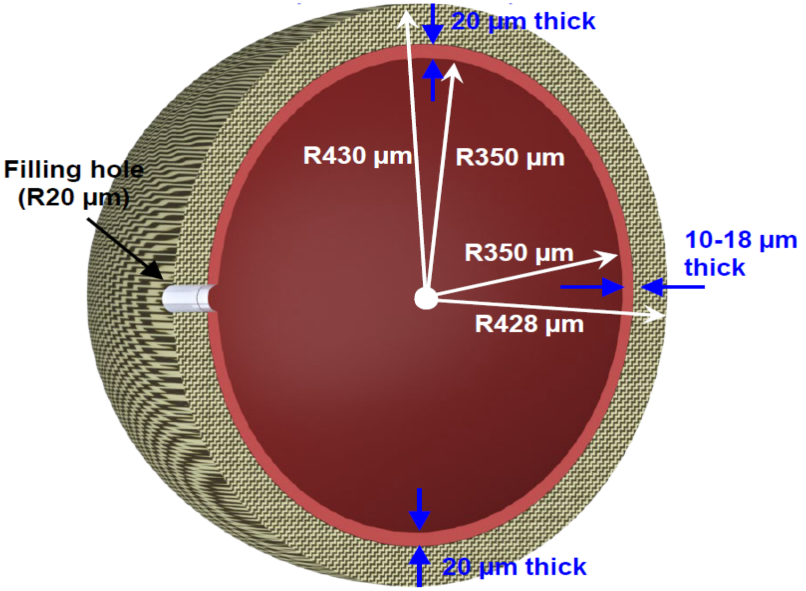
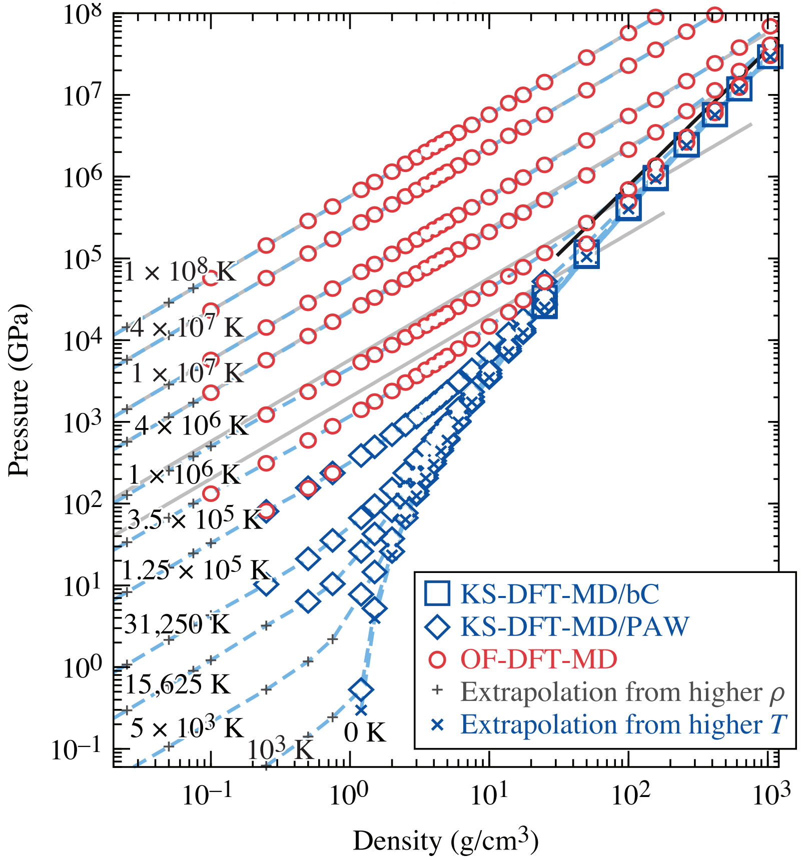
First-Principles Equation of State of CHON for Two-Photon-Polymerization-Fabricated Inertial Confinement Fusion Targets





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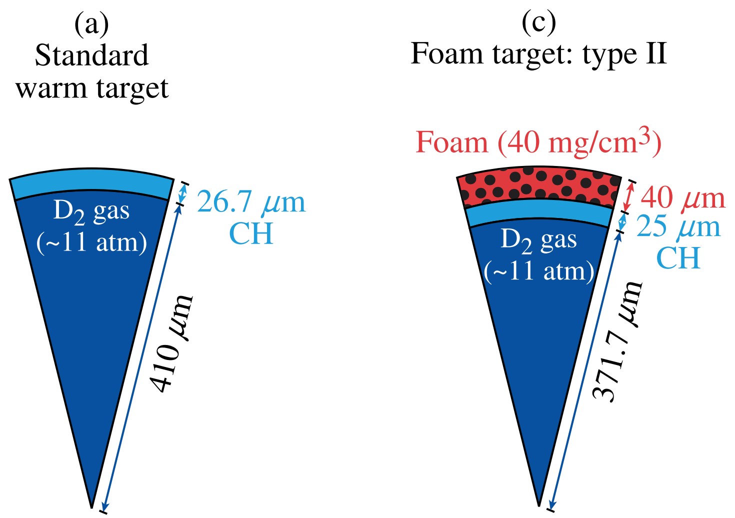
Summary

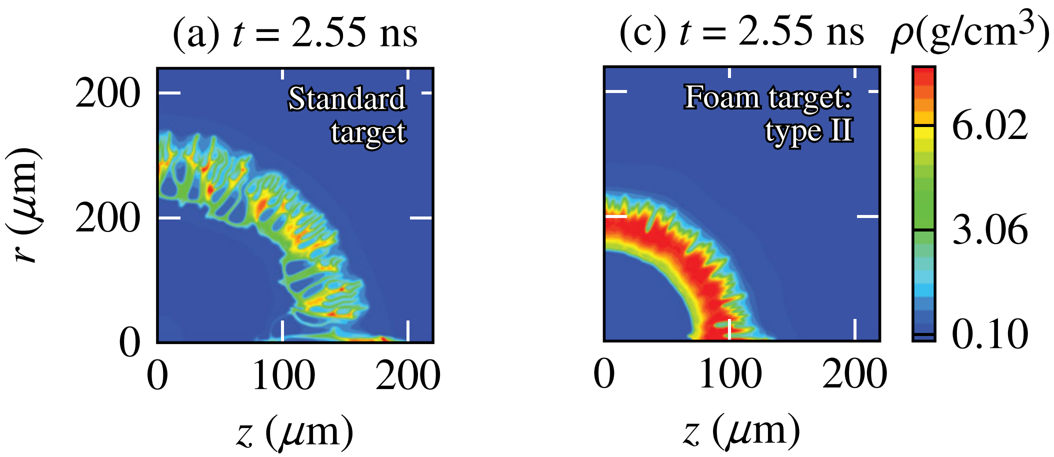
A first-principles EOS table has been constructed for CHON for ICF and HED applications

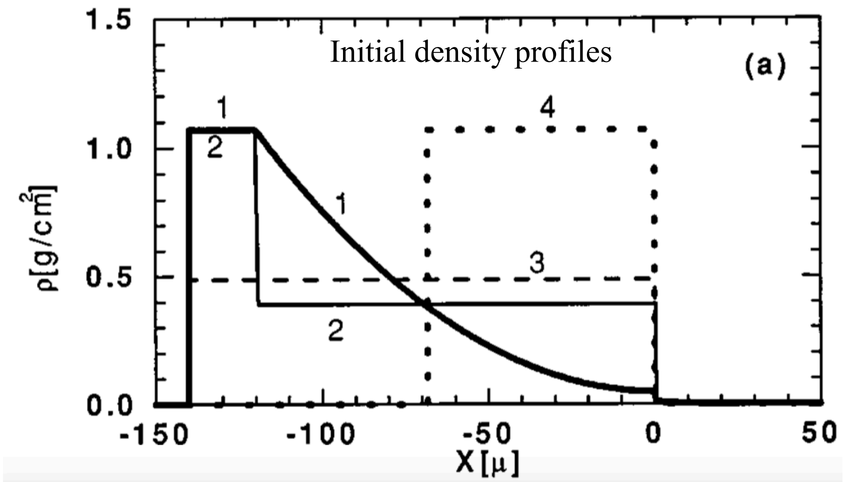
- We construct a wide-range (0–1044 g/cm^3 and 0–10^9 K) EOS table for a C-H-O-N quaternary compound ($CH_{1.72}O_{0.37}N_{0.086}$).
- The EOS is generated by calculations and numerical extrapolation based on first-principles approaches: KS-DFT-MD with T-SCAN-L xc functional and OF-DFT-MD with LKTγTF tunable free-energy functionals.
- We have made detailed comparisons with model predicted EOS, and with CH on shock Hugoniots, thermodynamic properties, and target performances.
- Radiation hydrodynamic simulations show CHON slightly outperforms CH as the ablator for LDD targets, which further prompts TPP fabrication of the CHON shell with a foam layer for laser imprint mitigation.

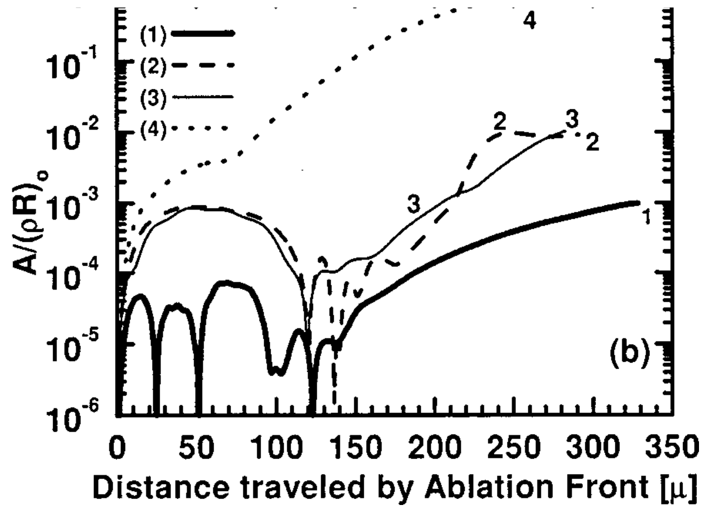
Ref.: S. Zhang, *et al*. Phys. Rev. E 106, 045207 (2022)

Foam ablators* or tailored density profiles† can mitigate laser imprint and hydrodynamic instabilities in LDD experiments



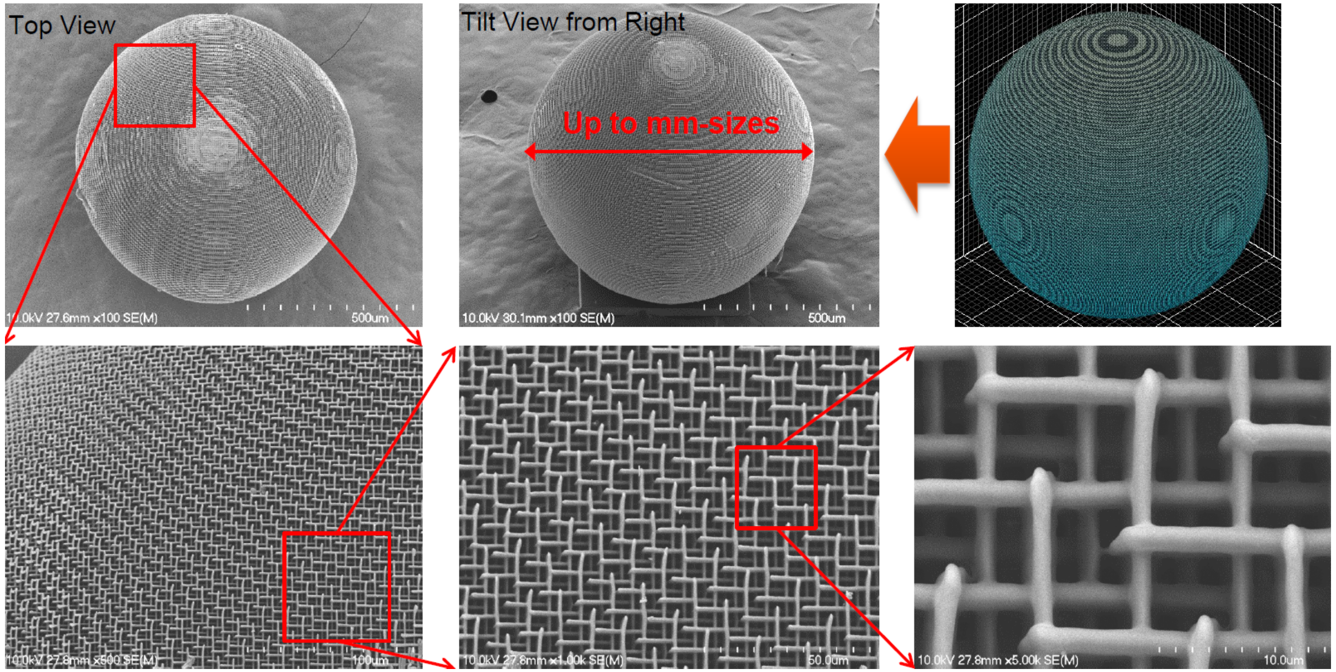


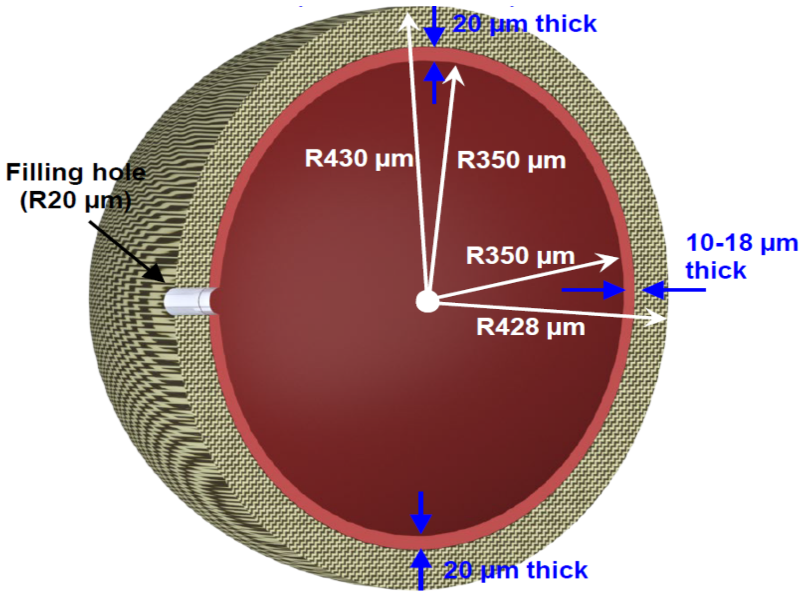




* Hu et al., Phys. Plasmas 25, 082710 (2018); † Metzler et al., Phys. Plasmas 6, 3283 (1999).

LLE has collaborated with UNL to fabricate shell-structured targets with density gradient by direct laser writing using two-photon polymerization (TPP)





High-quality equations of state (EOS) of the target materials are required to test new ideas and optimize designs for relevant ICF and HED experiments

Resins for TPP printing

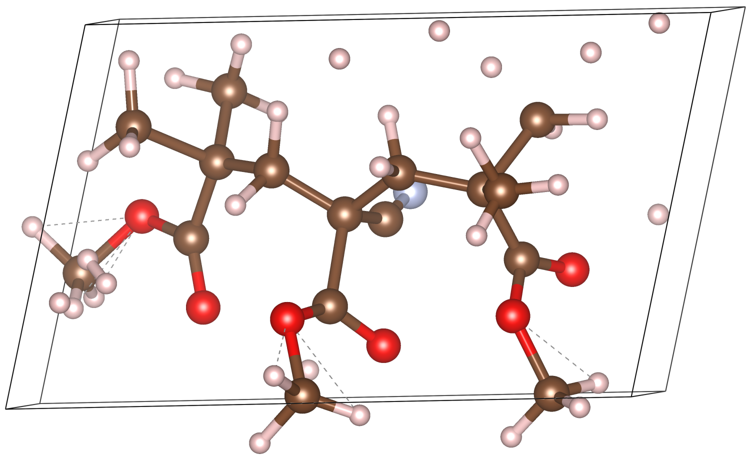
Elemental composition of the resin (at. %)					
Resin	C	H	O	N	Empirical Formula
CHON	31.5	54.05	11.8	5.77	$CH_{1.72}N_{0.086}O_{0.37}$

* Stein et al., Fusion Sci. Technol. 73, 153 (2018).

We construct a high-accuracy EOS for CHON resin based on first principles molecular dynamics simulations

- **Structure model: based on acrylic resin, 1.2 g/cm^3, $CH_{1.72}O_{0.37}N_{0.086}$, 50-400 atom cell**

$C_{16}H_{27}O_6N_1$



A snapshot during a KS-DFT-MD simulation @ 17.5 g/cc, 1000 K

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- **Methods based on KS-DFT-MD (T-SCAN-L), OF-DFT-MD (LKTγTF), and extrapolation (to low ρ and low T)**

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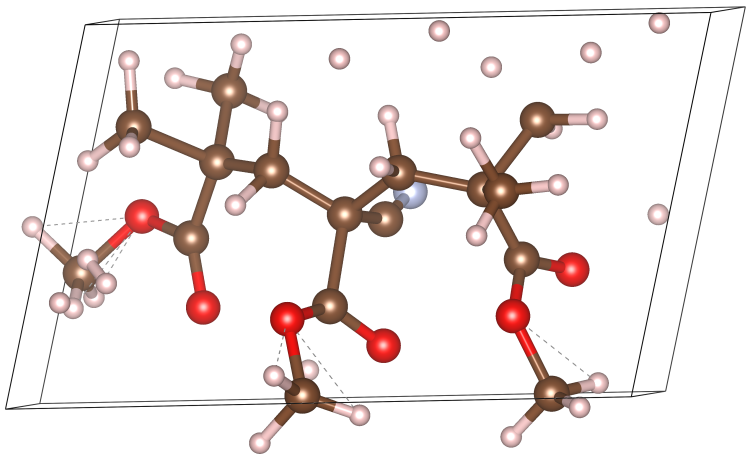

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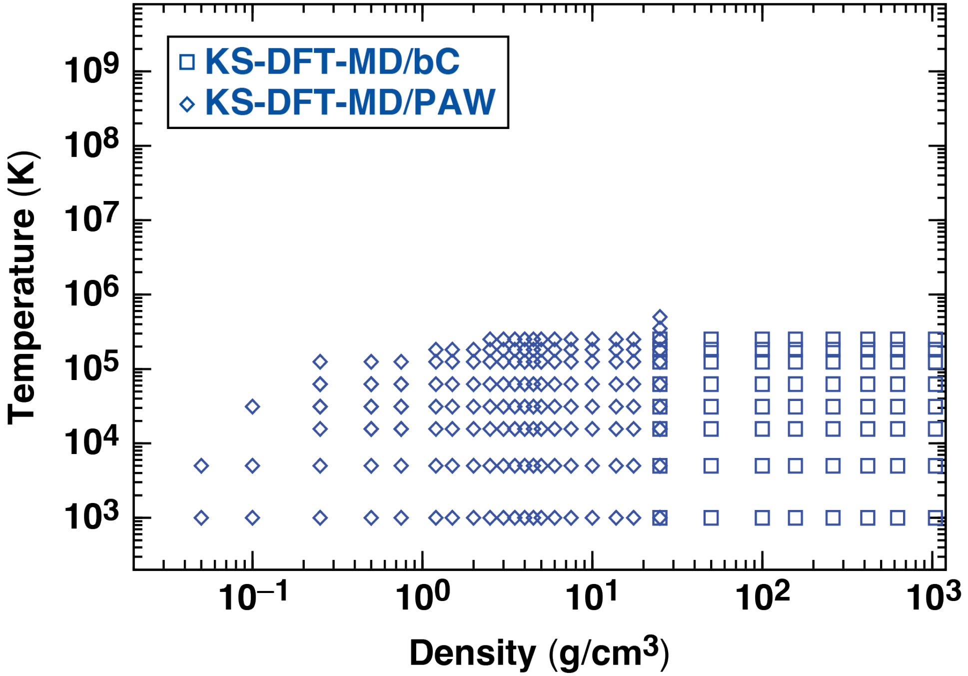

E30409a

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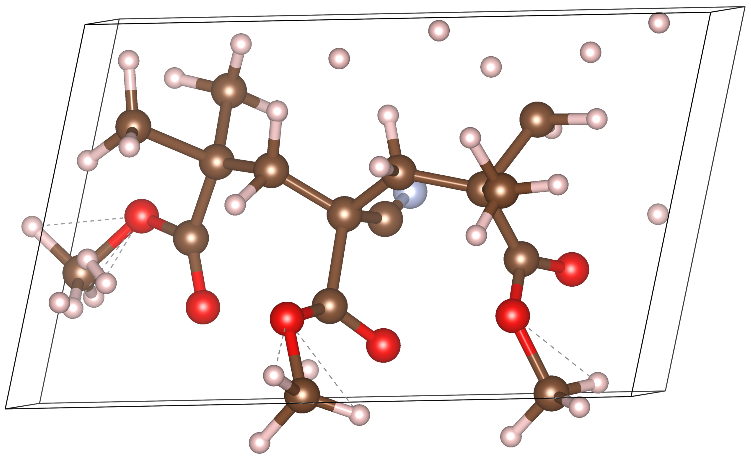
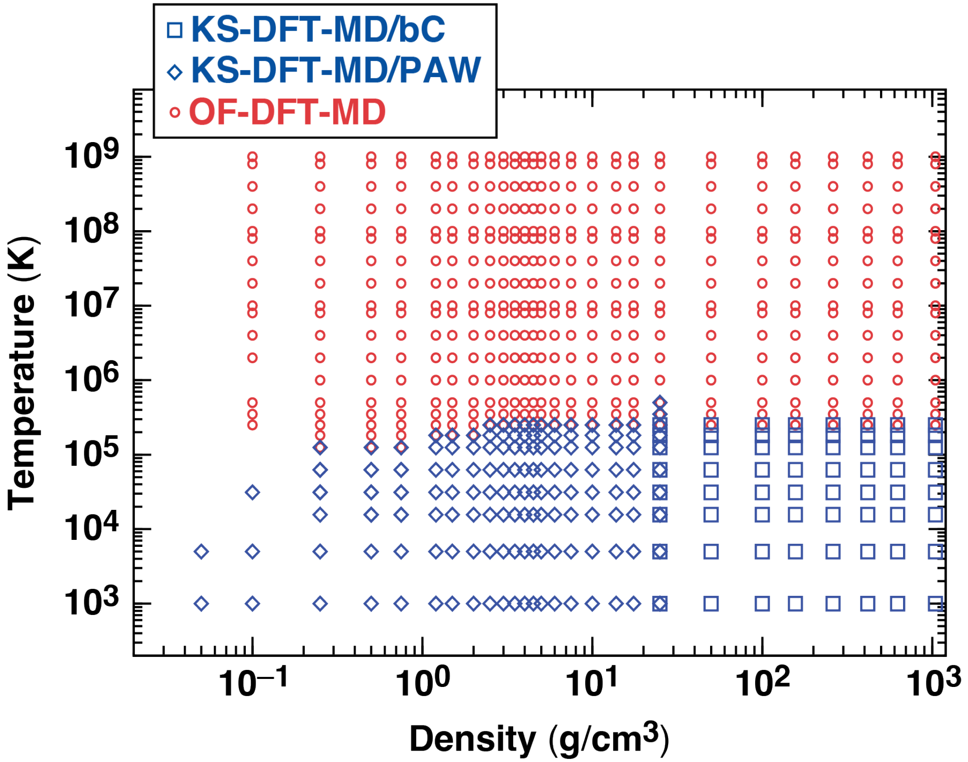
$C_{16}H_{27}O_6N_1$



A snapshot during a KS-DFT-MD simulation @ 17.5 g/cc, 1000 K



E30409b

We construct a high-accuracy EOS for CHON resin based on first principles molecular dynamics simulations

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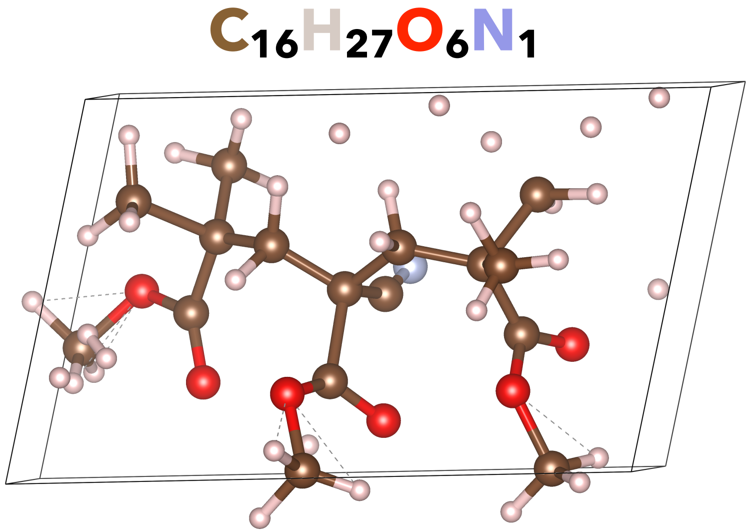
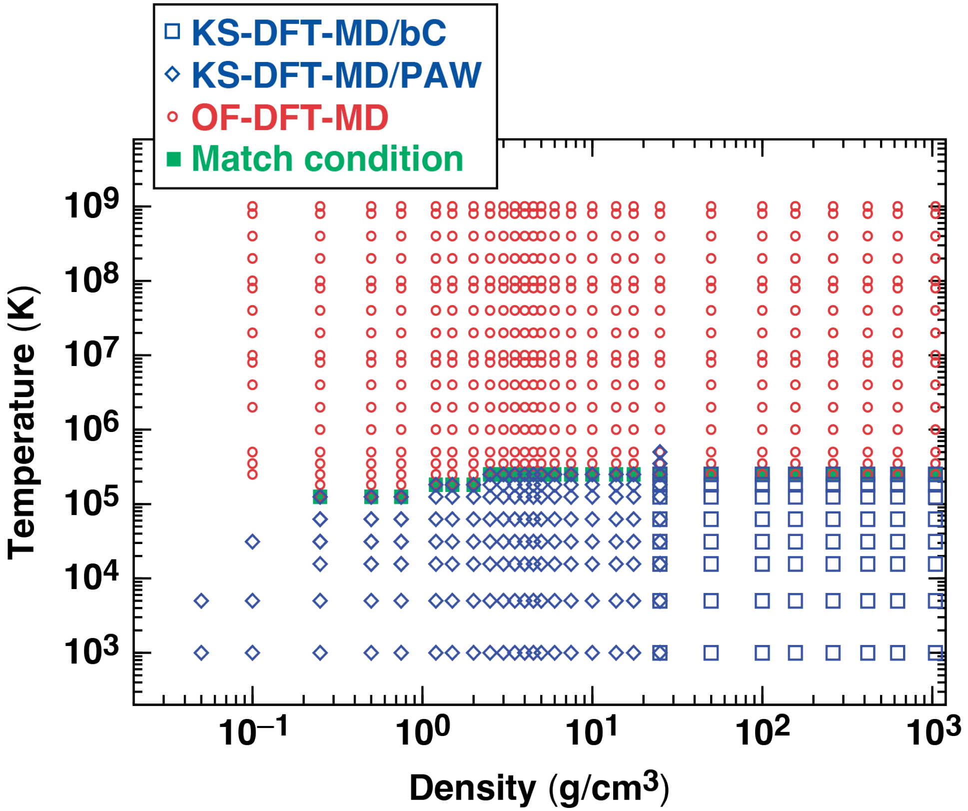
- **Methods based on KS-DFT-MD (T-SCAN-L), OF-DFT-MD (LKTγTF), and extrapolation (to low ρ and low T)**



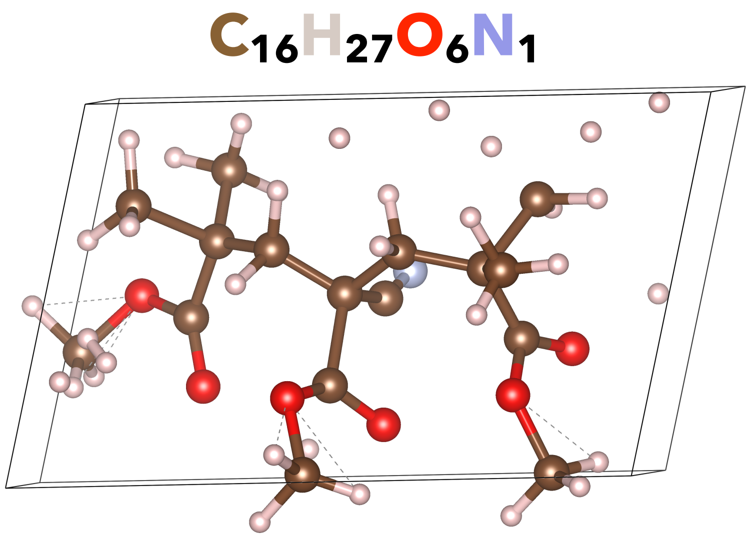
A snapshot during a KS-DFT-MD simulation @ 17.5 g/cc, 1000 K



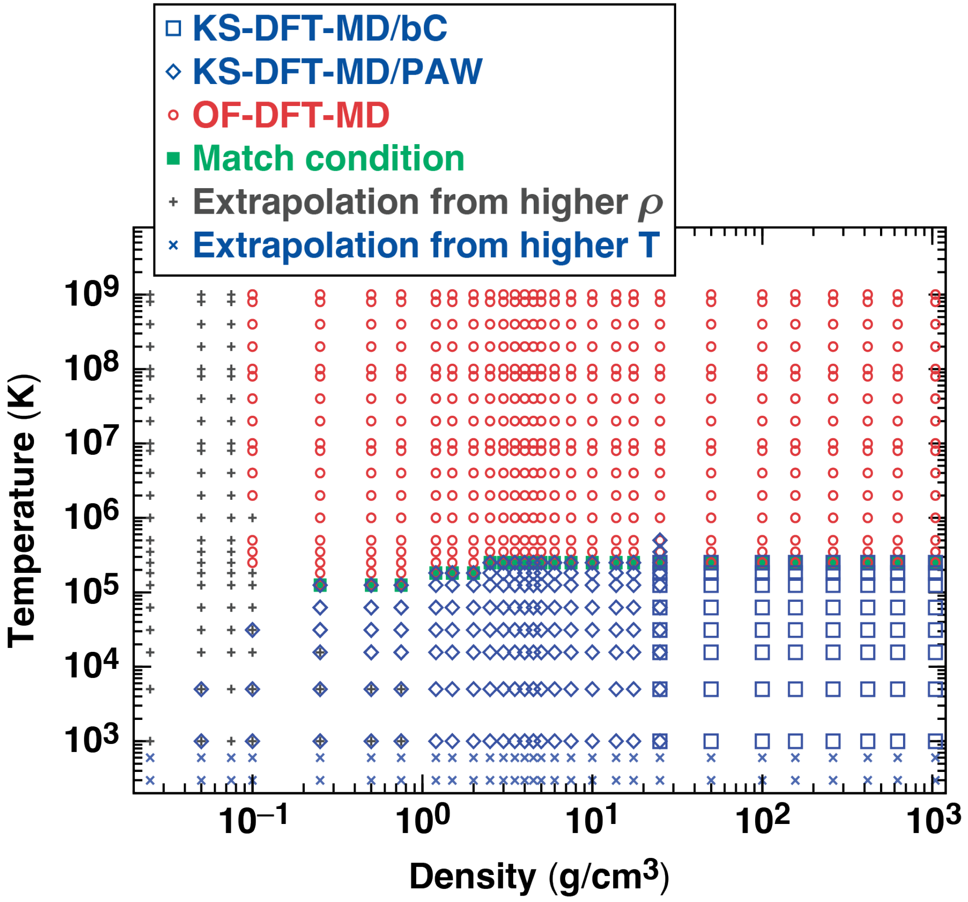
E30409c

We construct a high-accuracy EOS for CHON resin based on first principles molecular dynamics simulations

- **Structure model: based on acrylic resin, 1.2 g/cm^3, $CH_{1.72}O_{0.37}N_{0.086}$, 50-400 atom cell**
- **Methods based on KS-DFT-MD (T-SCAN-L), OF-DFT-MD (LKTγTF), and extrapolation (to low ρ and low T)**
- **Wide-range EOS: 0–1044 g/cm^3, 0–10^9 K**



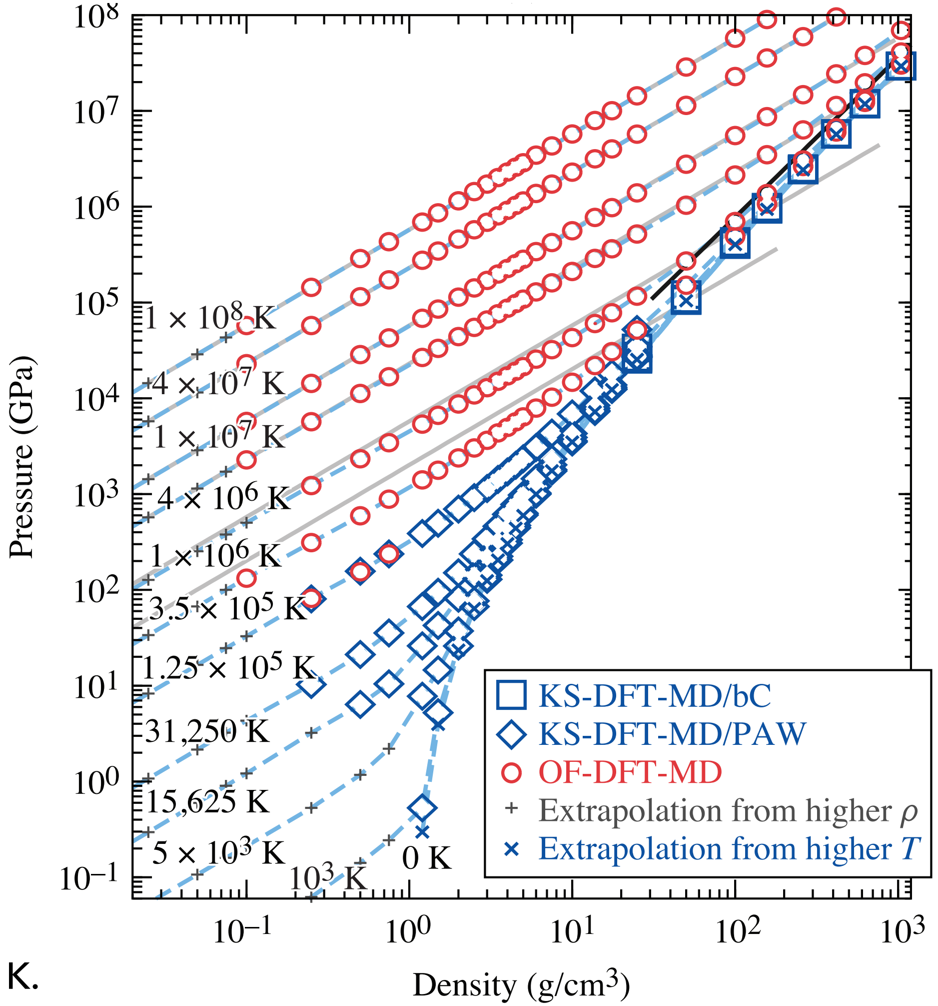
A snapshot during a KS-DFT-MD simulation @ 17.5 g/cc, 1000 K



E30409e

EOS is compared between different approaches and models at various densities and temperatures

- **Smooth bridging of KS and OF data at the matching condition (P differ by <2.5%)**
- **EOS reaches the fully ionized ideal gas values at high T (10^6–10^7 K)**
- **EOS approaches the Fermi degenerate electron gas values at high ρ (>10^3 g/cm^3)**
- **EOS variations are due to the interplay of ion thermal vibration, electron thermal excitation, and electron degeneracy. These lead to variations in thermodynamic properties (e.g., heat capacity and Grüneisen parameter).**

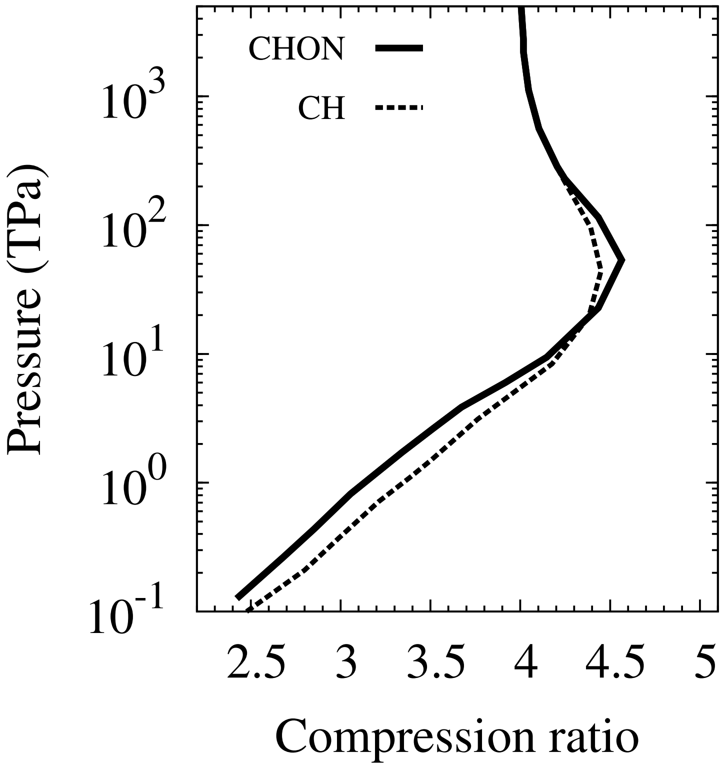


Gray lines: fully ionized ideal gas values;

Black line: Fermi degenerate electron gas values@0 K.

Comparison to CH shows overall similar Hugoniot profiles

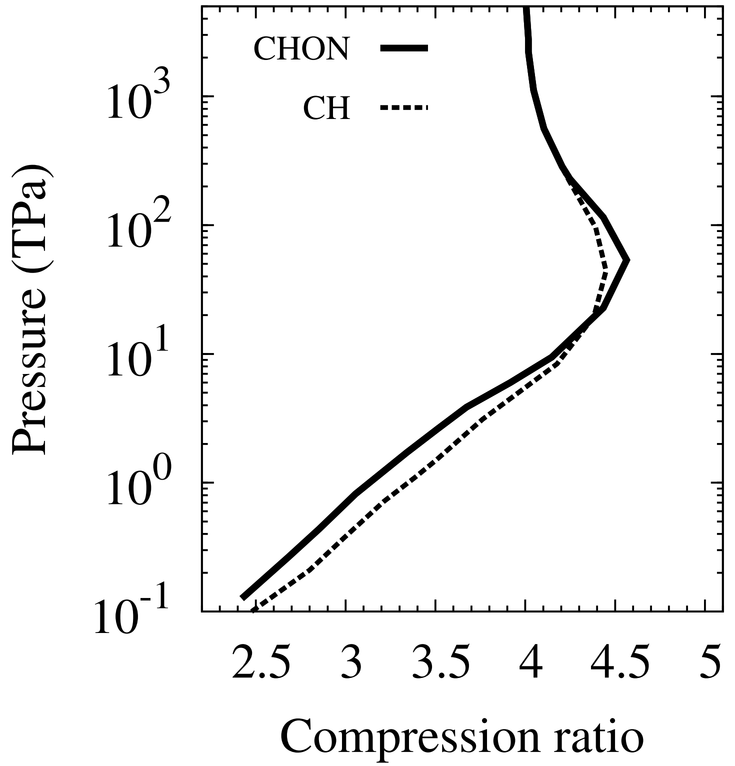
- Compared with the Hugoniot of CH, CHON is stiffer at up to 10 TPa (due to higher ρ_0) and has narrower and larger (by ~2%) compression peak (due to the existence of N and O)

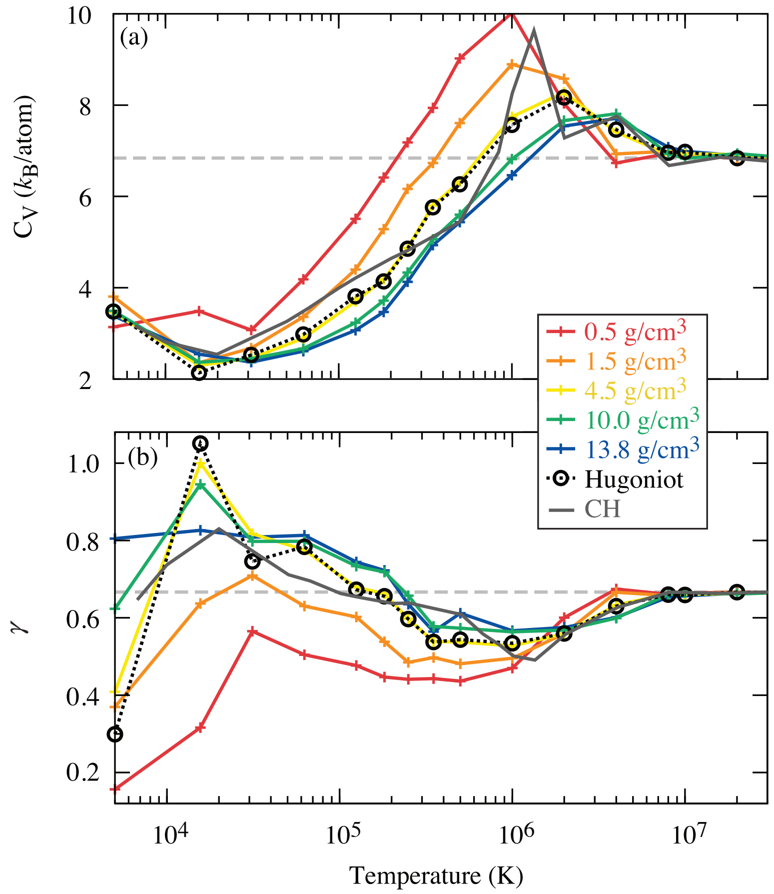


* CH Hugoniot: Hu et al., Phys. Rev. E 92, 043104 (2015).

Comparison to CH shows overall similar Hugoniot profiles and consistency in thermodynamic properties

- **Compared with the Hugoniot of CH, CHON is stiffer at up to 10 TPa (due to higher ρ_0) and has narrower and larger (by ~2%) compression peak (due to the existence of N and O)**
- **A minimum in C_V and local maximum in γ at 2–3×10^4 K, corresponding to bonded-atomic transition**
- **A peak in C_V and a basin in γ at 10^6 K, corresponding to ionization of the *K* shell**
- **C_V and γ reach the fully ionized ideal gas limit at T>10^7 K**

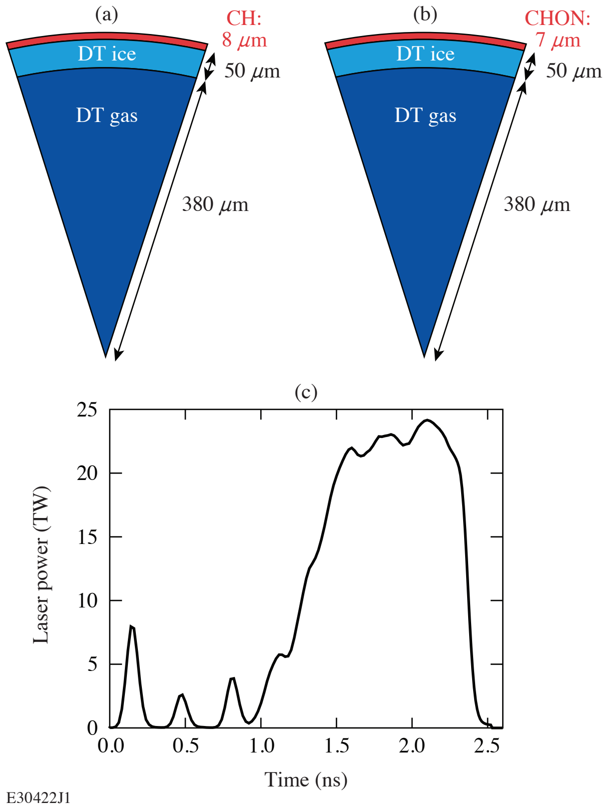


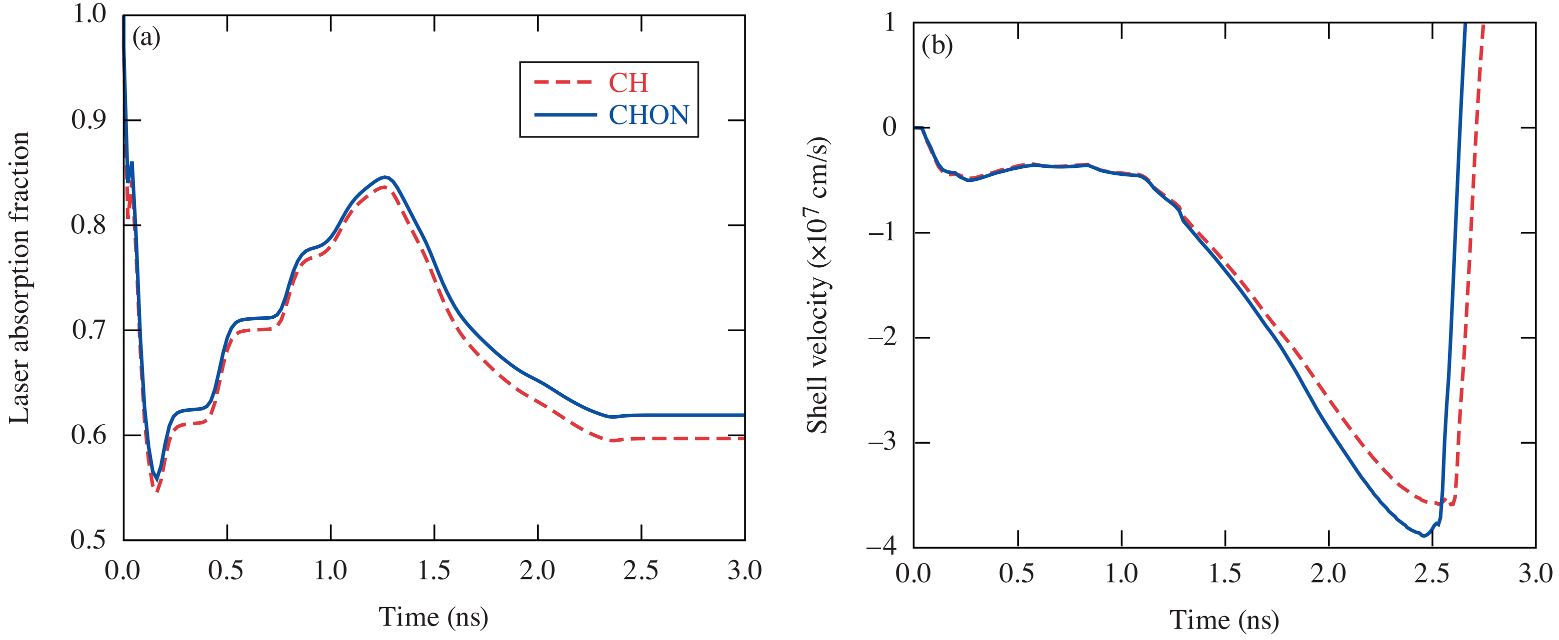


* **CH Hugoniot: Hu et al., Phys. Rev. E 92, 043104 (2015).**
* **CH thermodynamic properties: Zhang *et al.*, Phys. Rev. E 96, 013204 (2017); J. Chem. Phys. 148, 102318 (2018).**

LDD targets using CHON ablators outperform CH according to 1D radiation hydrodynamic simulations

- **LILAC simulations with OMEGA-scale cryo-DT target and state-of-the-art physics models (CBET, iSNB, first-principles EOS and OT; collisional-radiative-equilibrium model for the opacity); total UV laser energy ~27 kJ**
- **CHON outperforms CH due to slight increase in the laser absorption fraction**





	CH	CHON
DT-neutron Yield	8.8×10^{13}	1.3×10^{14}

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