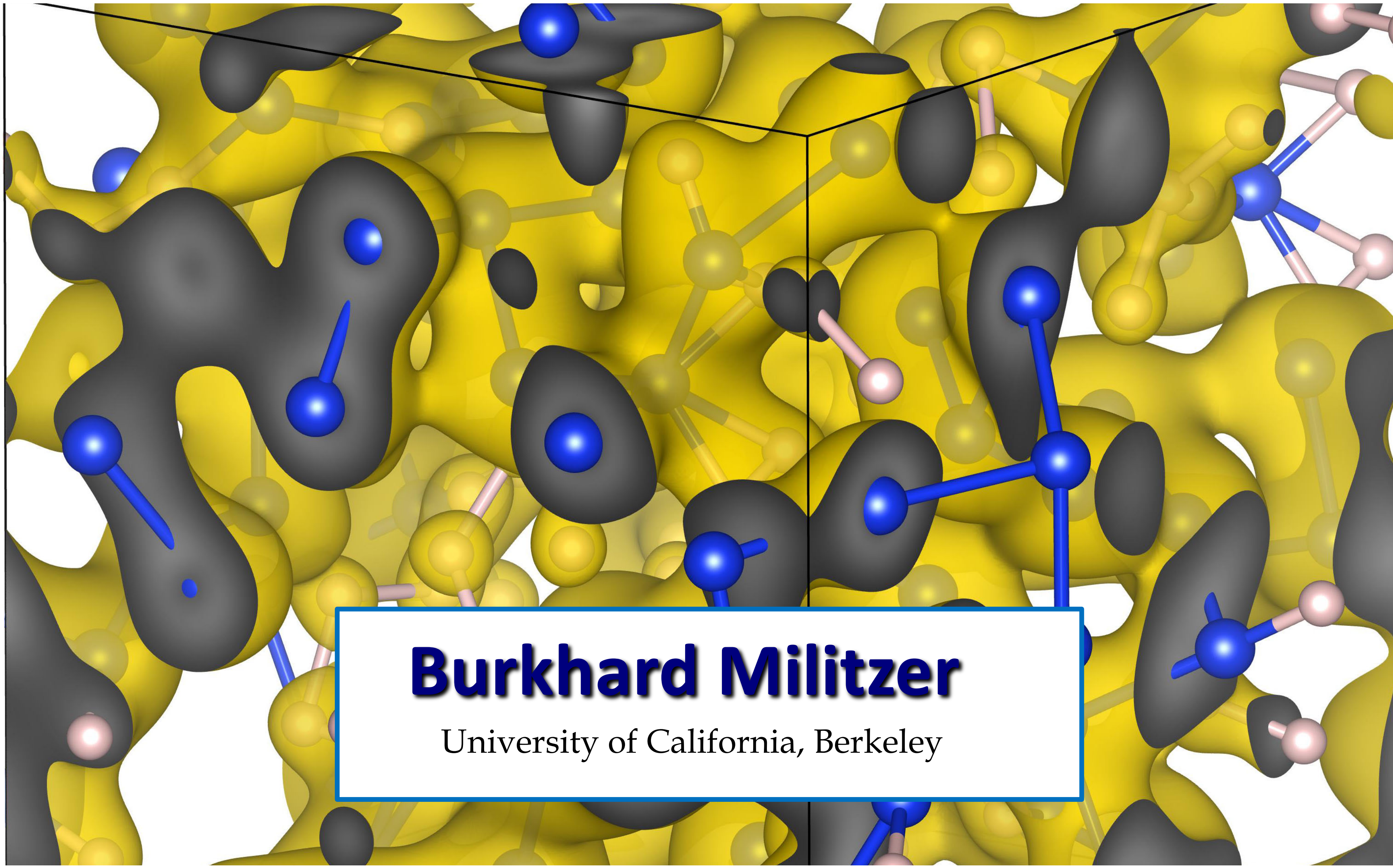
Path Integral Monte Carlo Simulations of Warm Dense Matter



Burkhard Militzer
University of California, Berkeley

Plan for L5, L9, L12 and T1 & T3

L5: Path integral Monte Carlo (PIMC) simulations and First Principles Equation of state (FPEOS) database

L9: NASA mission Juno to Jupiter, dilute core

T1: “Build that Planet” with SPH method

L12: NASA mission Cassini to Saturn. How did that planet become the Lord of the Rings?

T3: FPEOS tutorial

Software needed for T1 & T3

T1: "Built that Planet" with SPH method

Python + Jupyter notebooks (installation on laptop required, for example with Anaconda)

Alternative: use Google Colab (no installation, no animation)

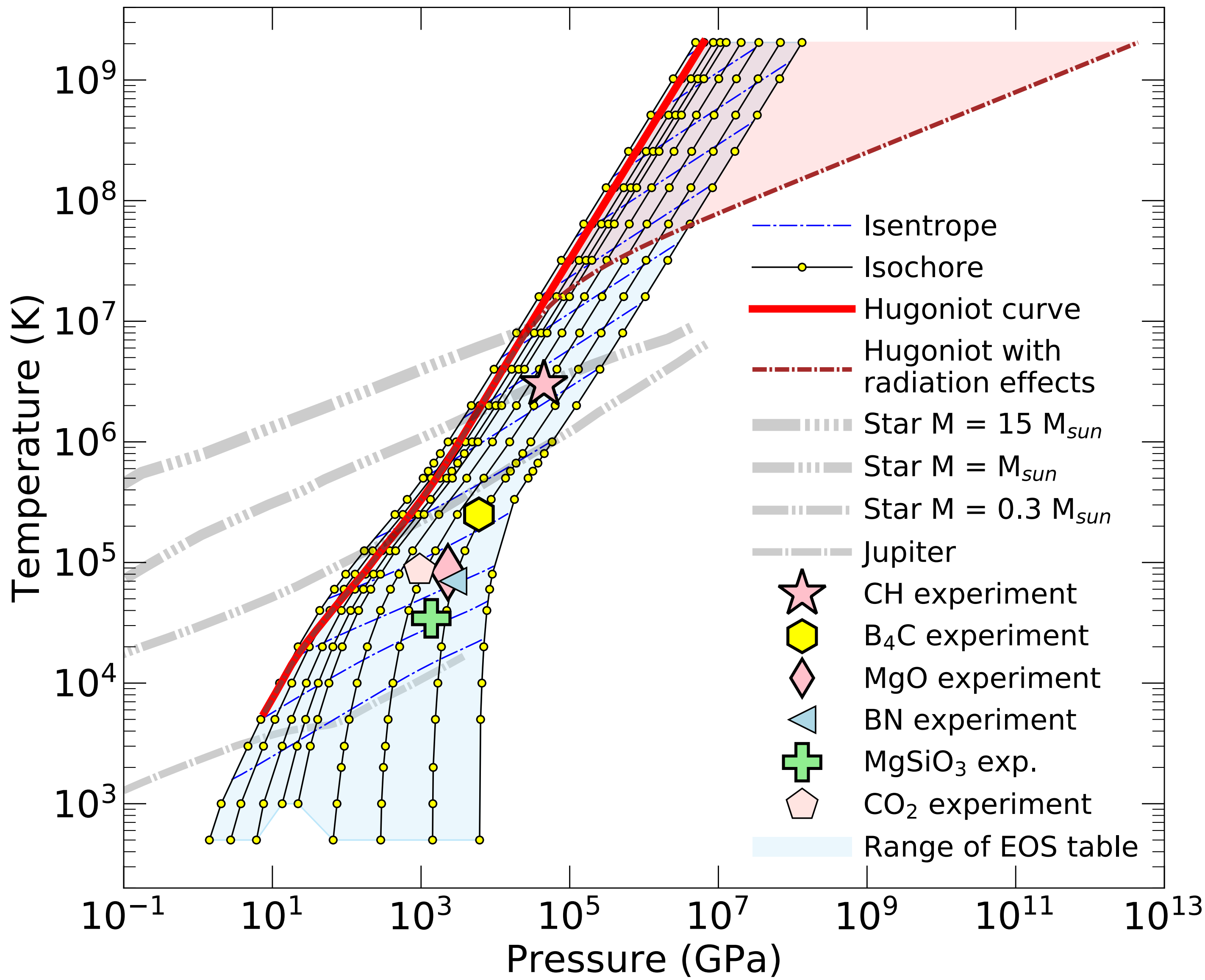
T3: FPEOS tutorial

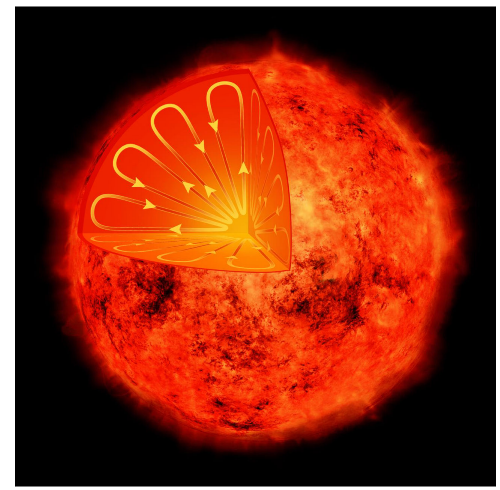
Requires a C++ compiler for all calculations, uses Python for all graphics.

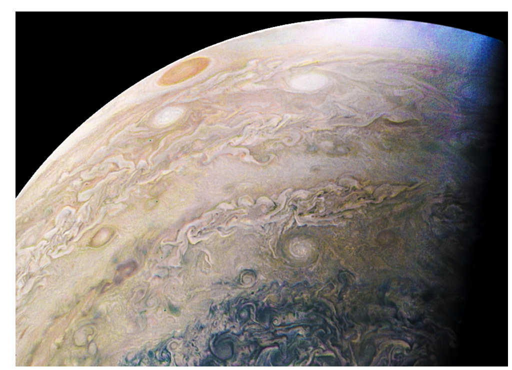
Outline of lecture 1

- Path integral Monte Carlo (PIMC) method
- Comparison with different experiments
- First Principles Equation of state (FPEOS) database

Center for Matter under Extreme Conditions (CMEC)

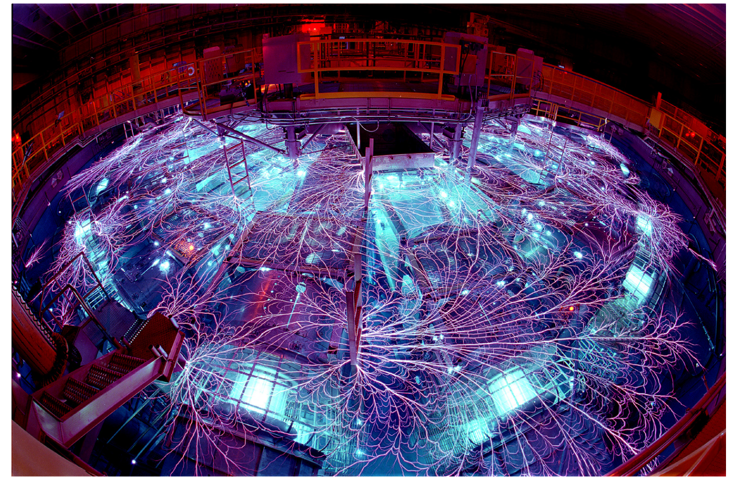




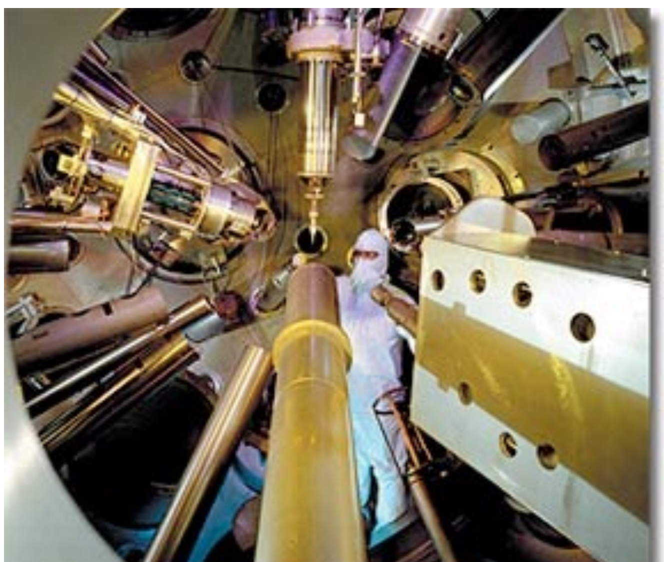


Study planetary interiors in the laboratory: shock wave experiments

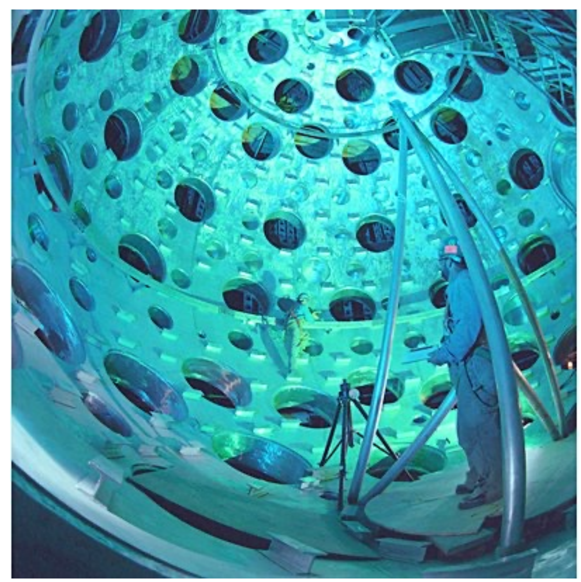
Two-stage gas gun (Livermore) 0.2 Mbar



Z capacitor bank (Sandia) 2 Mbar

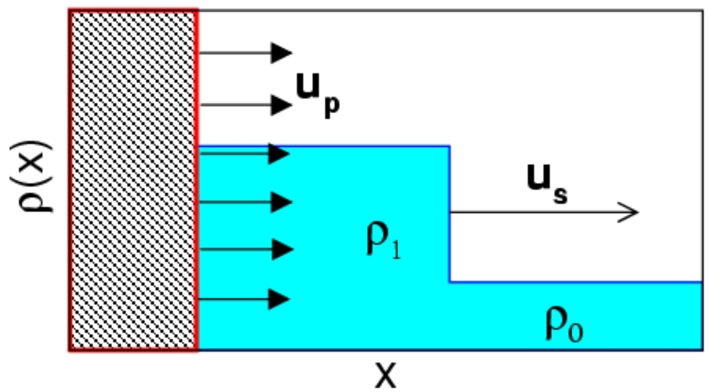


Nova laser (Livermore) 3.4 Mbar



National Ignition Facility 700 Mbar

Shock wave measurements determine the Equation of State on the Hugoniot curve

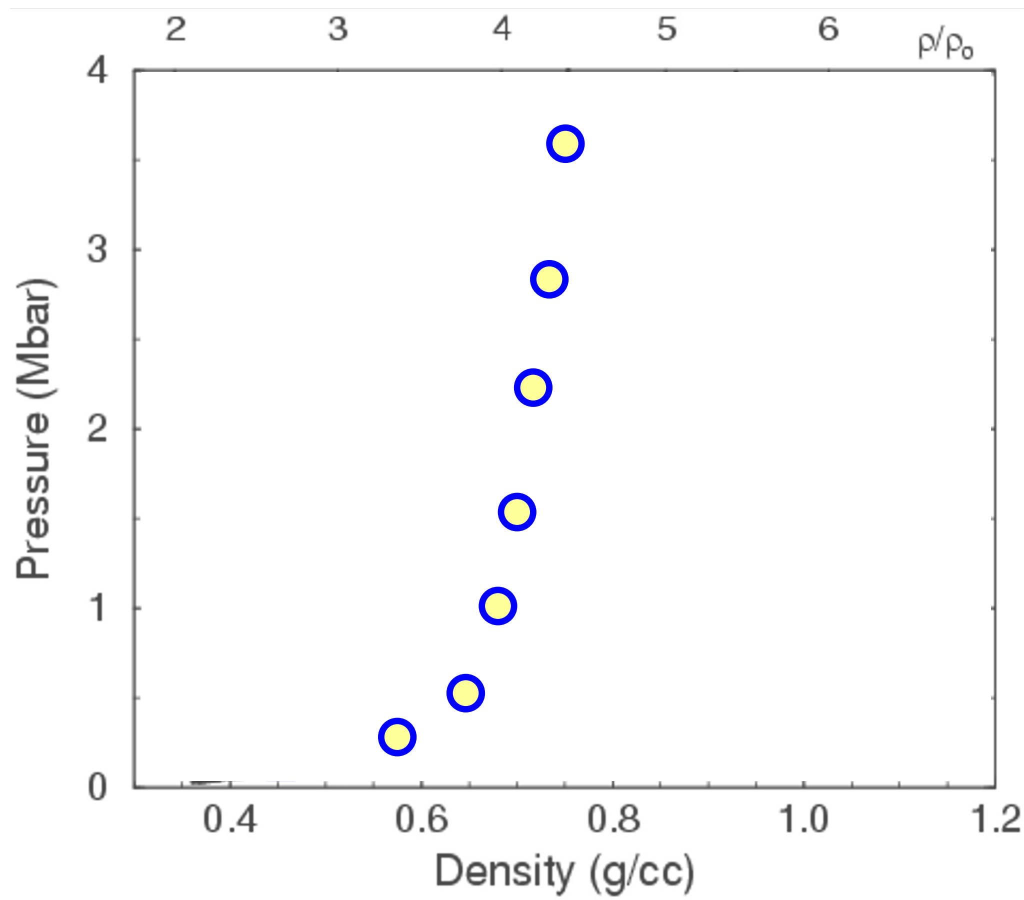


Conservation of mass, momentum and energy yields:

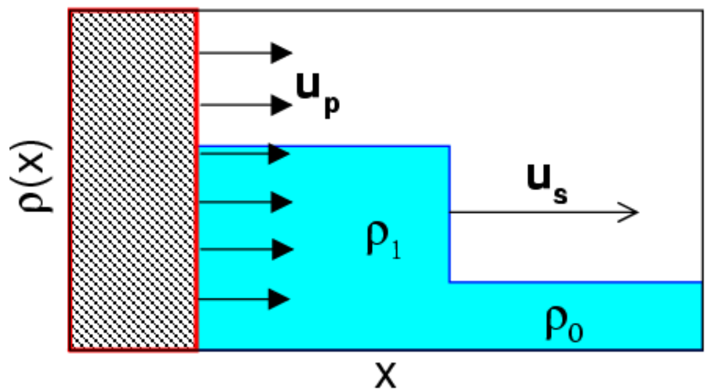
$$\rho = \rho_0 \frac{u_s}{u_s - u_p}$$

$$P = P_0 + \rho_0 u_s u_p$$

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



Shock wave measurements determine the Equation of State on the Hugoniot curve



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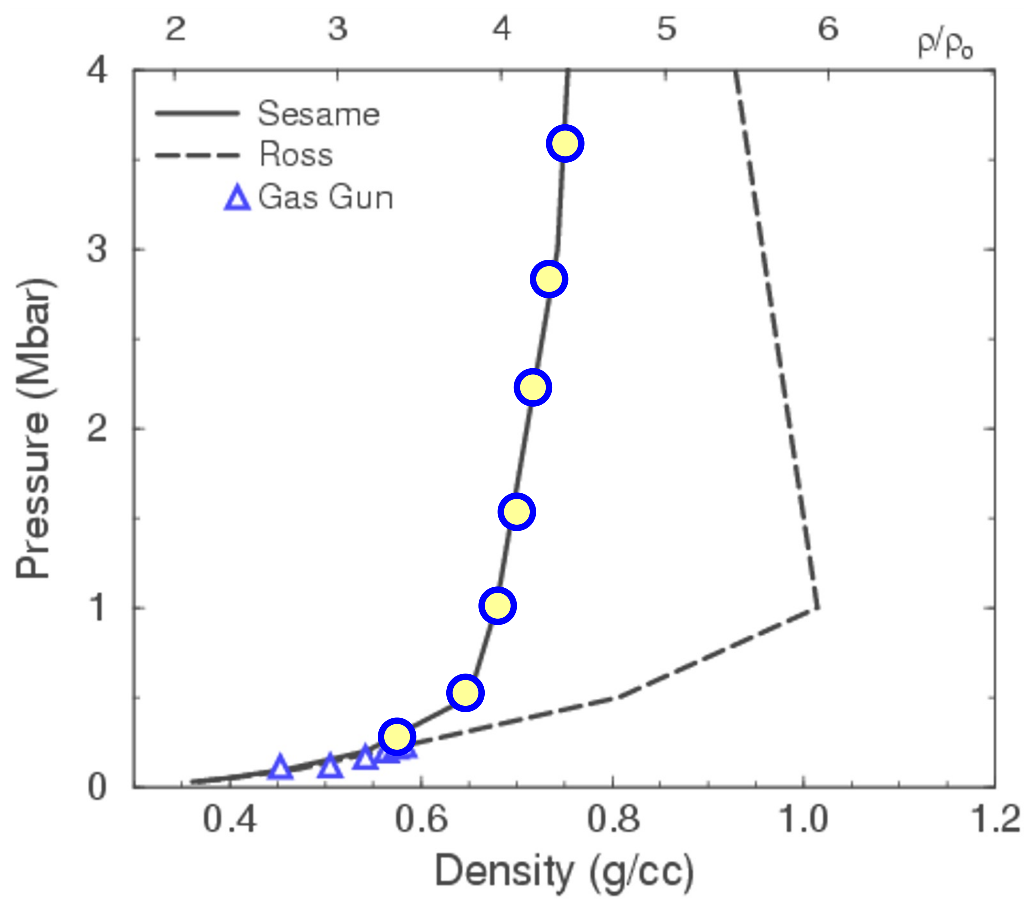
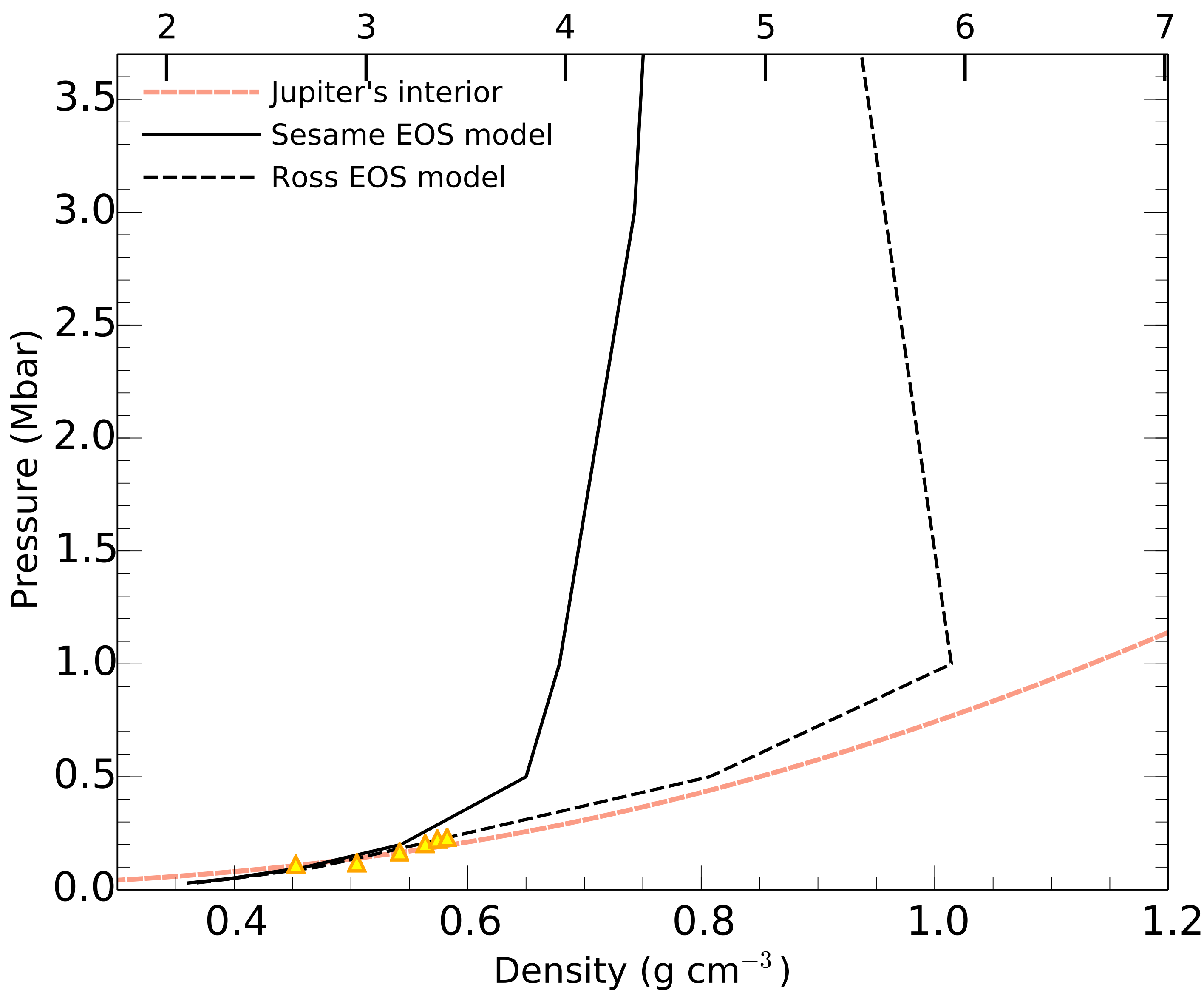


Comparison of Simulation Results and Shock Wave experiments of Deuterium



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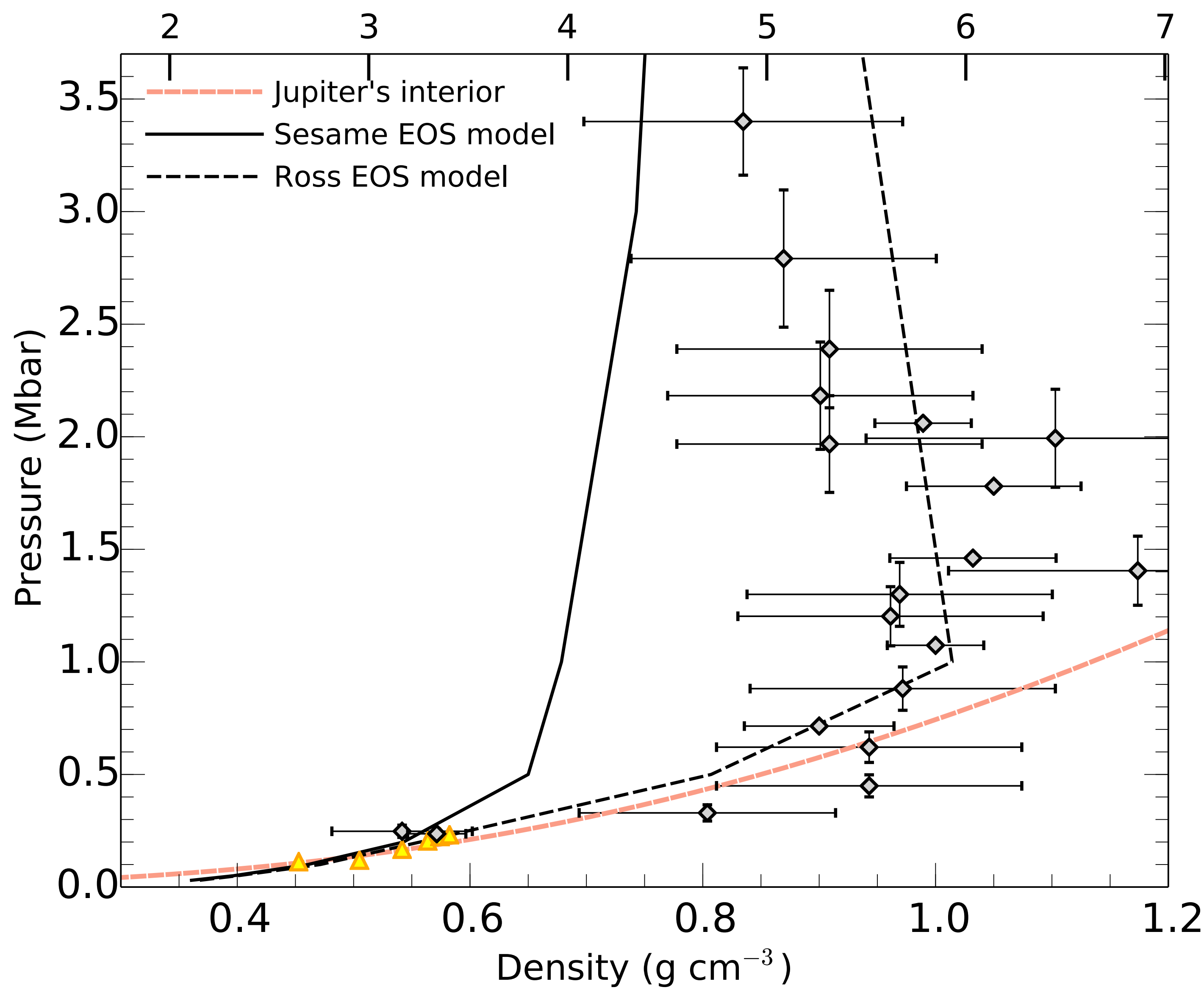

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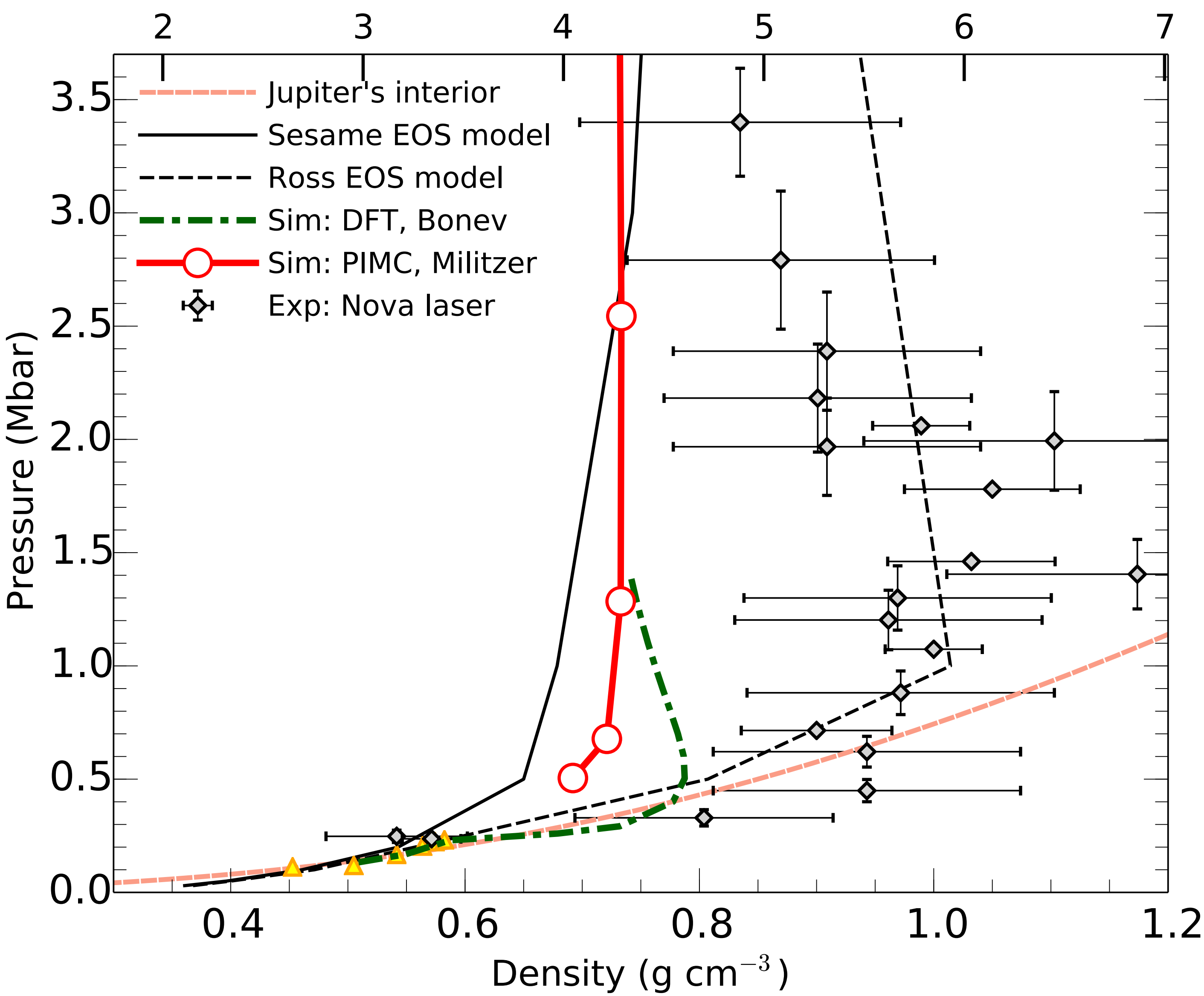

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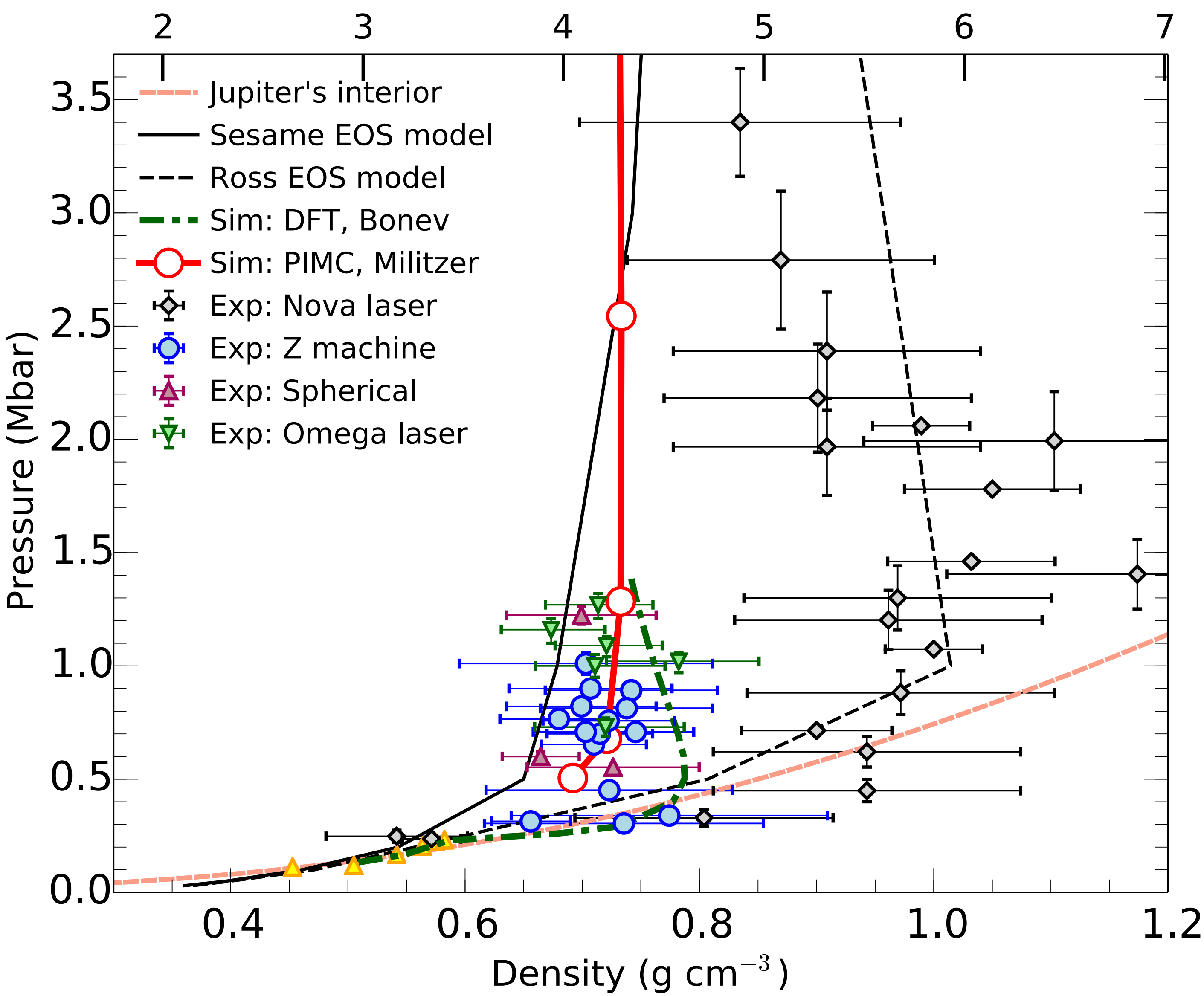
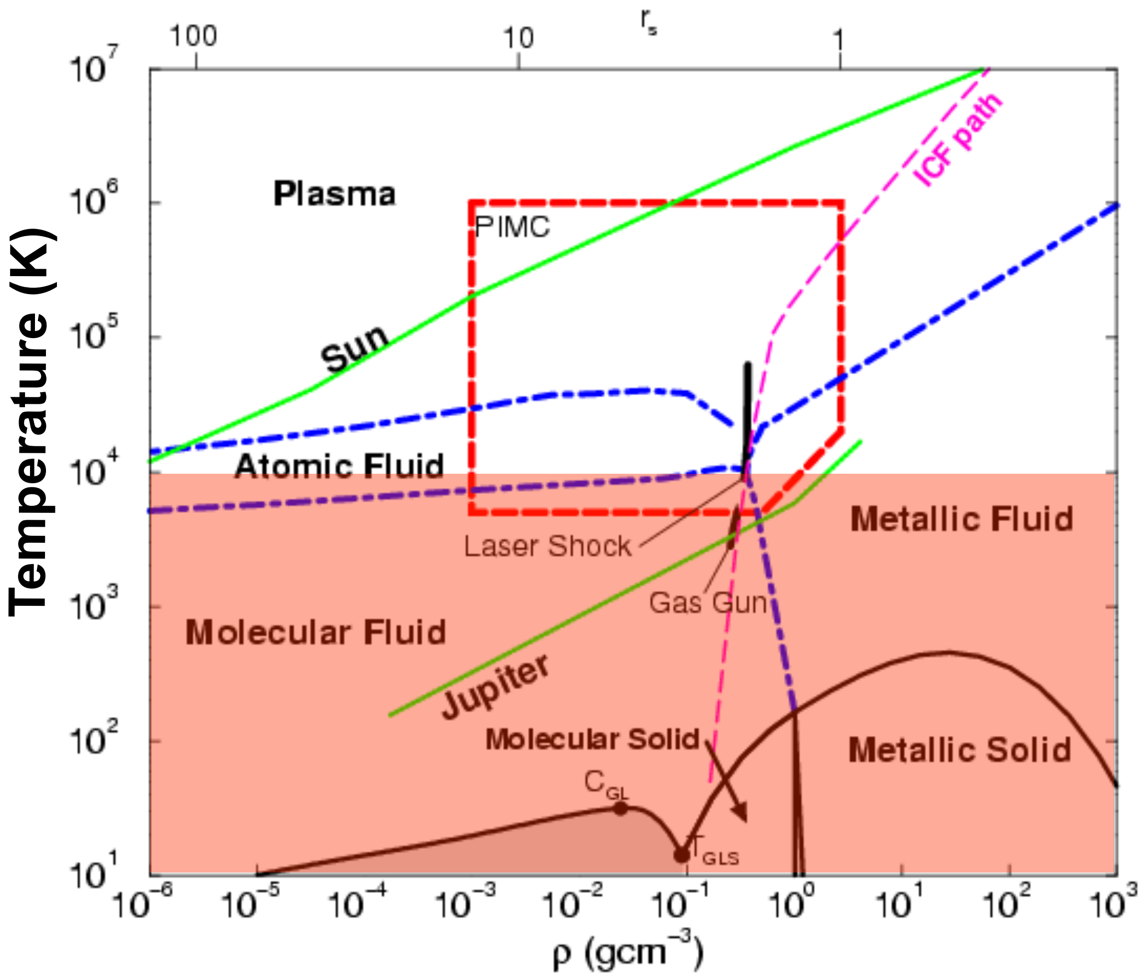
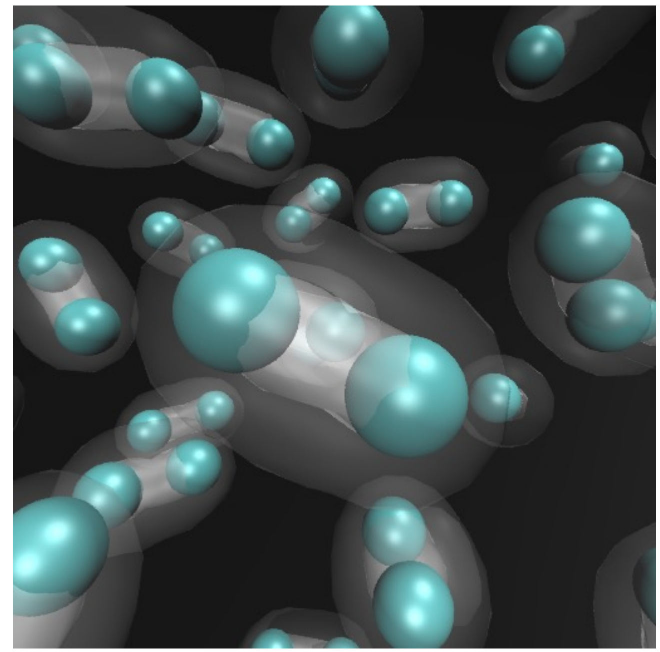


I.

Path Integral Monte Carlo

Density functional molecular dynamics at lower T



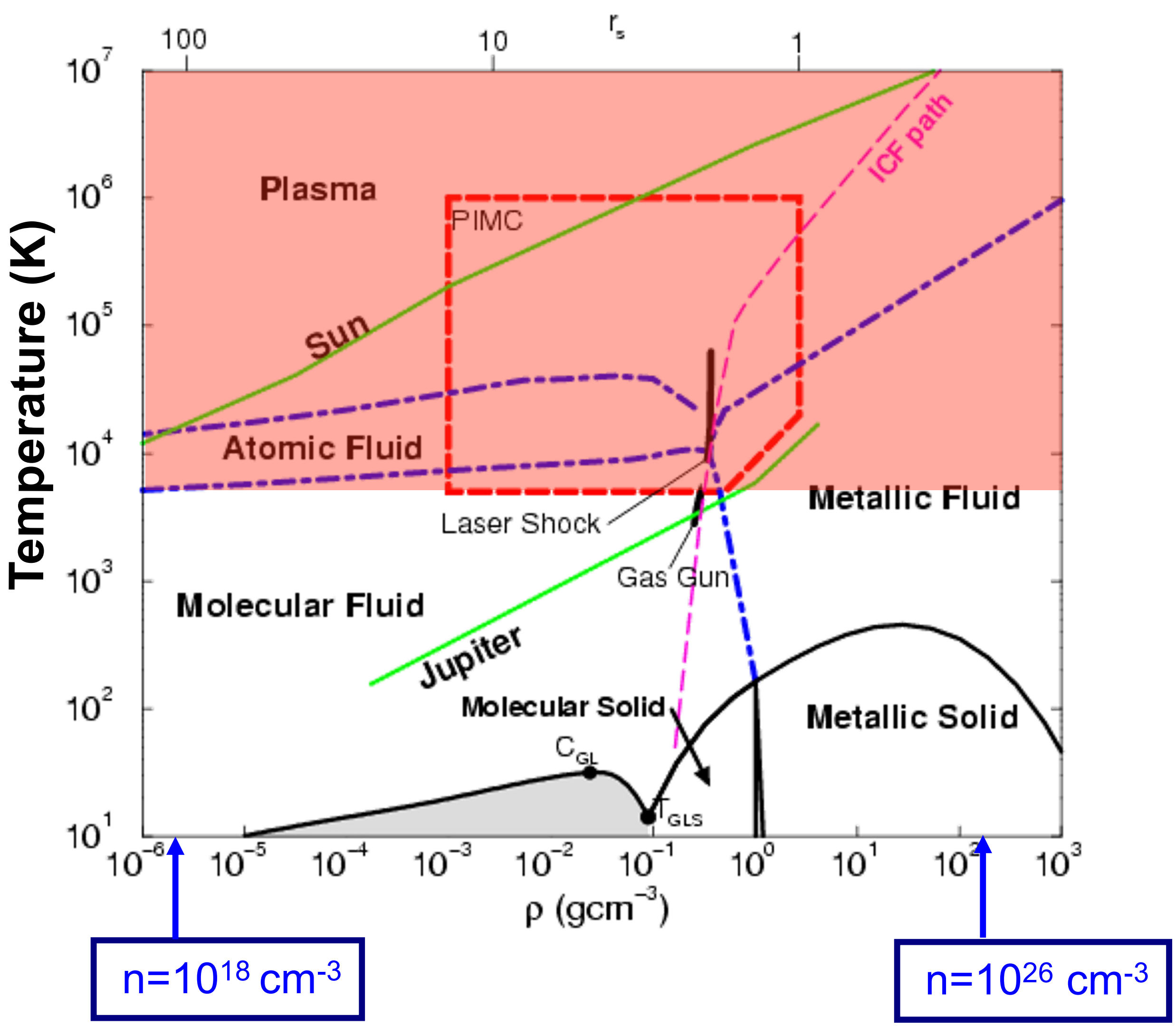


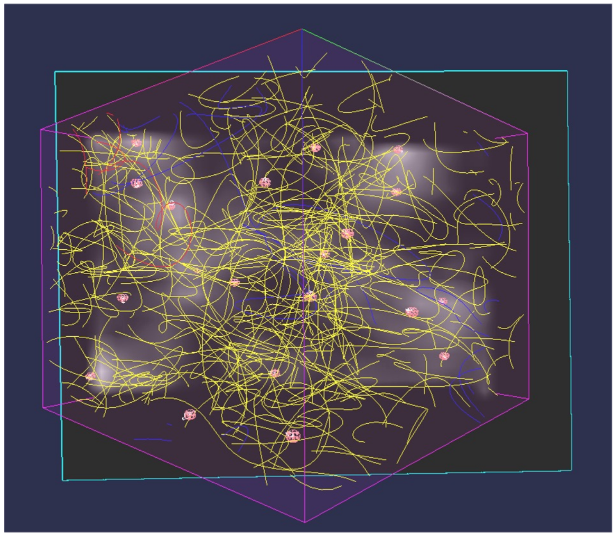
Born-Oppenheimer approx.
MD with classical nuclei:

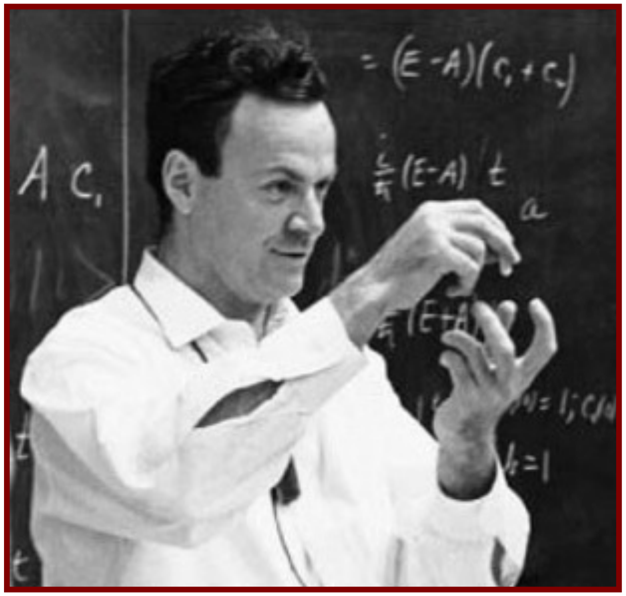
F = m a

Forces derived DFT with electrons in the instantaneous ground state.

Path integral Monte Carlo at high T > $10^4 \ldots 10^6$ K







Starting from Restricted PIMC Simulations of Hydrogen

PHYSICAL REVIEW LETTERS

VOLUME 73 | 17 OCTOBER 1994 | NUMBER 16

Equation of State of the Hydrogen Plasma by Path Integral Monte Carlo Simulation

C. Pierleoni,[1,2,*] D. M. Ceperley,[3] B. Bernu,[1] and W. R. Magro[3]

VOLUME 76, NUMBER 8 | PHYSICAL REVIEW LETTERS | 19 FEBRUARY 1996

Molecular Dissociation in Hot, Dense Hydrogen

W. R. Magro,[1] D. M. Ceperley,[2] C. Pierleoni,[3] and B. Bernu[4]

Canonical Ensembles:

Classical

Boltzmann factor

$$e^{-E / k_B T}$$

Thermodynamic averages:

$$Z_{Cl} = \sum_{S} e^{-\beta E_S}$$

Canonical Ensembles:

Classical

Quantum

Boltzmann factor

$$e^{-E / k_B T}$$

Density matrix

$$\hat{\rho} = e^{-\beta \hat{H}}$$

$$\rho(R,R',\beta) = \langle R | e^{-\beta \hat{H}} | R' \rangle$$

$$\rho(R,R',\beta) = \sum_S e^{-\beta E_S} \Psi_S^*(R) \Psi_S(R')$$

Thermodynamic averages:

$$Z_{Cl} = \sum_S e^{-\beta E_S}$$

$$Z_Q = Tr[\hat{\rho}] = \int dR \langle R | e^{-\beta \hat{H}} | R \rangle$$

$$\langle \hat{O} \rangle = \frac{Tr[\hat{O} \hat{\rho}]}{Tr[\hat{\rho}]}$$

Step 1 towards the path integral

Matrix squaring property of the density matrix

Matrix squaring in operator notation:

$$\hat{\rho} = e^{-\beta\hat{\mathrm{H}}} = \left(e^{-(\beta/2)\hat{\mathrm{H}}}\right)\left(e^{-(\beta/2)\hat{\mathrm{H}}}\right), \quad \beta = \frac{1}{k_B T}$$

Matrix squaring in real-space notation:

$$\langle R \,|\, \hat{\rho} \,|\, R' \rangle = \int dR_1 \; \langle R \,|\, e^{-(\beta/2)\hat{\mathrm{H}}} \,|\, R_1 \rangle \; \langle R_1 \,|\, e^{-(\beta/2)\hat{\mathrm{H}}} \,|\, R' \rangle$$

Matrix squaring in matrix notation:

$$\begin{bmatrix} \dots & R' & \dots \\ R & \ddots & \vdots \\ \dots & \dots & \dots \end{bmatrix} = \begin{bmatrix} \dots & R_1 & \dots \\ R & \ddots & \vdots \\ \dots & \dots & \dots \end{bmatrix} * \begin{bmatrix} \dots & R' & \dots \\ R_1 & \ddots & \vdots \\ \dots & \dots & \dots \end{bmatrix}$$

Repeat the matrix squaring step

Matrix squaring in operator notation:

$$\hat{\rho} = e^{-\beta\hat{\mathrm{H}}} = \left(e^{-(\beta/4)\hat{\mathrm{H}}}\right)^4, \;\; \beta = \frac{1}{k_B T}$$

Matrix squaring in real-space notation:

$$\langle R \,|\, \hat{\rho} \,|\, R' \rangle = \int dR_1 \int dR_2 \int dR_3 \langle R \,|\, e^{-(\beta/4)\hat{\mathrm{H}}} \,|\, R_1 \rangle \langle R_1 \,|\, e^{-(\beta/4)\hat{\mathrm{H}}} \,|\, R_2 \rangle \langle R_2 \,|\, e^{-(\beta/4)\hat{\mathrm{H}}} \,|\, R_3 \rangle \langle R_3 \,|\, e^{-(\beta/4)\hat{\mathrm{H}}} \,|\, R' \rangle$$

Path Integrals in Imaginary Time

Every particle is represented by a path, a ring polymer.

Density matrix:

$$\hat{\rho} = e^{-\beta \hat{\mathrm{H}}} = \left(e^{-\tau \hat{\mathrm{H}}}\right)^{M}, \quad \beta = \frac{1}{k_B T}, \quad \tau = \frac{\beta}{M}$$

$$\langle \hat{O} \rangle = \frac{\mathrm{Tr}[\hat{O}\hat{\rho}]}{\mathrm{Tr}[\hat{\rho}]}$$

Trotter break-up:

$$\langle R | \hat{\rho} | R' \rangle = \langle R | (e^{-\tau \hat{\mathrm{H}}})^{M} | R' \rangle = \int dR_1 \ldots \int dR_{M-1} \langle R | e^{-\tau \hat{\mathrm{H}}} | R_1 \rangle \langle R_1 | e^{-\tau \hat{\mathrm{H}}} | R_2 \rangle \ldots \langle R_{M-1} | e^{-\tau \hat{\mathrm{H}}} | R' \rangle$$

Path Integrals in Imaginary Time

Simplest form for the paths' action: primitive approx.

Density matrix:

$$\hat{\rho} = e^{-\beta \hat{\mathrm{H}}} = \left(e^{-\tau \hat{\mathrm{H}}}\right)^M \,, \quad \beta = \frac{1}{k_B T} \,, \quad \tau = \frac{\beta}{M}$$

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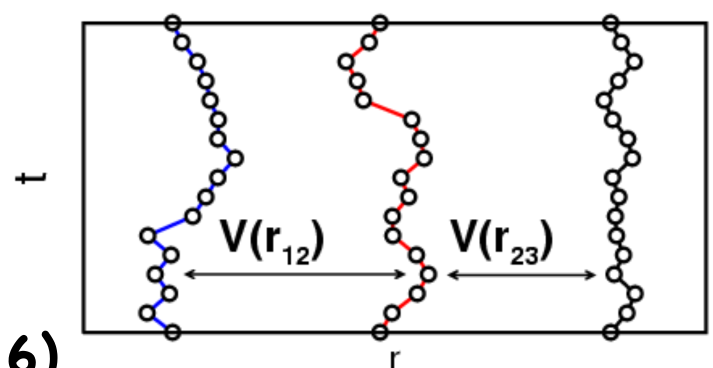
Trotter formula:

$$e^{-\beta(\hat{T}+\hat{V})} = \lim_{M \to \infty} \left[e^{-\tau \hat{T}} e^{-\tau \hat{V}} \right]^M$$

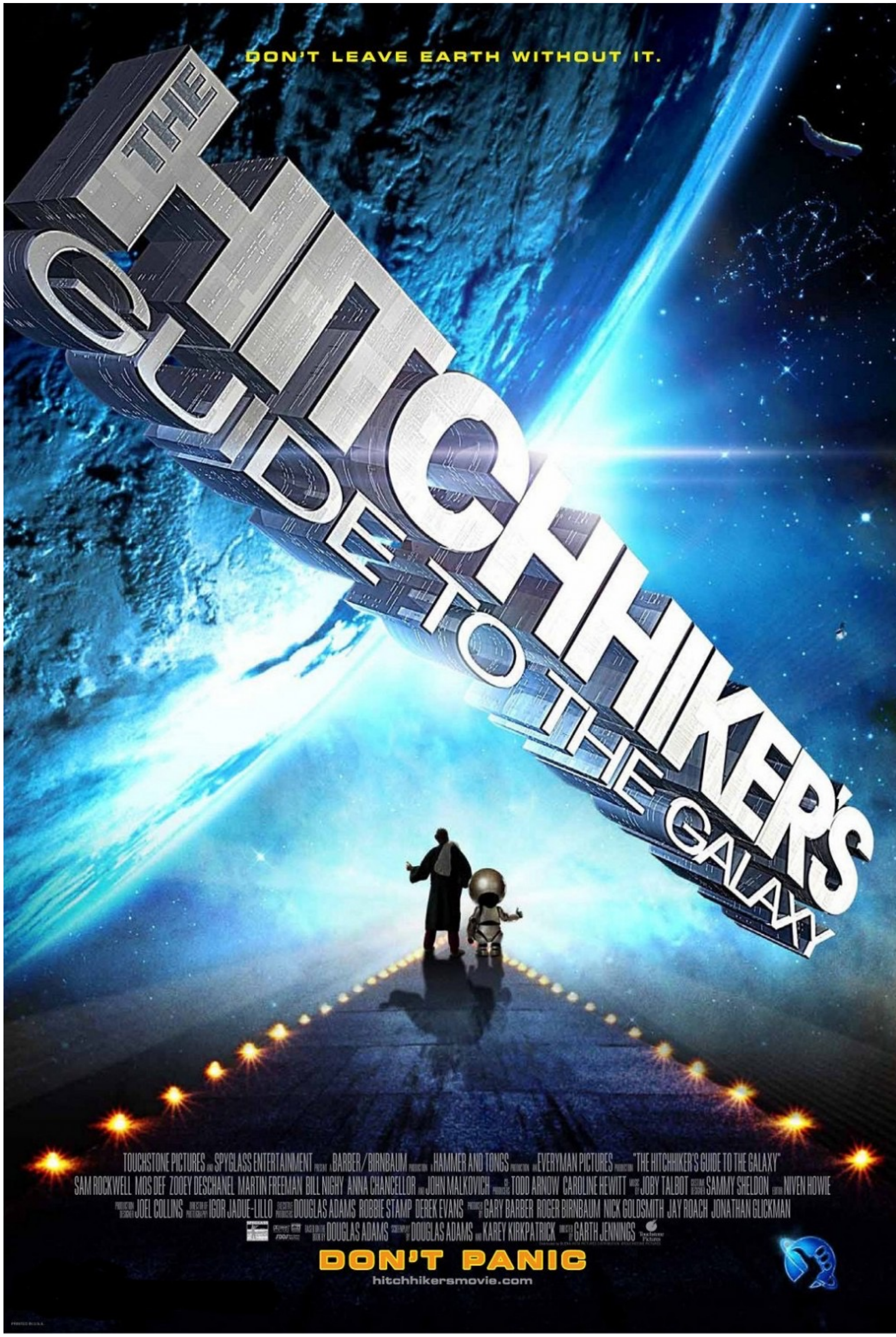
Path integral and primitive action S :

$$\langle R | \hat{\rho} | R' \rangle = \oint_{R \to R'} dR_t \, e^{-S[R_t]}$$

$$S[R_t] = \sum_{i=1}^{M} \frac{(R_{i+1} - R_i)^2}{4\lambda\tau} + \frac{\tau}{2}\left[V(R_i) + V(R_{i+1}) \right]$$



Pair action: Militzer, Comp. Phys. Comm. (2016)



Douglas Adams:

"Infinite Improbability Drive"

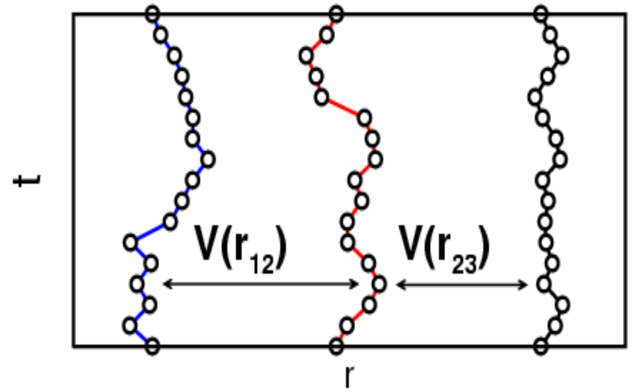
of spaceship

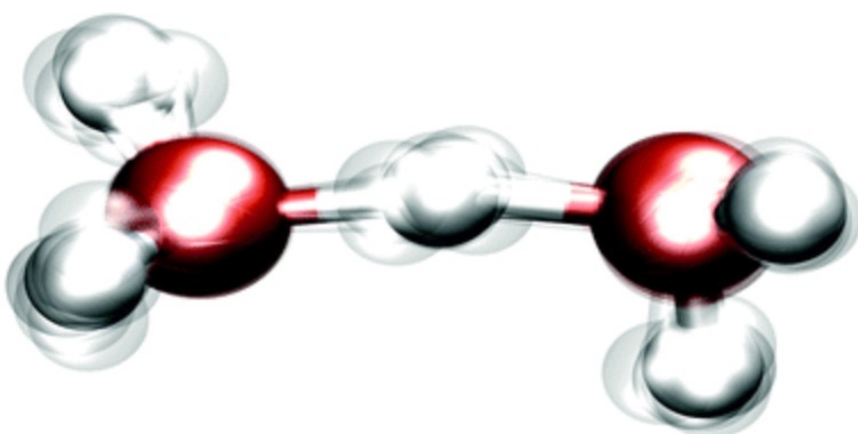
"Heart of Gold"

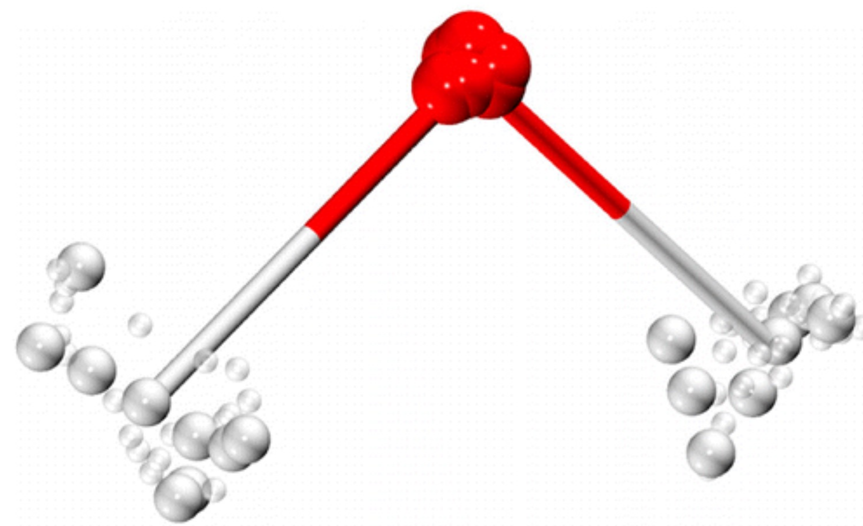
Path Integrals in Imaginary Time include Zero-Point Motion and some Tunnelling Effects

$$\langle R \mid \hat{\rho} \mid R' \rangle = \oint_{R \rightarrow R'} dR_t e^{-S[R_t]}$$

$$S[R_t] = \sum_{i=1}^{M} \frac{(R_{i+1} - R_i)^2}{4\lambda\tau} + \frac{\tau}{2}\left[V(R_i) + V(R_{i+1})\right]$$







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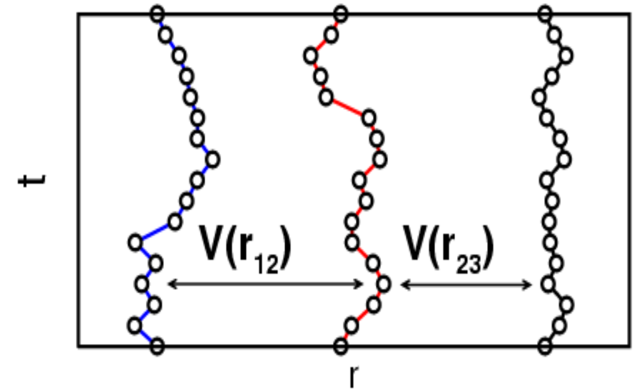

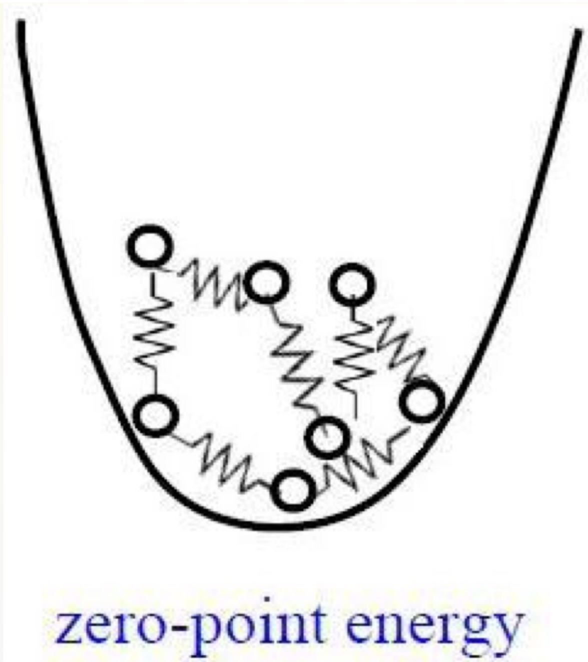

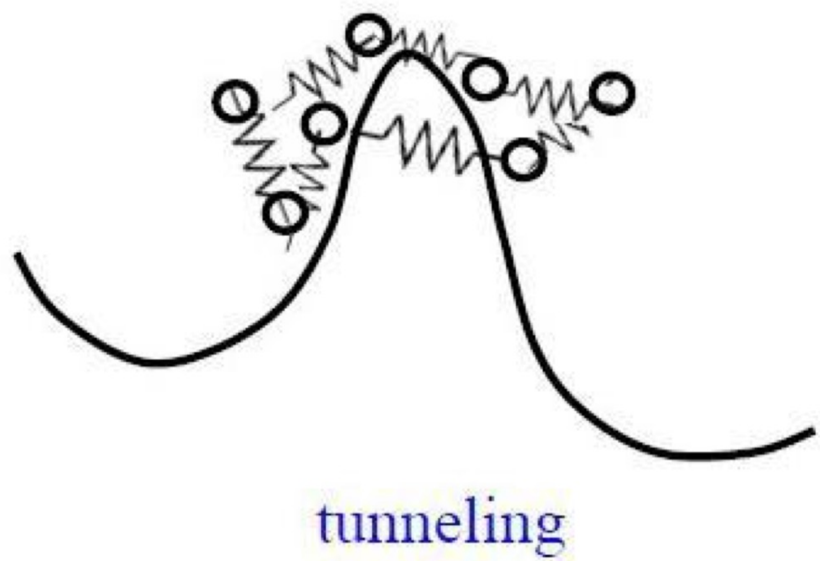

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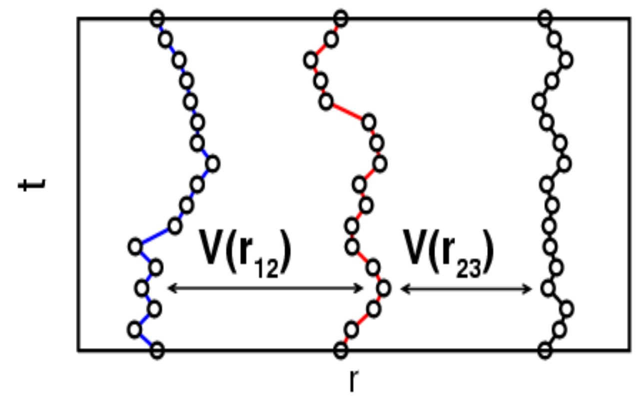

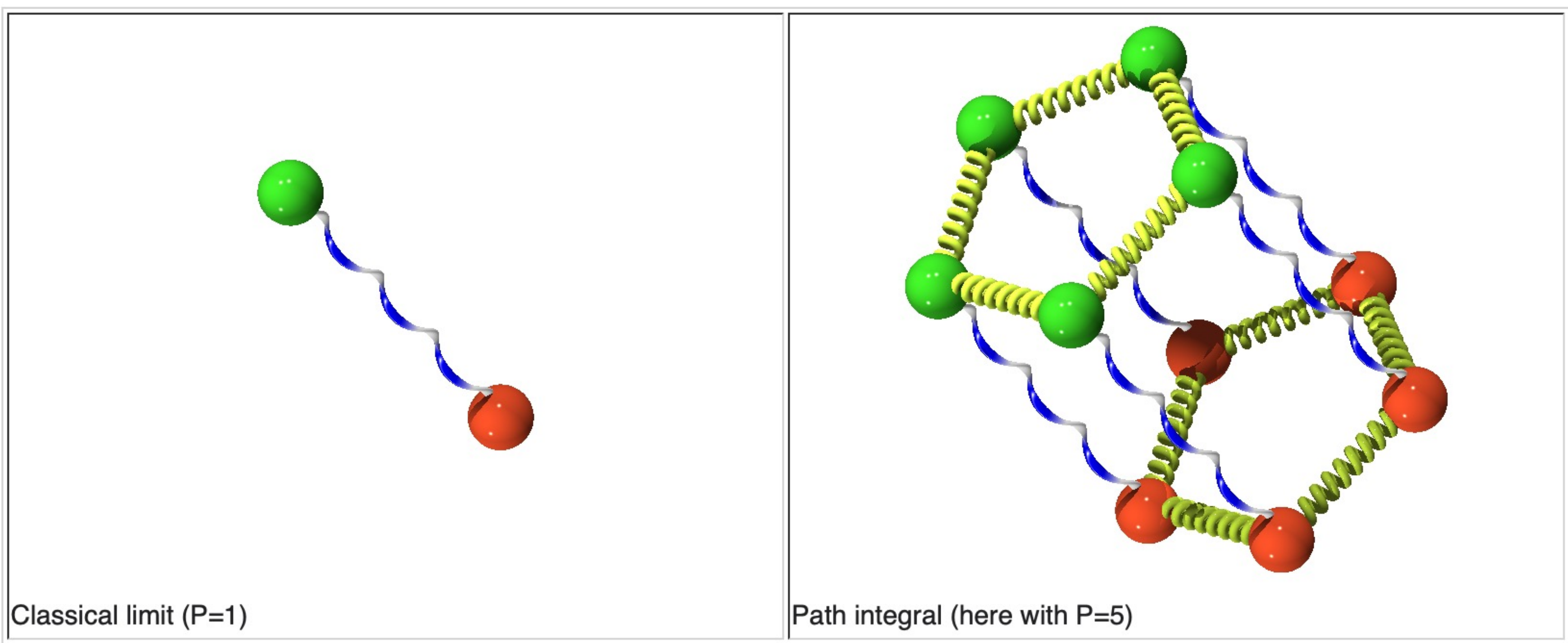

Bosonic and Fermionic Density Matrices

Bosonic density matrix:
Sum over all symmetric eigenstates.

$$\rho_B(R,R',\beta) = \sum_i e^{-\beta\ E_i}\ \ \Psi_S^{[i]*}(R)\ \ \Psi_S^{[i]}(R')$$

Fermionic density matrix:
Sum over all antisymmetric eigenstates.

$$\rho_F(R,R',\beta) = \sum_i e^{-\beta\ E_i}\ \ \Psi_{AS}^{[i]*}(R)\ \ \Psi_{AS}^{[i]}(R')$$

Bosonic and Fermionic Path Integrals

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Fermionic density matrix:
Sum over all antisymmetric eigenstates.

$$\rho_F(R,R',\beta) = \sum_i e^{-\beta E_i} \; \Psi_{AS}^{[i]*}(R) \; \Psi_{AS}^{[i]}(R')$$

Project out the symmetric states:

$$\rho_B(R,R',\beta) = \sum_P (+1)^P \; \rho_D(R,PR',\beta)$$

Project out the antisymmetric states:

$$\rho_F(R,R',\beta) = \sum_P (-1)^P \; \rho_D(R,PR',\beta)$$

$$\langle R \,|\, \hat{\rho}_{F/B} \,|\, R' \rangle = \sum_P (\pm 1)^P \int dR_1 \ldots \int dR_{M-1} \langle R \,|\, e^{-\tau \hat{\mathrm{H}}} \,|\, R_1 \rangle \ldots \langle R_{M-1} \,|\, e^{-\tau \hat{\mathrm{H}}} \,|\, PR' \rangle$$

Bosonic and Fermionic Path Integrals

Bosonic density matrix:
Sum over all symmetric eigenstates.

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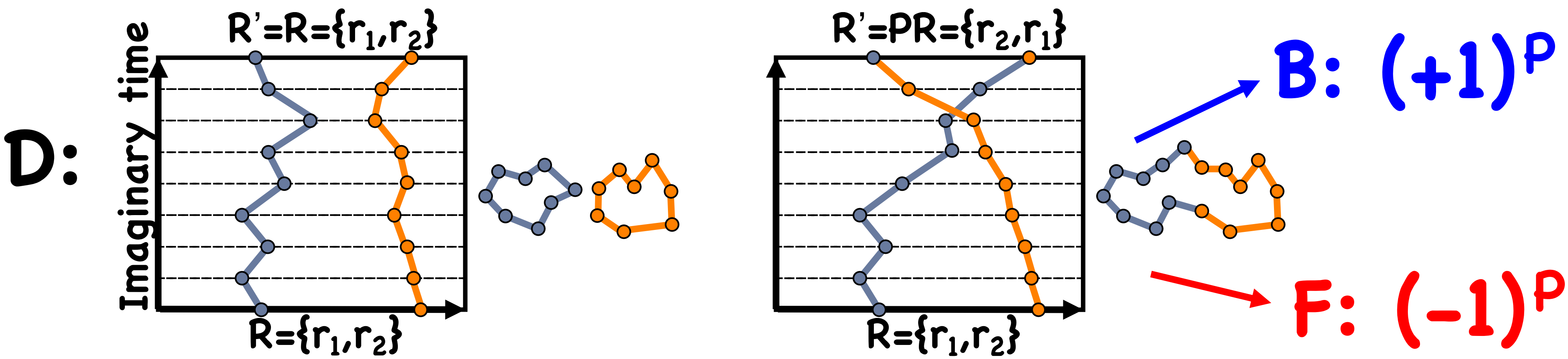


Bosonic and Fermionic P… …tegrals

Bosonic density matrix:
Sum over all symmetric eigensta…

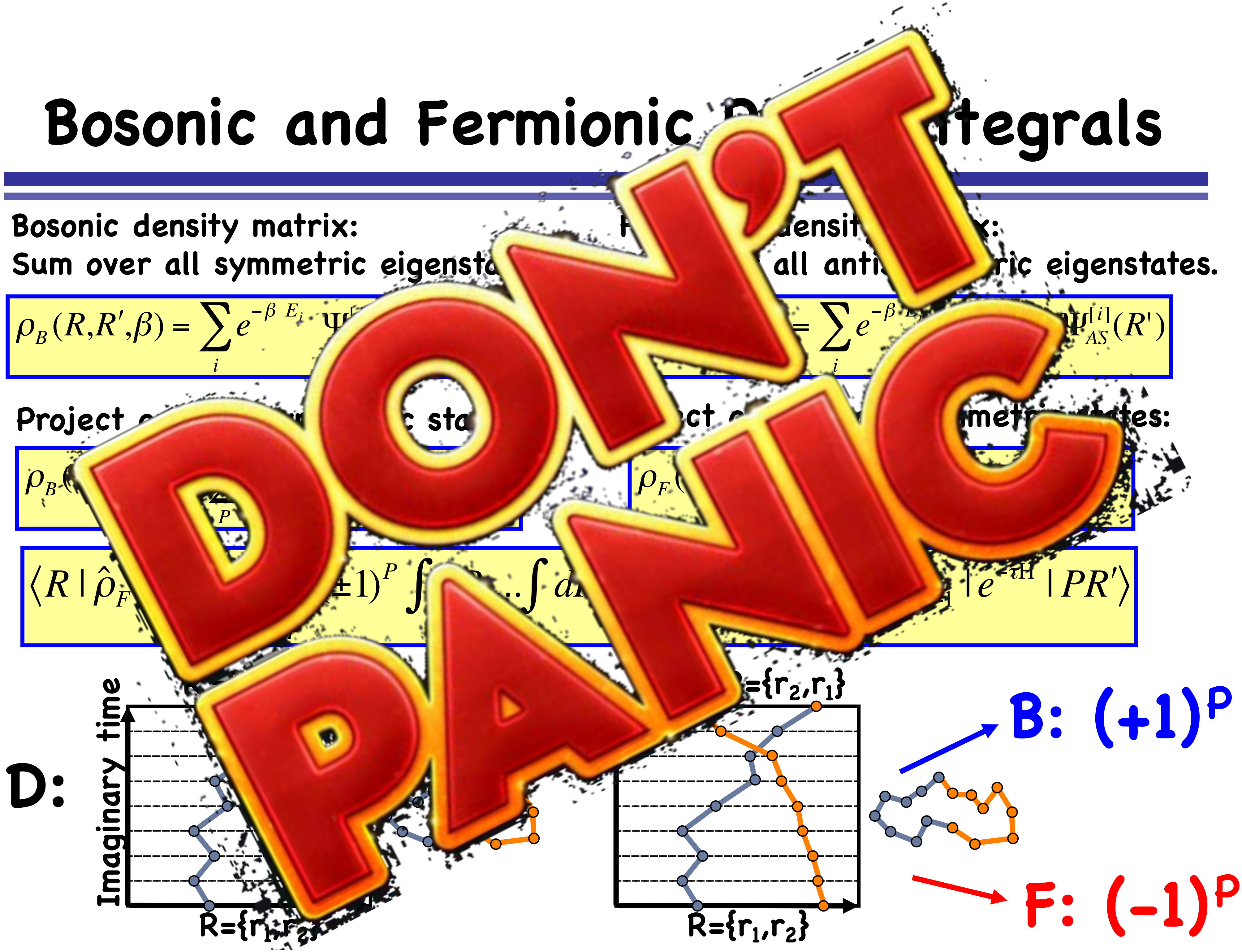
F… densit… …x:
… all anti… …ric eigenstates.

$$\rho_B(R,R',\beta) = \sum_i e^{-\beta E_i} \Psi^{[\ldots}$$ … $$= \sum_i e^{-\beta E_i} \ldots \Psi_{AS}^{[i]}(R')$$

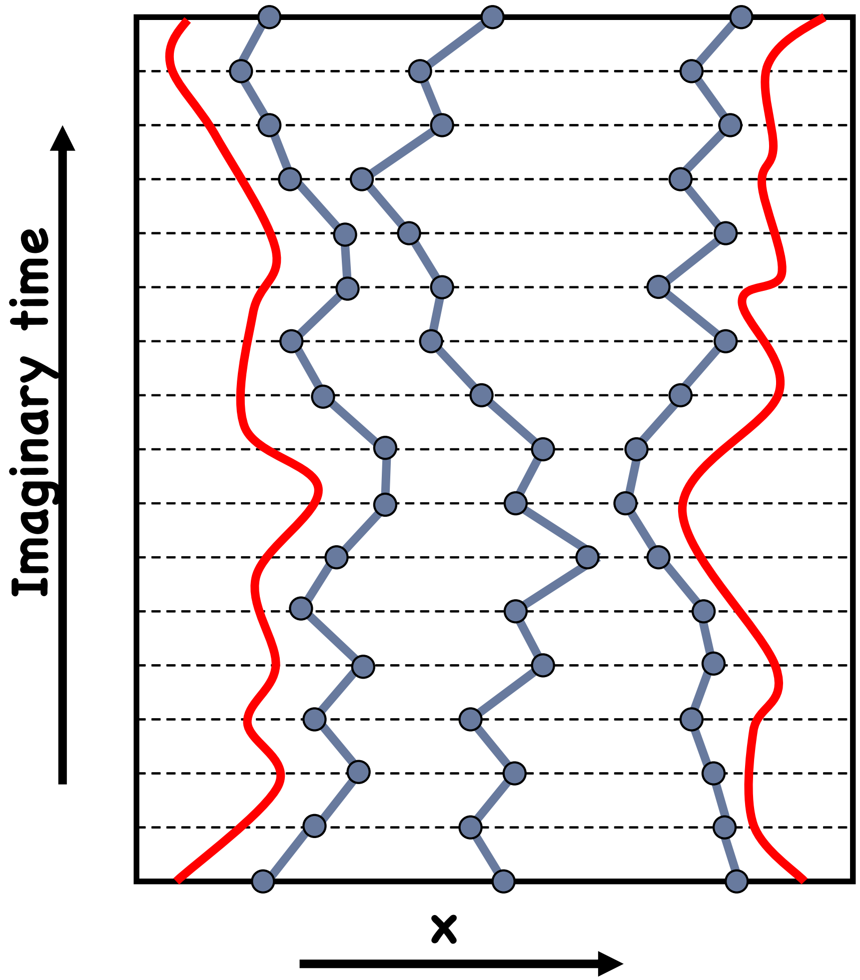
Project o… …c sta… …ect o… …metr… …tes:

$\rho_B($ … $\sum_P$ … $\rho_F($ …

$$\langle R|\hat{\rho}_F \ldots (\pm1)^P \int \ldots \int dR \ldots |e^{-\tau H}|PR'\rangle$$



Restricted PIMC for fermions: How is the restriction applied?



Construct a fermionic trial density matrix in form of a Slater determinant of single-particle density matrices:

$$\rho_T(R,R',\beta) = \begin{vmatrix} \rho(r_1,r_1',\beta) & \cdots & \rho(r_1,r_N',\beta) \\ \vdots & \ddots & \vdots \\ \rho(r_N,r_1',\beta) & \cdots & \rho(r_N,r_N',\beta) \end{vmatrix}$$

Enforce the following nodal condition for all time slices along the paths:

$$\rho_T\left[R(t),R(0),t\right] > 0$$

This 3N-dimensional conditions eliminates all negative and some positive contribution to the path → Solves the fermion sign problem approx.

Free-particle nodes:

$$\rho_0^{[1]}(r,r';\beta) = \sum_k e^{-\beta E_k}\,\Psi_k(r)\,\Psi_k^*(r')$$

Fermionic Path Integrals

Example: Closed paths of 2 free particles

Distinguishable particles:

Consider path types: NA + NX

Bosons:

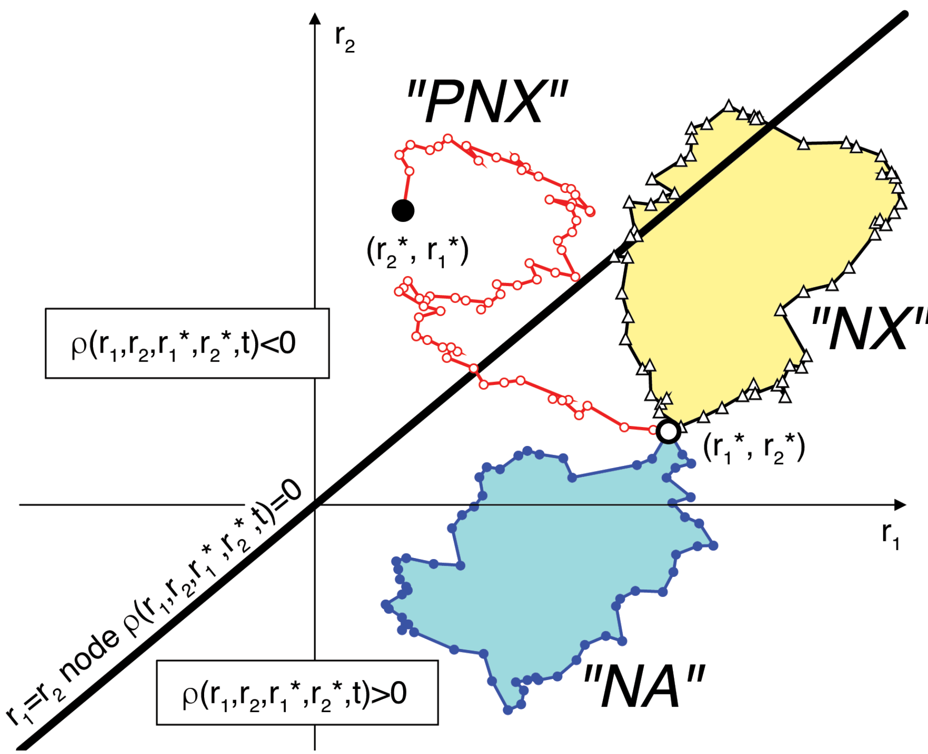
Consider path types: NA + NX + PNX

Direct fermions:

Consider path types: NA + NX - PNX

Restricted fermions:

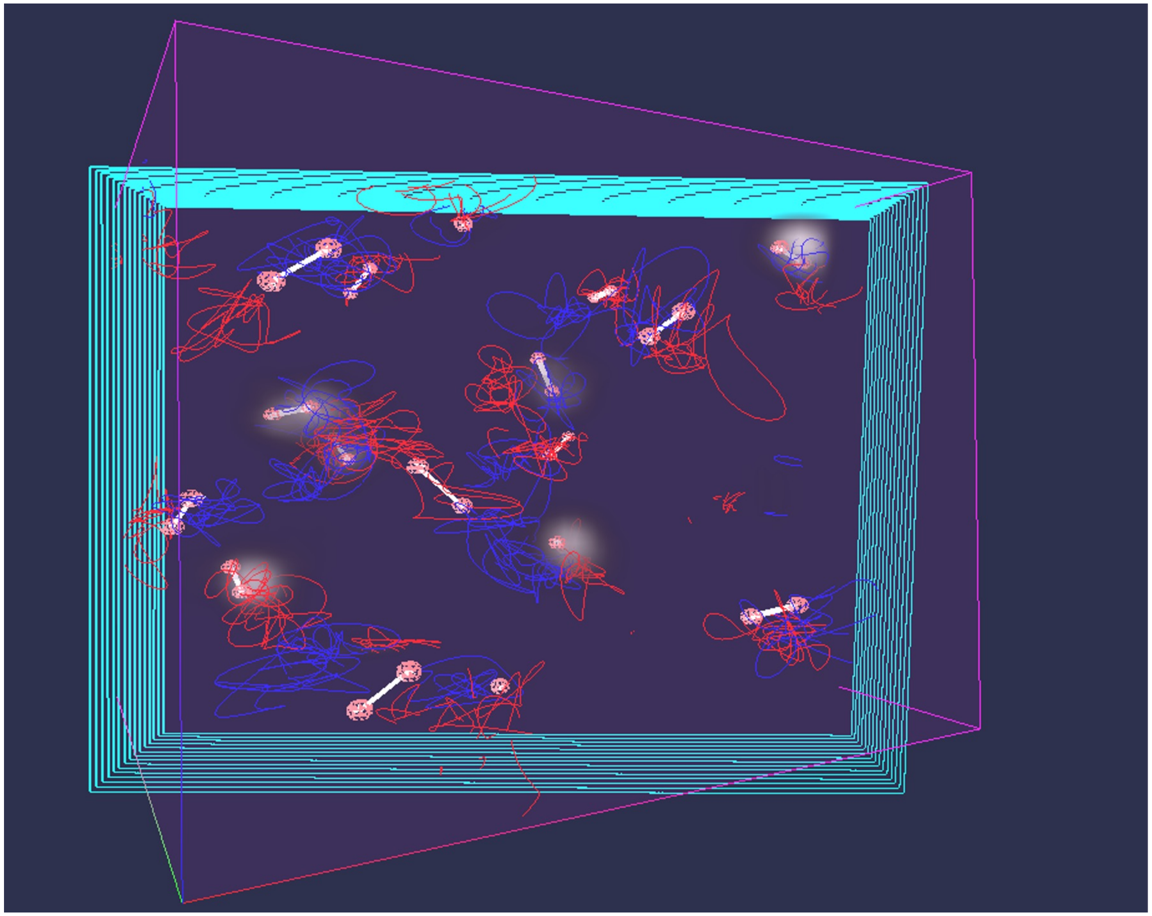
Consider only path type: NA



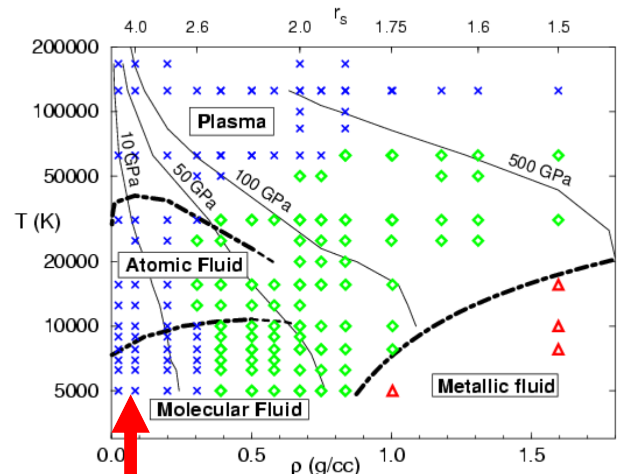
I. Hydrogen

Molecular Hydrogen

Snapshot from a PIMC simulation with 32 protons and electrons



2 protons (pink spheres) and spin-up and one spin-down electron form one H_2 molecule.

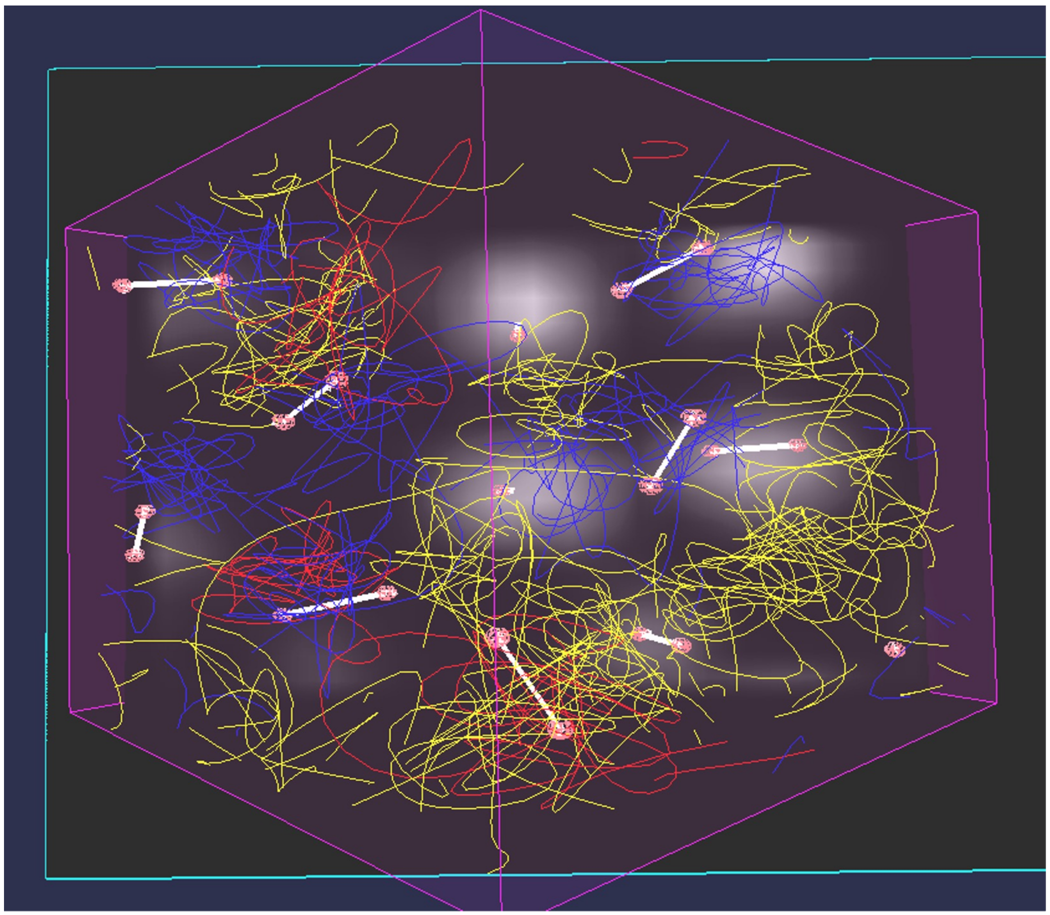


T=5000K, r_s=4

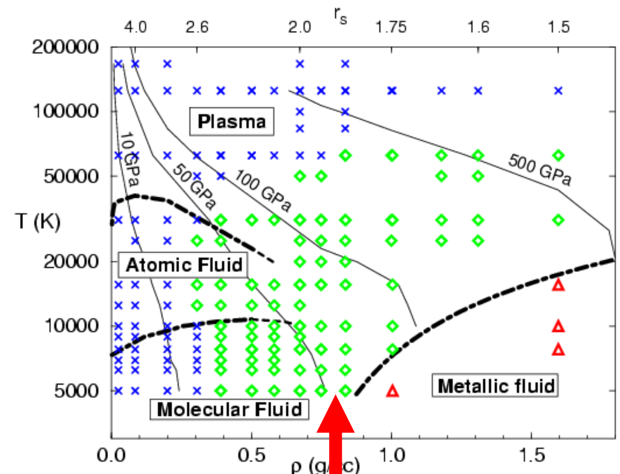
100% molecules, weakly interacting

Molecular Hydrogen

Snapshot from a PIMC simulation with 32 protons and electrons



2 protons (pink spheres) and spin-up and one spin-down electron form one H_2 molecule.

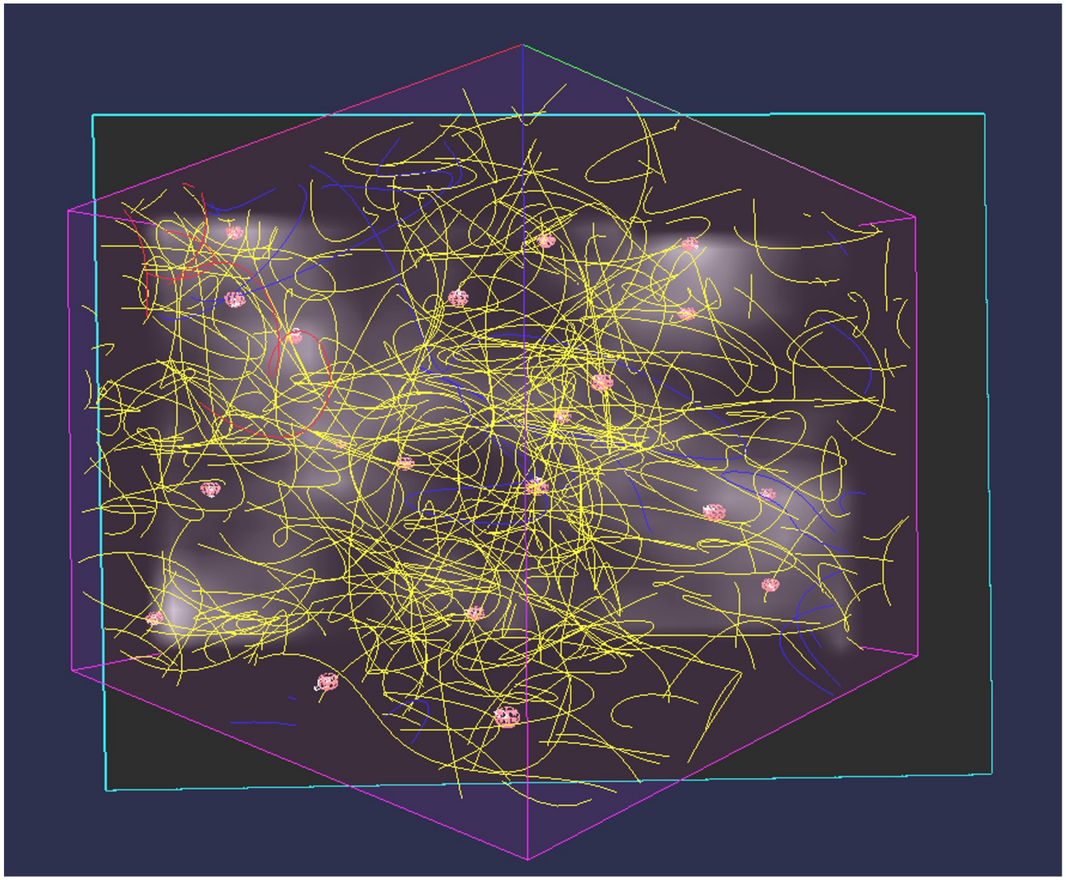


T=5000K, r_s=1.86

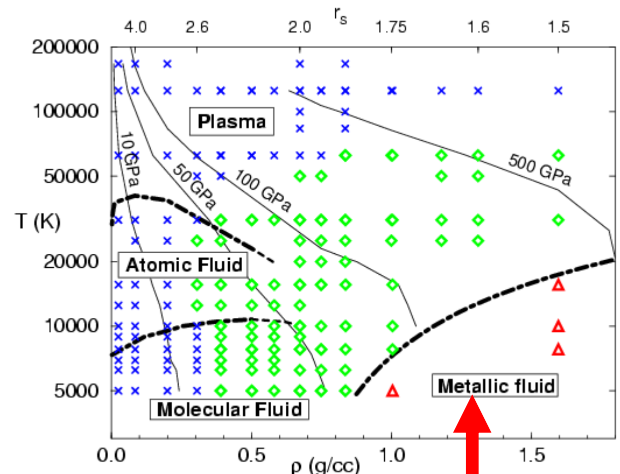
- strongly interacting molecules, close to pressure dissociation
- Electrons are degenerate, partially delocalized
- Electron paths are permuting

Metallic Hydrogen

Snapshot from a PIMC simulation with 32 protons and electrons



Free protons (pink spheres) and delocalized electrons.



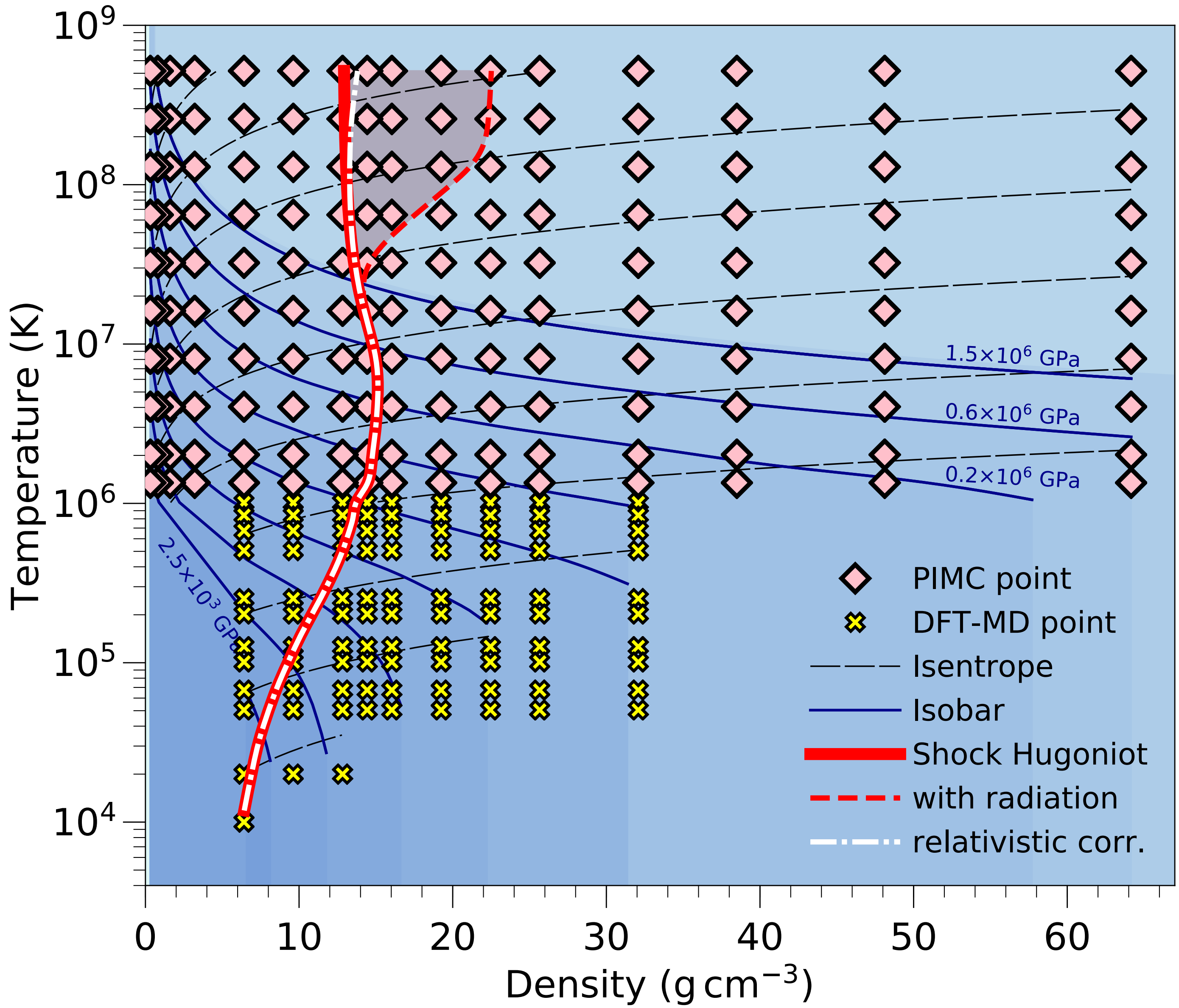
T=5000K, r_s=1.6

- Pressure dissociation, free protons
- Degenerate electron gas
- High number of permutations

Silicates:

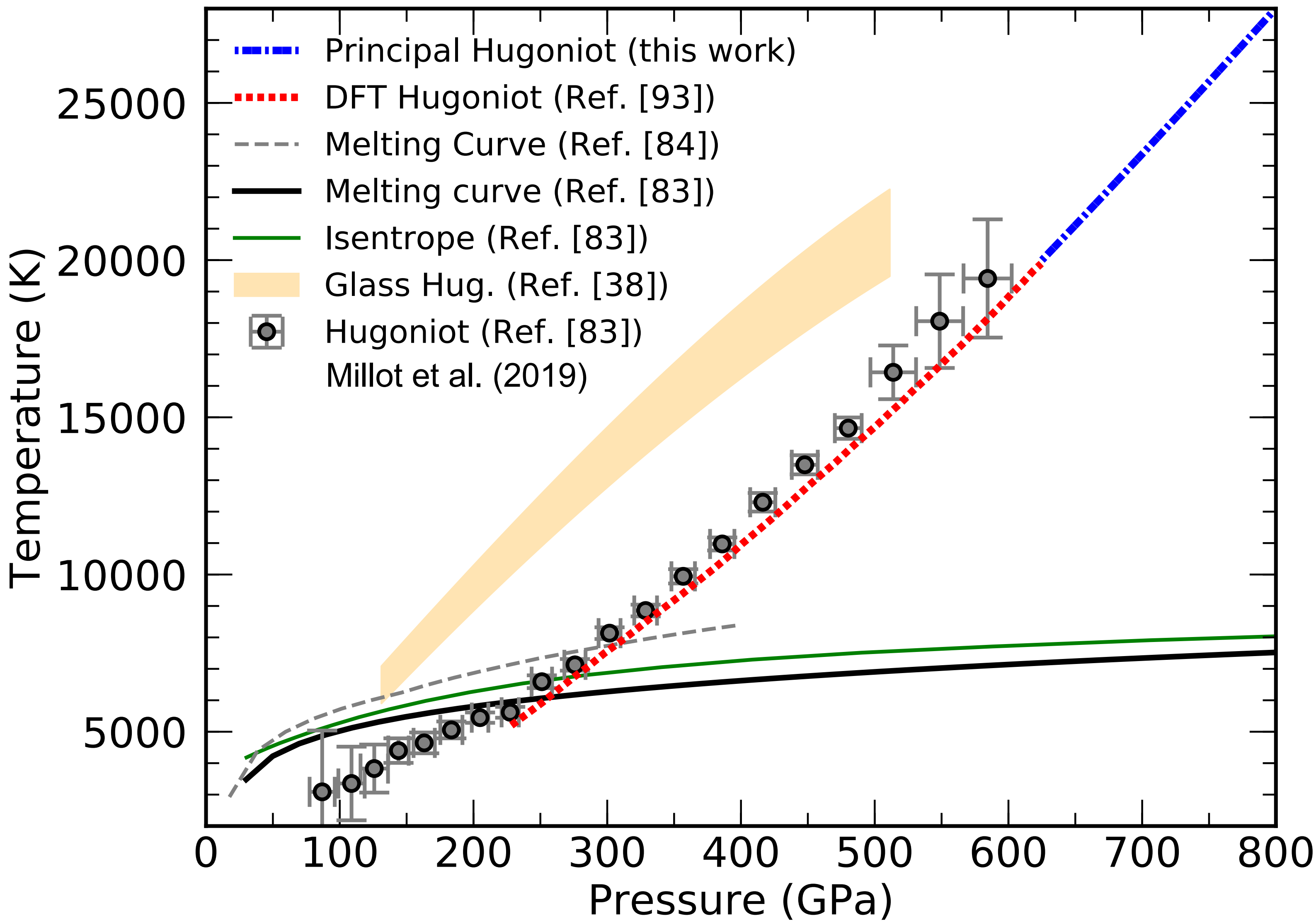
$MgSiO_3$

$MgSiO_3$: Principal Hugoniot Curve

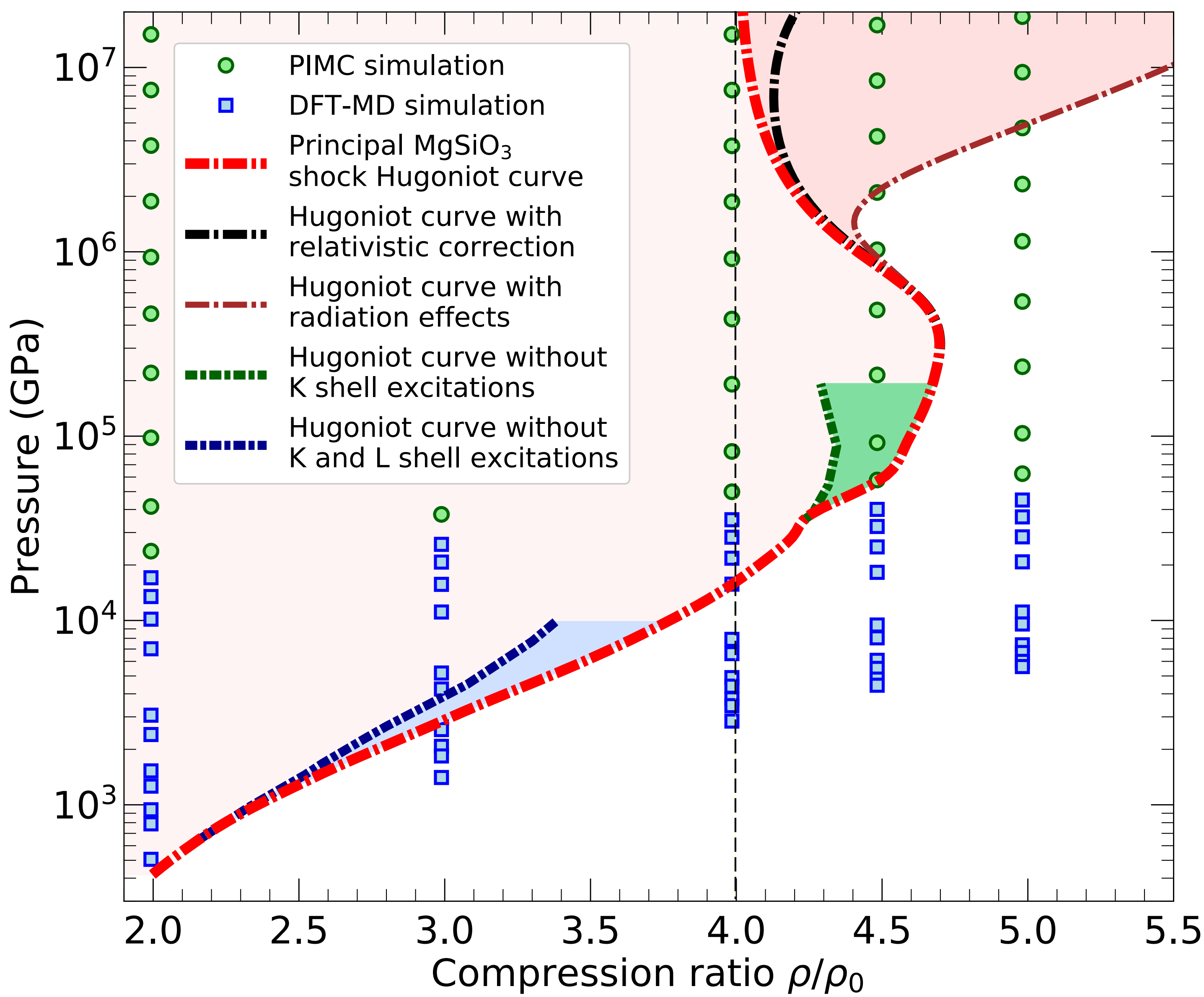


Gonzalez, Soubiran, Peterson, Militzer, *Phys. Rev. B* **101** (2020) 024107

$MgSiO_3$: Principal Hugoniot Curve



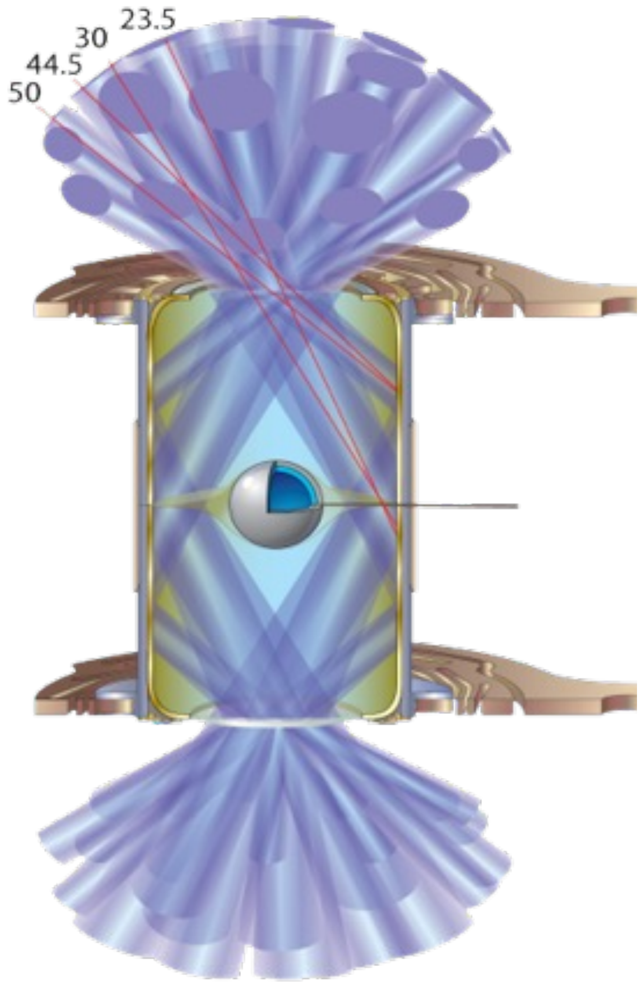
$MgSiO_3$: Principal Hugoniot Curve

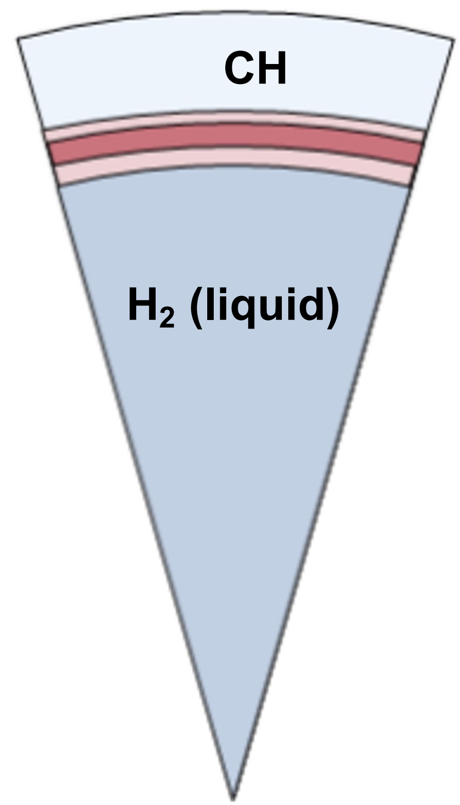


Gonzalez, Soubiran, Peterson, Militzer, *Phys. Rev. B* **101** (2020) 024107

CH plastics

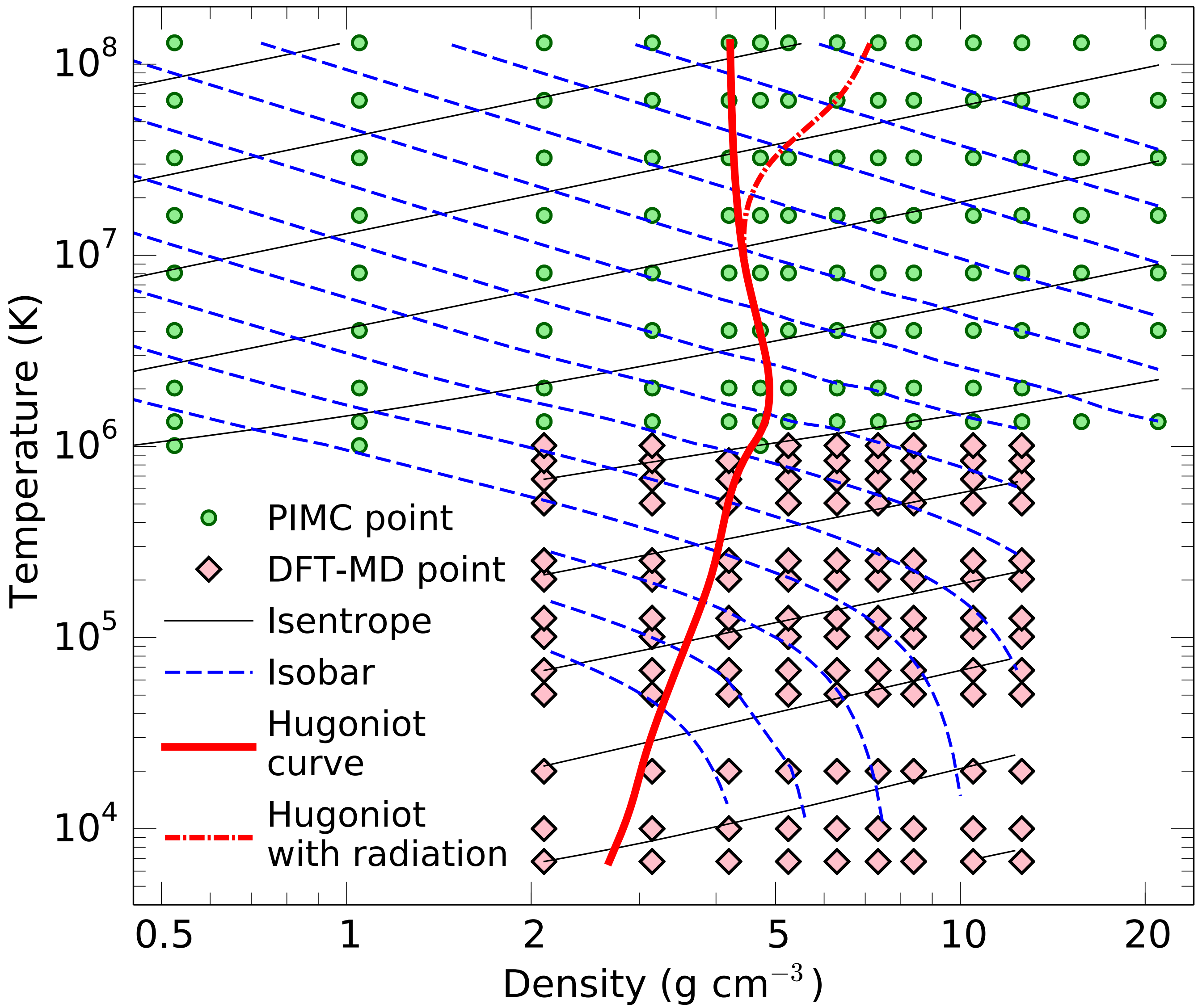
Inertial confinement fusion experiments with plastic coated spheres of liquid H_2





(Graphics: Bachmann et al. LLNL)

PIMC and DFT-MD simulations performed for C_2H, CH, C_2H_3, CH_3 and CH_4.



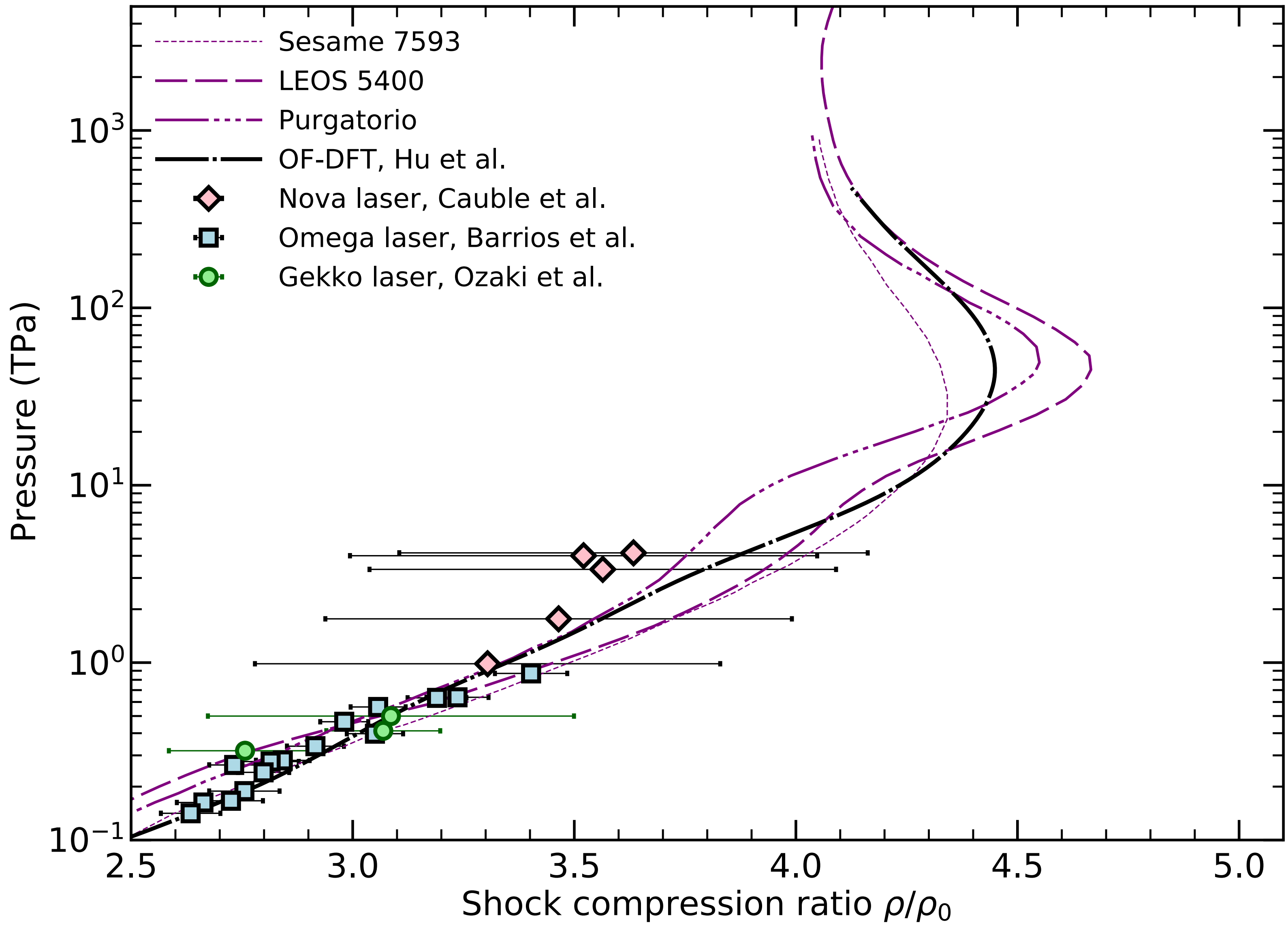
All calculations performed on

BLUE WATERS

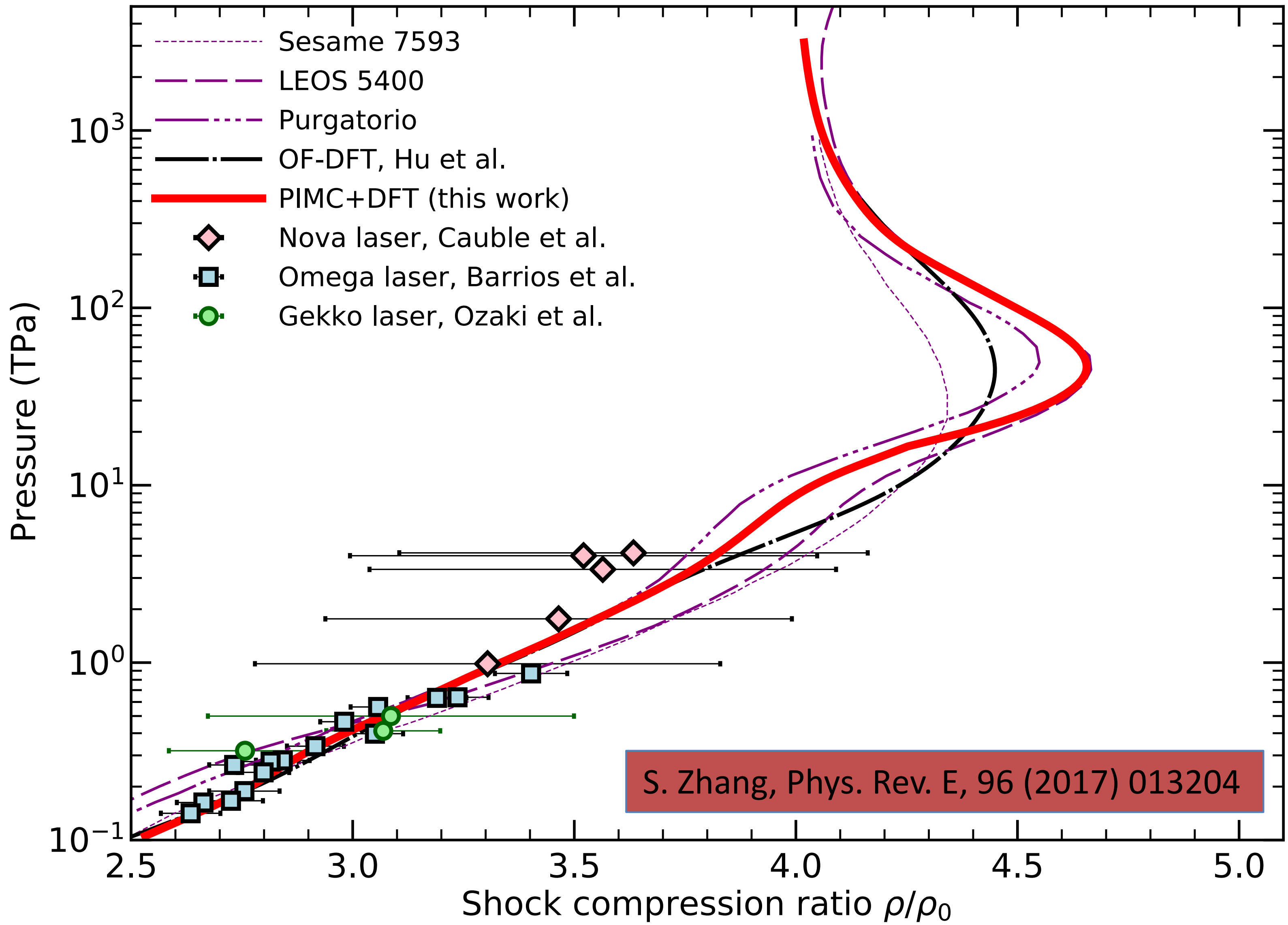
SUSTAINED PETASCALE COMPUTING

NCSA

CH Shock Hugoniot Curves: Comparison of Theory and Experiments



CH Shock Hugoniot Curves: Comparison of Theory and Experiments



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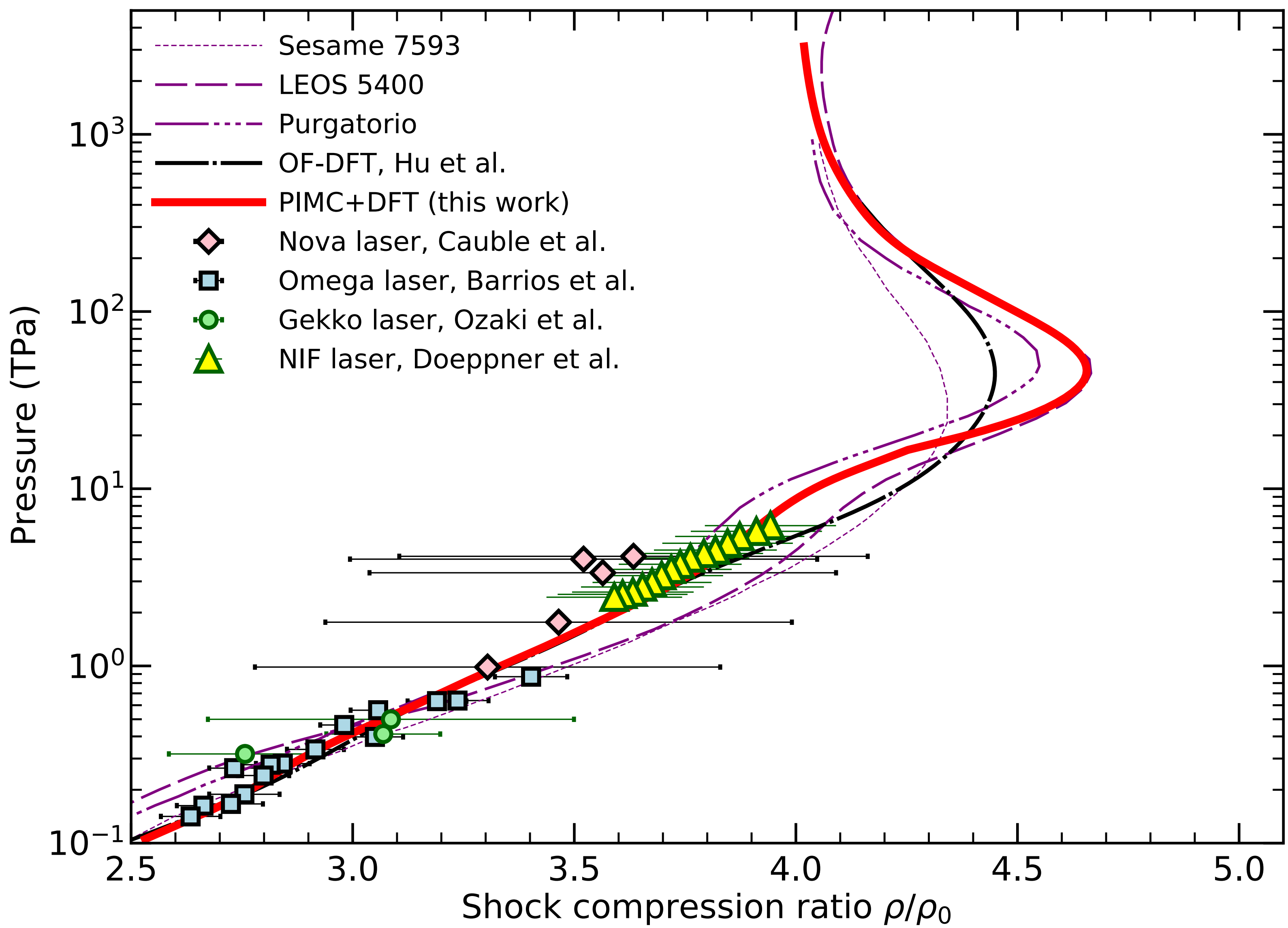
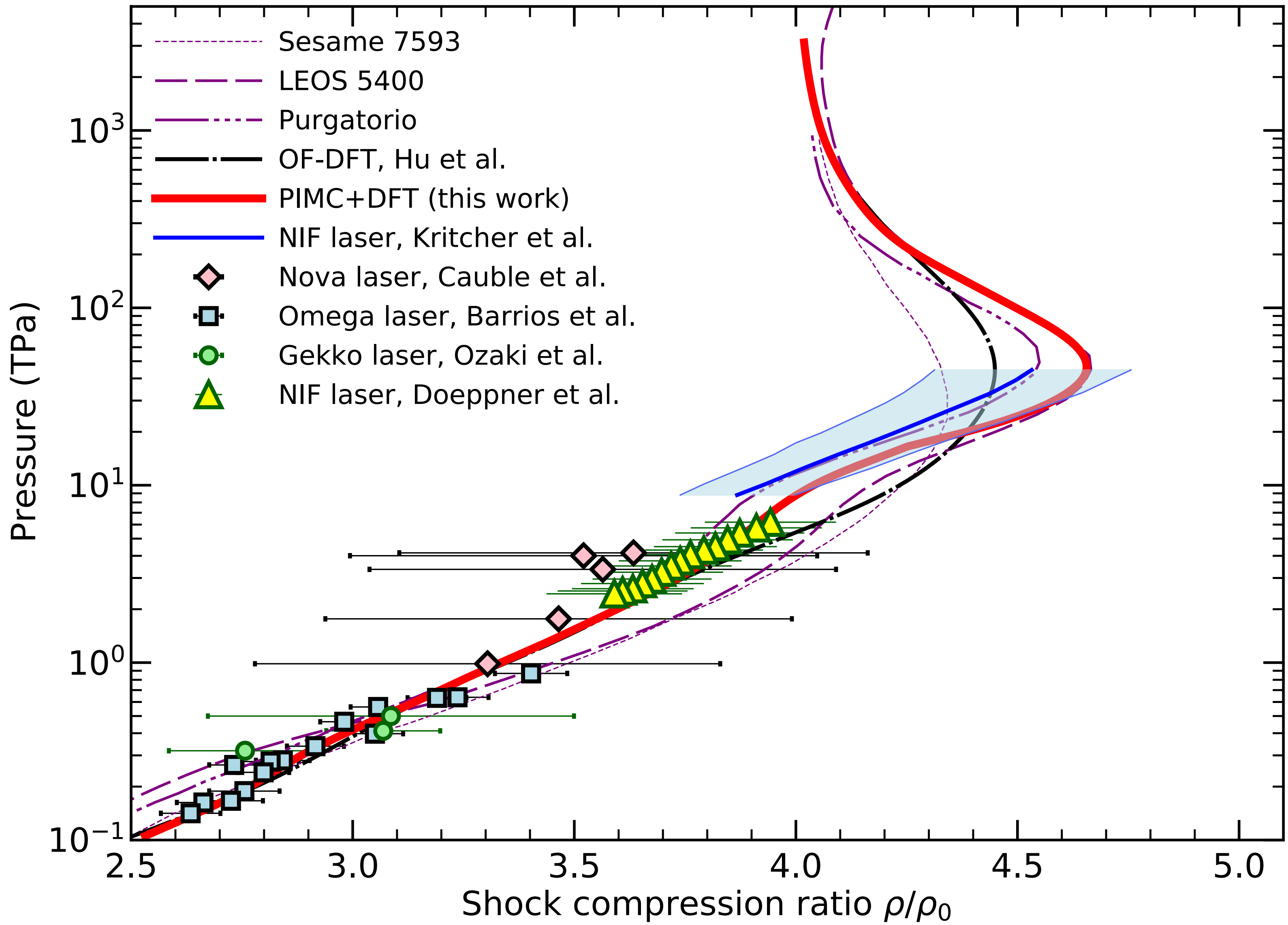


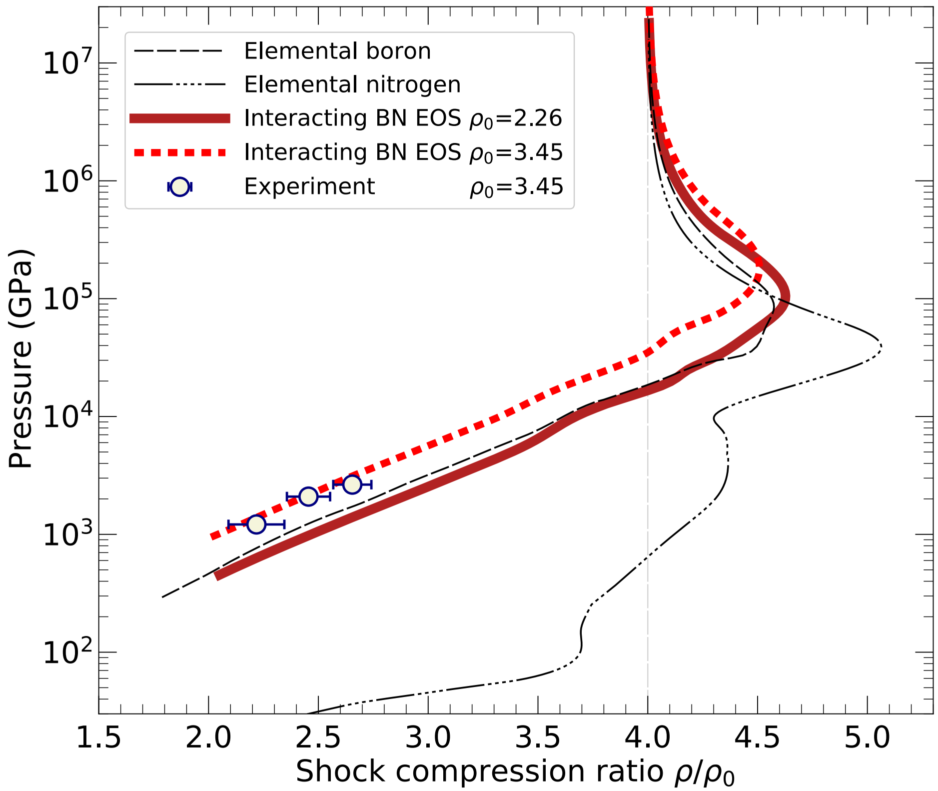
CH Shock Hugoniot Curves: Comparison of Theory and Experiments



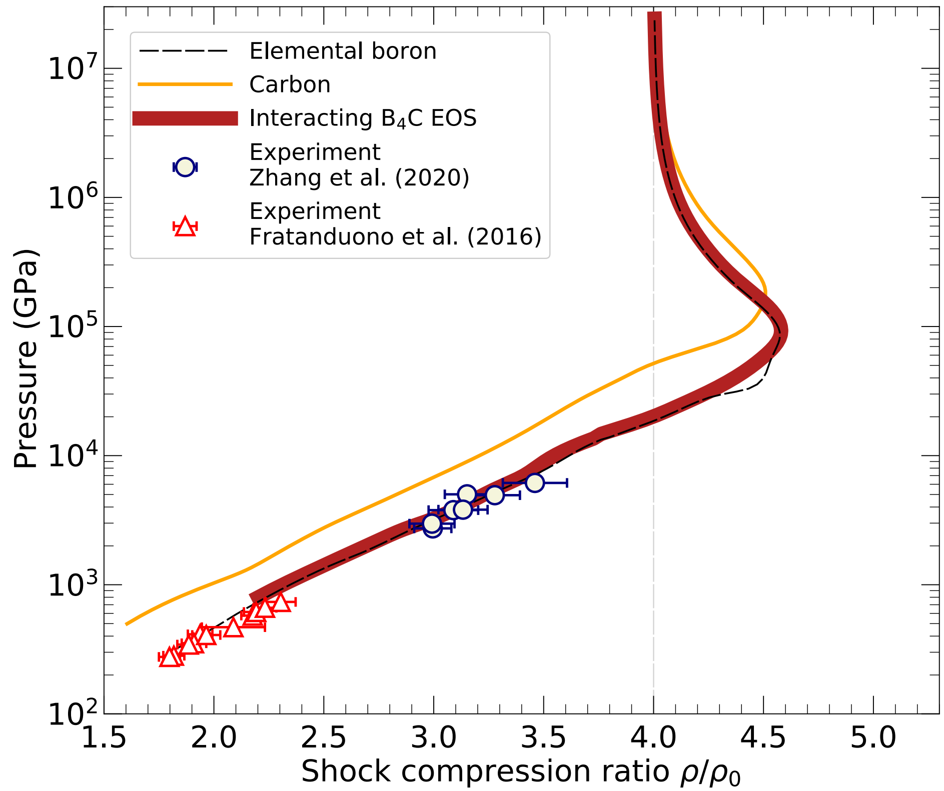
Hugoniot Curves of BN and B_4C

Fully interacting EOS and Linear Mixing agree quite well.

Boron nitride
Zhang et al. PRB 2019



Boron carbide
Zhang et al. PRE 2020



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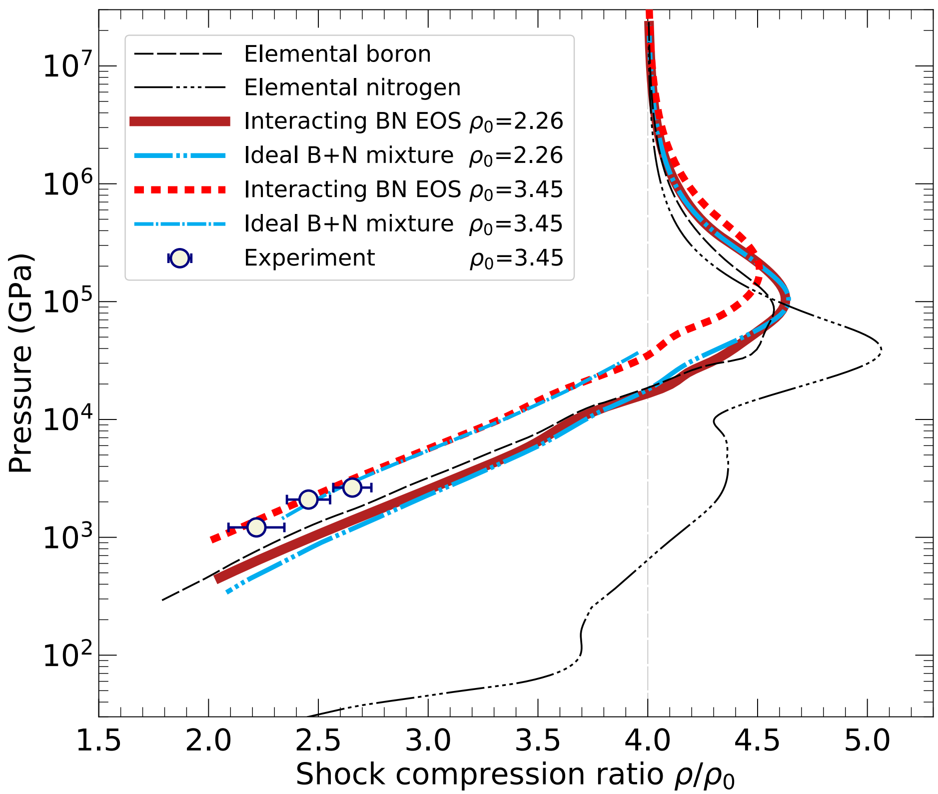
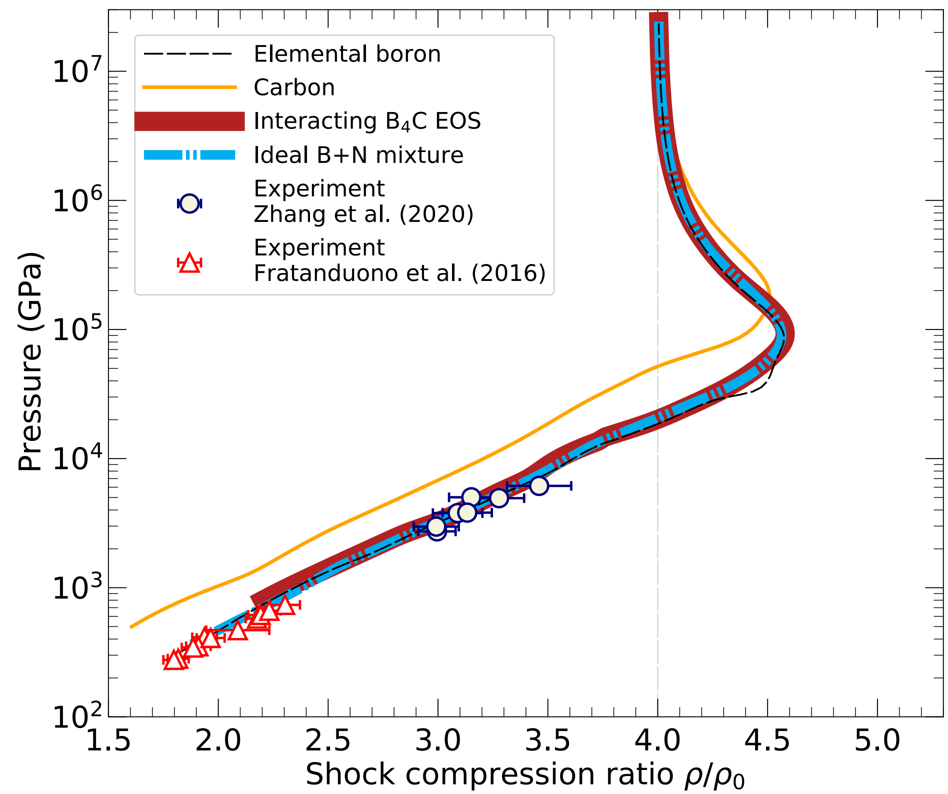
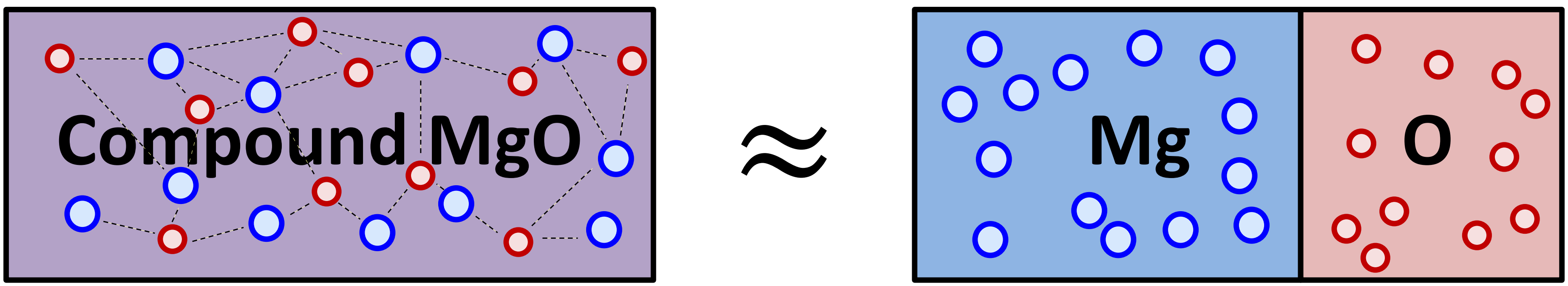


Boron carbide
Zhang et al. PRE 2020



Linear Mixing at Constant P and T
(Also called additive volume rule)



$$V_{\text{mix}} = N_1 V_1 + N_2 V_2 \; ,$$

$$m_{\text{mix}} = N_1 m_1 + N_2 m_2 \; ,$$

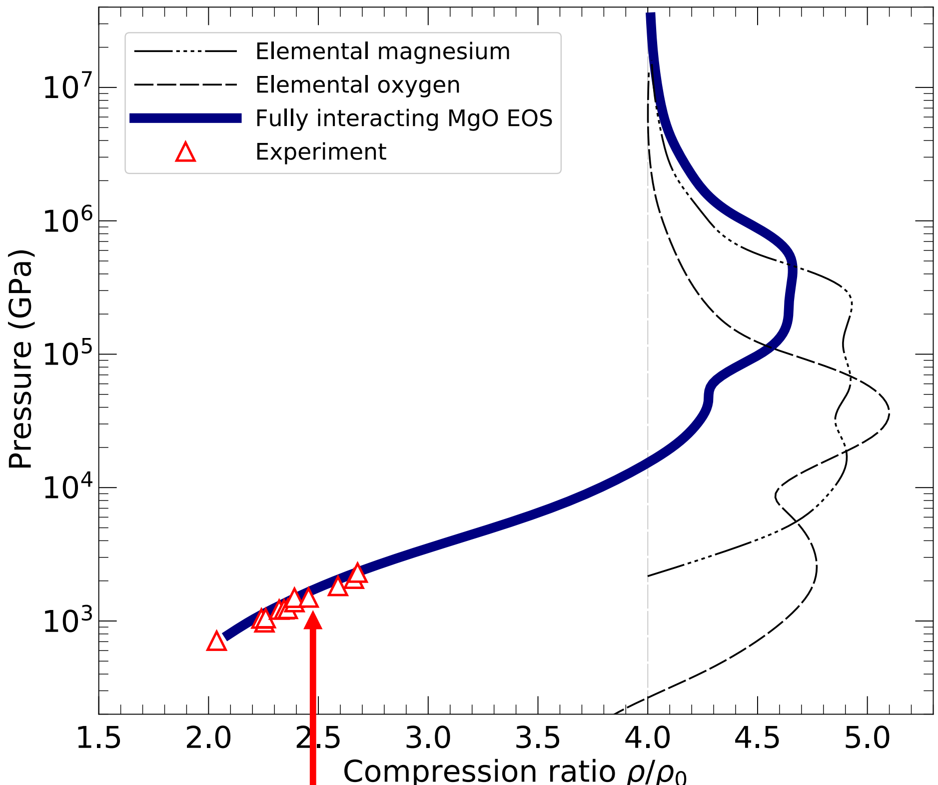
$$E_{\text{mix}} = N_1 E_1 + N_2 E_2 \; ,$$

$$\rho_{\text{mix}} = m_{\text{mix}} / V_{\text{mix}}$$

Hugoniot Curves of MgO and $MgSiO_3$

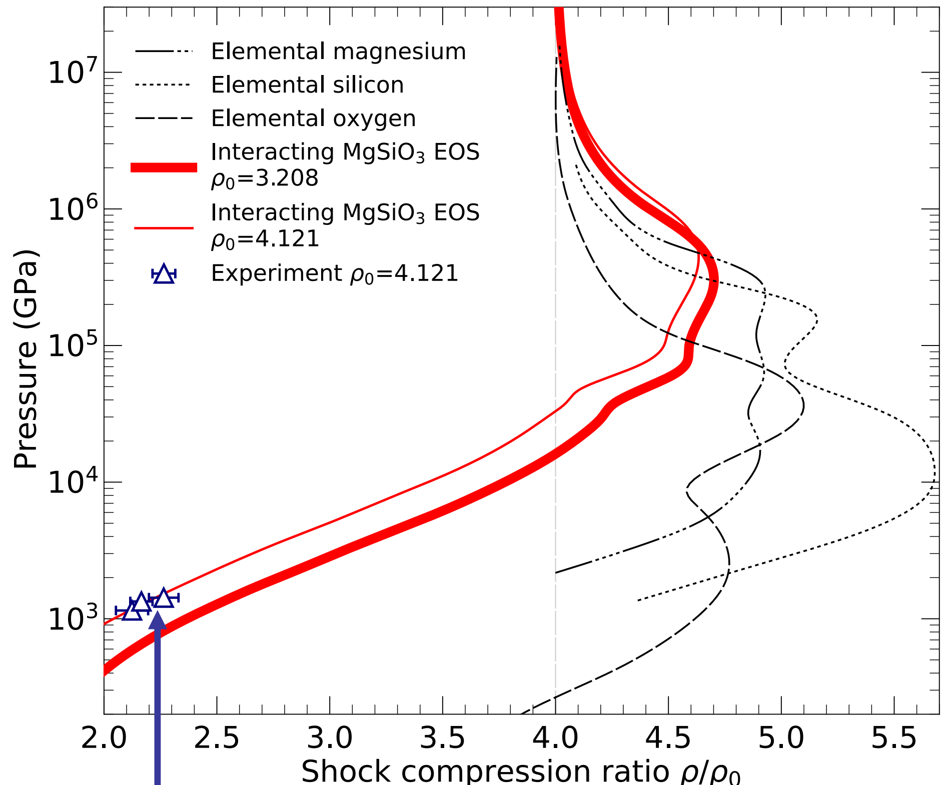
Results from fully interacting EOS and experiment.

Soubiran et al. JCP 2019



McCoy et al. PRB 2019

Gonzalez et al. PRB 2020



Millot et al. GRL 2020

Hugoniot Curves of MgO and $MgSiO_3$

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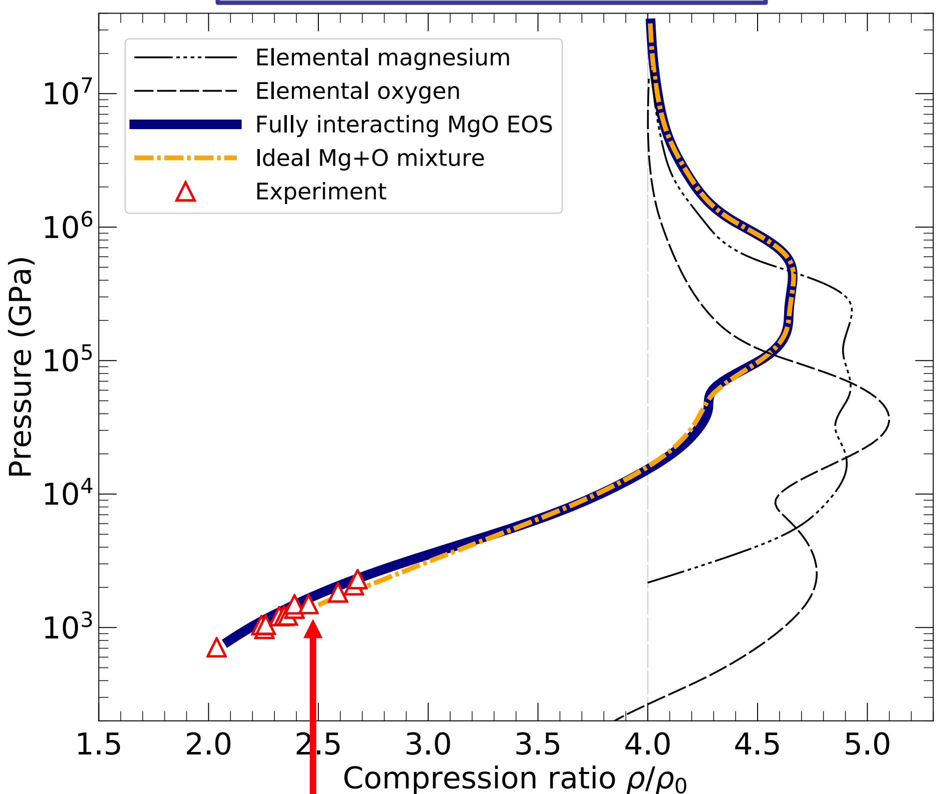
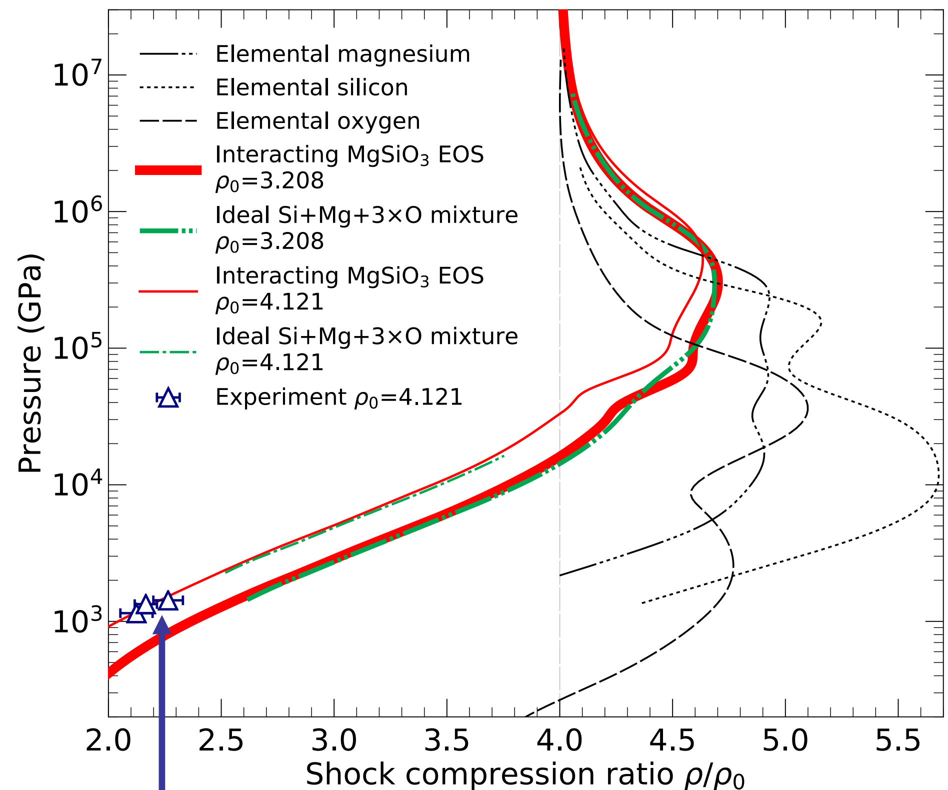
Soubiran et al. JCP 2019



McCoy et al. PRB 2019

Gonzalez et al. PRB 2020



Millot et al. GRL 2020

Linear mixing works well for $T \gtrsim 2\times10^5\mathrm{K}$ and $\varrho/\varrho_0 \gtrsim 3.2$

The Journal of Chemical Physics

Nonideal mixing effects in warm dense matter studied with first-principles computer simulations

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Published Online: 9 November 2020

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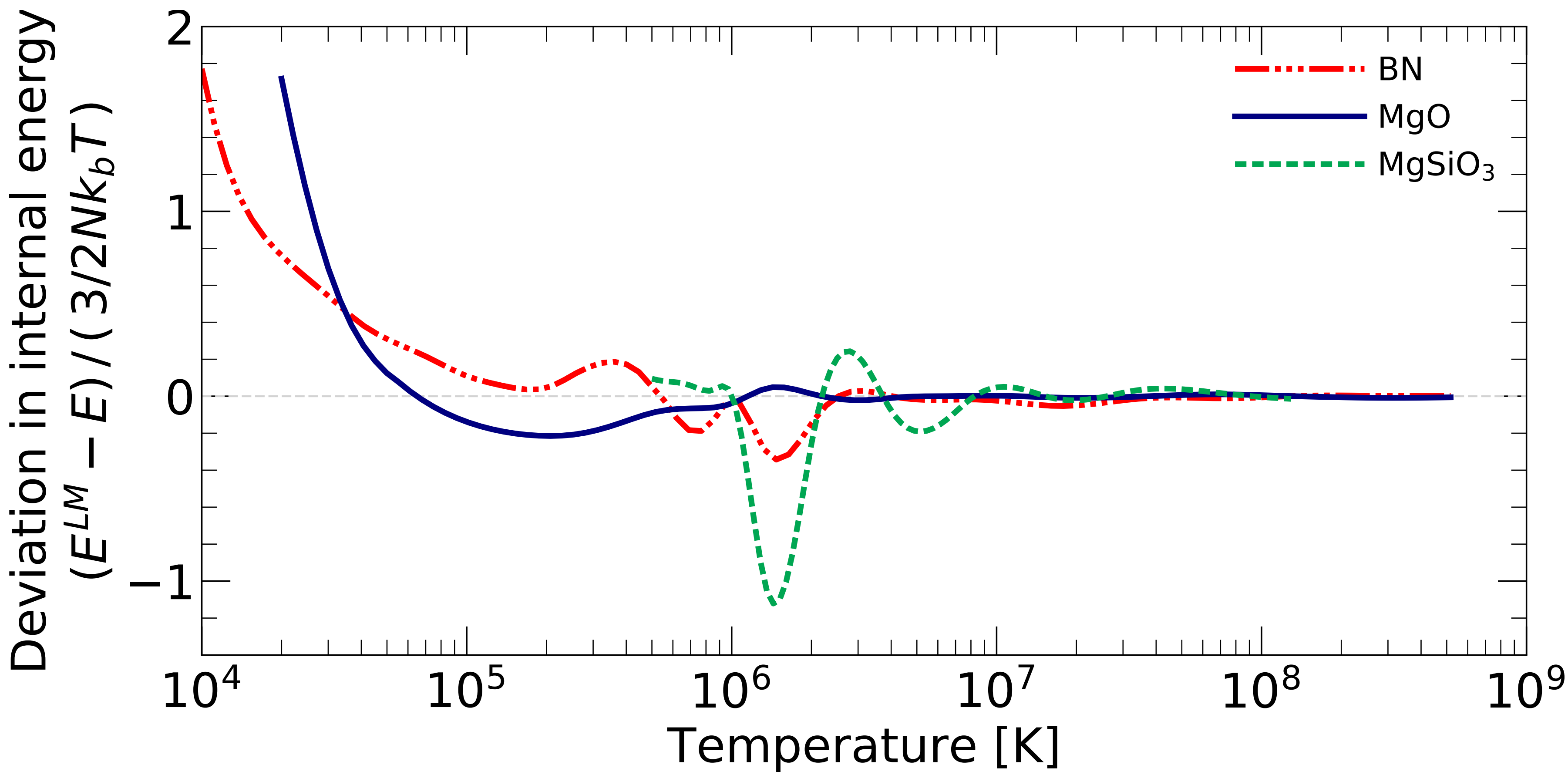
Burkhard Militzer,[1,2,a)] Felipe González-Cataldo,[1] Shuai Zhang,[3] Heather D. Whitley,[4] Damian C. Swift,[4] and Marius Millot[4]

Nonlinear Mixing Effects in $MgSiO_3$

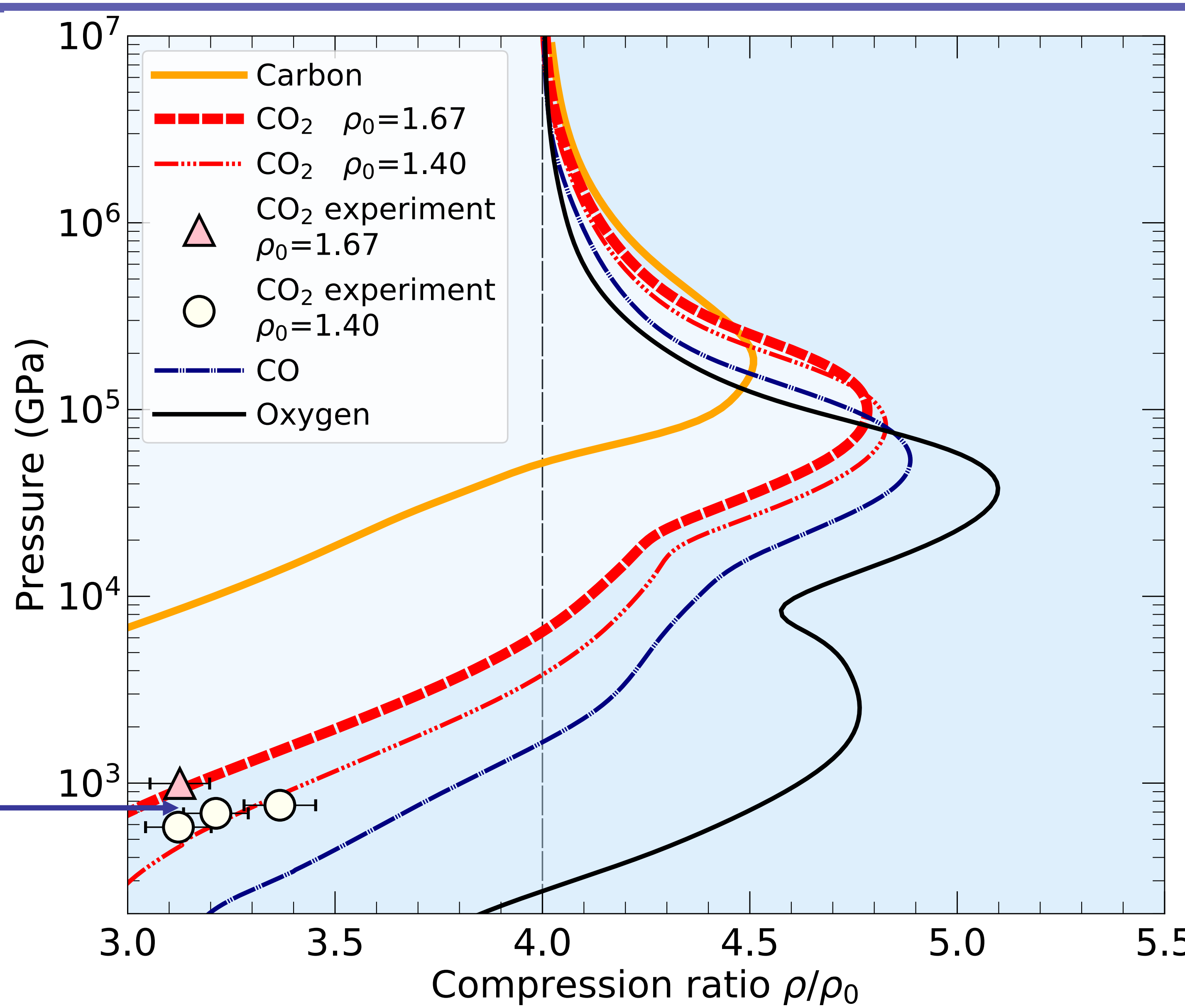
Fully interacting EOS and Linear Mixing agree quite well.



Linear mixing works well for $T \gtrsim 2{\times}10^5$K and $\varrho/\varrho_0 \gtrsim 3.2$

Hugoniot Curves of CO and CO_2

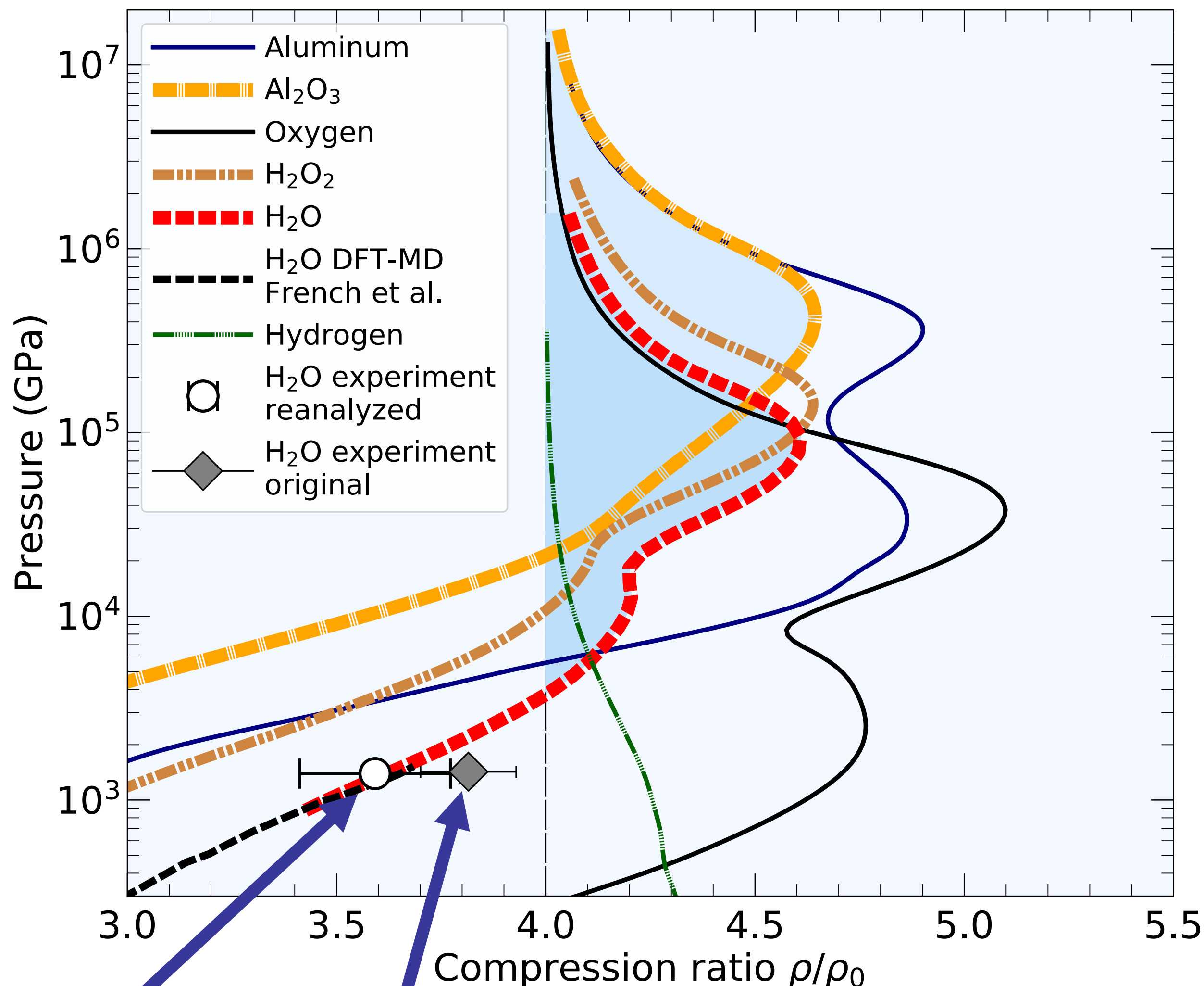
Experimental CO_2 Hugoniot agree with Linear Mixing result



Crandall et al.
PRL 2020

Hugoniot Curves of H_2O, H_2O_2, and Al_2O_3

Experimental H_2O Hugoniot agree with Linear Mixing result



Reanalyzed by Knudson et al.

Experiments by Podurets et al. 1972

FPEOS: 11+10 Available Tables

Material	Number of isochores	Minimum density [g cm^{-3}]	Maximum density [g cm^{-3}]	Minimum temperature [K]	Maximum temperature [K]	Number of EOS points	References
Hydrogen	33	0.001	798.913	15625	6.400×10^{7}	401	[69–74]
Helium	9	0.387	10.457	500	2.048×10^{9}	228	[75, 76]
Boron	16	0.247	49.303	2000	5.174×10^{8}	314	[77]
Carbon	9	0.100	25.832	5000	1.035×10^{9}	162	[78, 79]
Nitrogen	17	1.500	13.946	1000	1.035×10^{9}	234	[80]
Oxygen	6	2.486	100.019	10000	1.035×10^{9}	76	[81]
Neon	4	0.895	15.026	1000	1.035×10^{9}	67	[82]
Sodium	9	1.933	11.600	1000	1.293×10^{8}	193	[83, 84]
Magnesium	23	0.431	86.110	20000	5.174×10^{8}	371	[85]
Aluminum	15	0.270	32.383	10000	2.156×10^{8}	240	[86]
Silicon	7	2.329	18.632	50000	1.293×10^{8}	85	[87, 88]
LiF	8	2.082	15.701	10000	1.035×10^{9}	91	[89]
B_4C	16	0.251	50.174	2000	5.174×10^{8}	291	[90]
BN	16	0.226	45.161	2000	5.174×10^{8}	311	[91]
CH_4	16	0.072	14.376	6736	1.293×10^{8}	247	[92, 93]
CH_2	16	0.088	17.598	6736	1.293×10^{8}	248	[92, 93]
C_2H_3	16	0.097	19.389	6736	1.293×10^{8}	247	[92, 93]
CH	16	0.105	21.000	6736	1.293×10^{8}	248	[92, 93]
C_2H	16	0.112	22.430	6736	1.293×10^{8}	245	[92, 93]
MgO	19	0.357	71.397	20000	5.174×10^{8}	286	[94]
$MgSiO_3$	16	0.321	64.158	6736	5.174×10^{8}	284	[95, 96]

First-Principles Equation of State Database online http://militzer.berkeley.edu/FPEOS

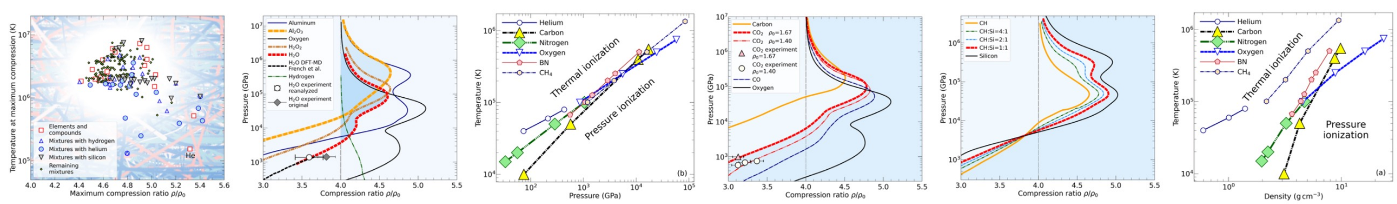
militzer.berkeley.edu

First-Principles Equation of State (FPEOS) Database for Warm Dense Matter Computation

Authors: B. Militzer, F. Gonzalez-Cataldo, S. Zhang, K. P. Driver, F. Soubiran

With the goal in mind of making WDM computations more reliable and efficient, we make available our EOS tables for 11 elements and 10 compounds as well as the C++ computer codes for their interpolation. Python code is provided to generate graphs of shock Hugoniot curve, isentropes, isobars, and isotherms for compounds and user-defined mixtures. We put together this first-principles equation of state (FPEOS) database for matter at extreme conditions by combining results from path integral Monte Carlo and density functional molecular dynamics simulations of the elements H, He, B, C, N, O, Ne, Na, Mg, Al and Si as well as the compounds LiF, B_4C, BN, CH_4, CH_2, C_2H_3, CH, C_2H, MgO, and $MgSiO_3$. For all these materials, we provide the pressure and internal energy over a wide density-temperature range from ~0.5 to 50 g/cc and from ~10^4 to 10^9 K. This database encompasses the results from approximately 5000 different first-principles simulations. It allows one to compute isobars, adiabats, and shock Hugoniot curves in the regime of L and K shell ionization. Invoking the linear mixing approximation, one can study the properties of user-defined mixtures at high density and temperature.

Recommended citation: B. Militzer, F. Gonzalez-Cataldo, S. Zhang, K. P. Driver, F. Soubiran, "First-Principles Equation of State Database for Warm Dense Matter Computation", *Physical Review E* **103** (2021) 013203.

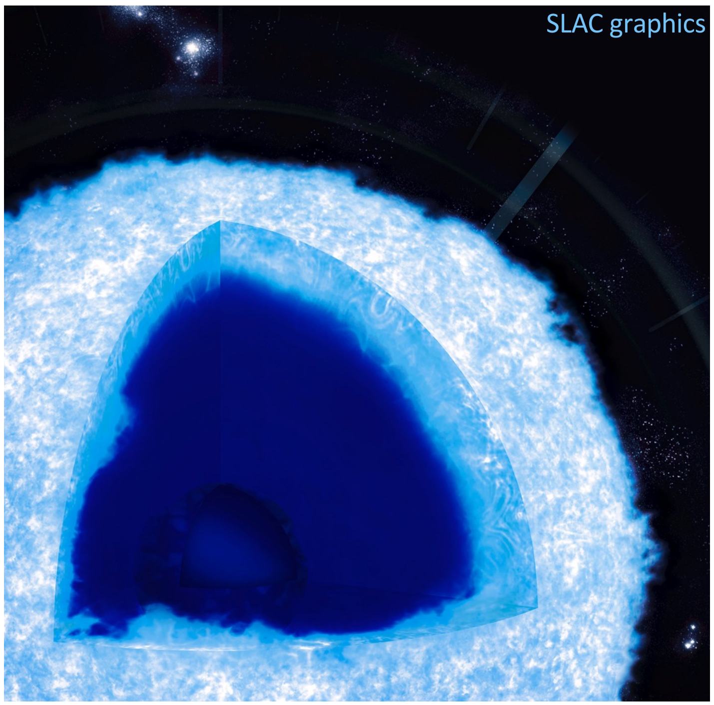


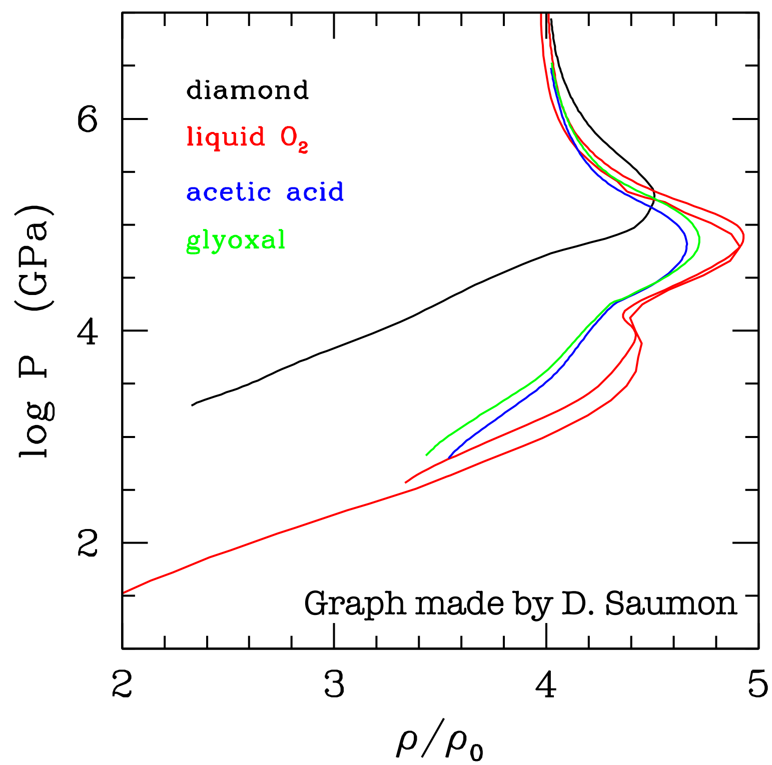
5000 first-principles calculations have been combined into our FPEOS database. So anyone can predict shock Hugoniot curves for a variety of compounds and mixtures. This will make warm dense matter calculations more reliable and efficient.

NIF Gbar Experiment: Equations of State of C-O Mixtures in White Dwarf Stars

PI: D. Saumon (LANL), Blouin, Glenzer, Swift, Kritcher, Doppner, Whitley, Lazicki, Falcone, Militzer

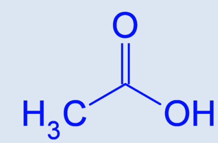
We propose to make EOS measurements along the Hugoniot with the Gbar platform of carbon-oxygen rich materials that resemble conditions in White Dwarf stars.





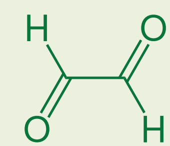
Acetic acid

$C_2O_2H_4$



Glyoxal

$C_2O_2H_2$



Glyoxal $C_2O_2H_2$ `comp:~/fpeos> fpeos binaryMixture EOS1=6 2.0 EOS2=18 2.0 rho0=1.27 E0=-227.8`

Acetic acid $C_2O_2H_4$ `comp:~/fpeos> fpeos binaryMixture EOS1=6 2.0 EOS2=16 2.0 rho0=1.049 E0=-229.0`

FPEOS demo

The End