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

Shuai Zhang
University of Rochester
Laboratory for Laser Energetics

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University of Rochester
Laboratory for Laser Energetics

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

Burkhard Militzer, Kevin Driver, François Soubiran (University of California, Berkeley)

Abhiraj Sharma, Phanish Suryanarayana (Georgia Institute of Technology)

Duane D. Johnson, Andrey V. Smirnov (Ames Laboratory)

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, B₄C) over wide \( T \) \( (10^3\text{–}10^8 \text{K}) \), \( \rho \) \( (0.1\text{–}100 \text{ g/cm}^3) \) 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:

B₄C: Zhang et al., to be published.
FIRST-PRINCIPLES METHODOLOGY

WE COMBINE QUANTUM-MECHANICAL METHODS TO CALCULATE THE EOS

**DFT-MD: for low-T**

\[ M_i \dot{R}_i = -\frac{\partial E}{\partial R_i} = F_i \{ R_j \} \]

\[ \hat{H} \psi_i(r) = \epsilon \psi_i(r) \]

**PIMC: for high-T**

\[ \langle O \rangle = Z^{-1} \int dRdR' \rho (R, R'; \beta) \left< R \left| \hat{O} \right| R' \right> \]

\[ \rho (R, R'; \beta) = \left< R \left| e^{-\beta \hat{H}} \right| R' \right> e^{-\beta \hat{H}} = \left( e^{-\tau \hat{H}} \right)^M, \tau = \beta / M \]

\[ \rho (R, R'; \beta) = \int dR_1 \ldots dR_{M-1} e^{-\sum_{m=1}^{M-1} S_n} \]

- 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**
RESULTS: EOS

**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

* Boron $\rho_0 = 2.465$ g/cc
RESULTS: EOS

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\[ |\Delta E| < 1.5 \text{ Ha}/B, \quad |\Delta P/P| < 5\% \]

Note: 1.5 Hartree/B \(\approx \) 5%*E$_{\text{ideal gas}}$
RESULTS: EOS

OUR RECENT DEVELOPMENTS EMPLOY ADDITIONAL METHODS FOR BN & B4C

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>Density (g/cm³)</th>
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<td>10⁸</td>
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PIMC
PAWpw

BN

B₄C
OUR RECENT DEVELOPMENTS EMPLOY ADDITIONAL METHODS FOR BN & B\textsubscript{4}C

* ONCV\textsubscript{pw}/PAW\textsubscript{pw}: DFT-MD with ONCV/PAW potentials
OUR RECENT DEVELOPMENTS EMPLOY ADDITIONAL METHODS FOR BN & B4C

* **ONCVpw/PAWpw**: DFT-MD with ONCV/PAW potentials; **FOE**: Fermi-operator expansion
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RESULTS: EOS

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 ($21k_B T/BN$)
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RESULTS: HUGONIOT

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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
**APPLICATION#1: CONSTRUCTION OF NEW EOS TABLES**

**OUR DATA SET CONSTRAINTS FOR THE CONSTRUCTION OF ACCURATE EOS TABLES**

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

**QEoS**: 
\[
F(\rho, T) = E_{\text{cold}}(\rho) + F_{\text{ion}}(\rho, T) + F_{\text{ele}}(\rho, T)
\]

**Graphs**:
- Graph showing Electron relativistic effect.
- Graph showing P(ion)/P(total)*100% according to X2152.

**Tables**:
- Table showing Density (g/cm³) vs. Temperature (K) for different Compression Ratios.
WE RUN 1D SIMULATIONS TO CLARIFY THE PERFORMANCE SENSITIVITY TO EOS

<table>
<thead>
<tr>
<th>EOS Model (P multiplier)</th>
<th>Neutron Yield</th>
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<tbody>
<tr>
<td>LEOS 50 (0.8)</td>
<td>2.15×10^{13}</td>
</tr>
<tr>
<td>LEOS 50 (1.0)</td>
<td>3.60×10^{13}</td>
</tr>
<tr>
<td>LEOS 50 (1.2)</td>
<td>5.70×10^{13}</td>
</tr>
<tr>
<td>X52 (1.0)</td>
<td>3.53×10^{13}</td>
</tr>
<tr>
<td>GDP</td>
<td>2.14×10^{13}</td>
</tr>
</tbody>
</table>

- 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.

Polar direct-drive exploding pusher expt. simulations based on 1D Ares model*

Capsule thickness:
- Boron: 6 μm
- GDP: 18 μm

SUMMARY

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$_4$C) over wide $T$ ($10^3$–$10^8$ K), $\rho$ (0.1–100 g/cm$^3$) regimes.
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Thank you!