SAND2013-5307C

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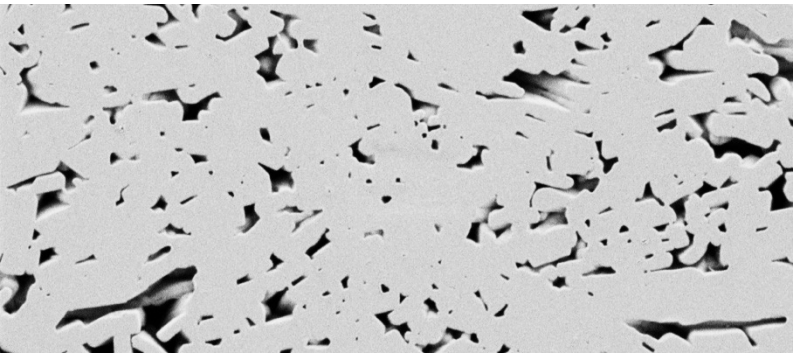
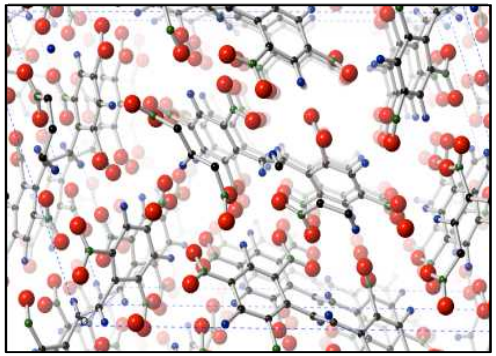
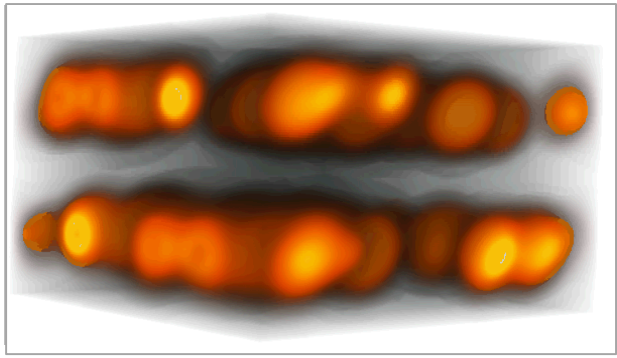

First-principles prediction of equations of state for molecular crystal explosives.

Ryan R. Wixom and David L. Damm

Ann Mattsson, Kyle Cochrane, Thomas Mattsson, Ray Shan, and Adian Thompson

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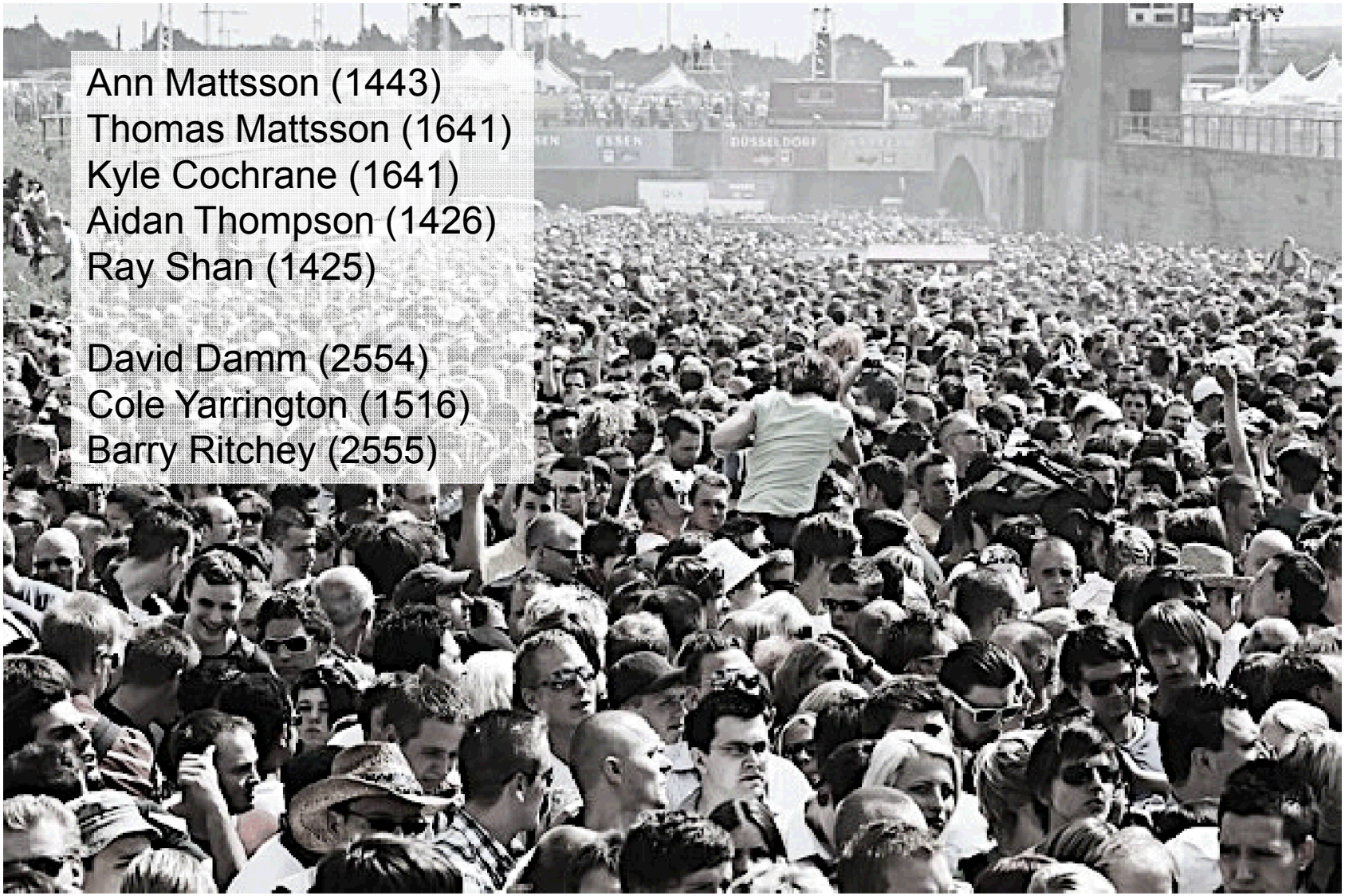
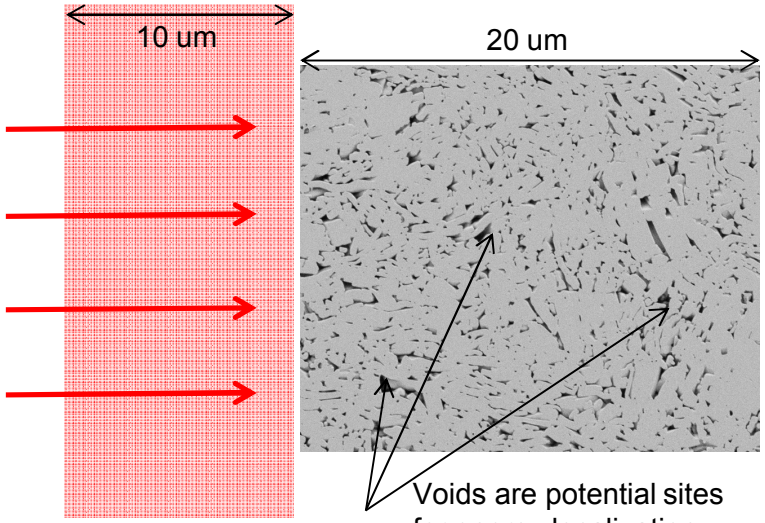
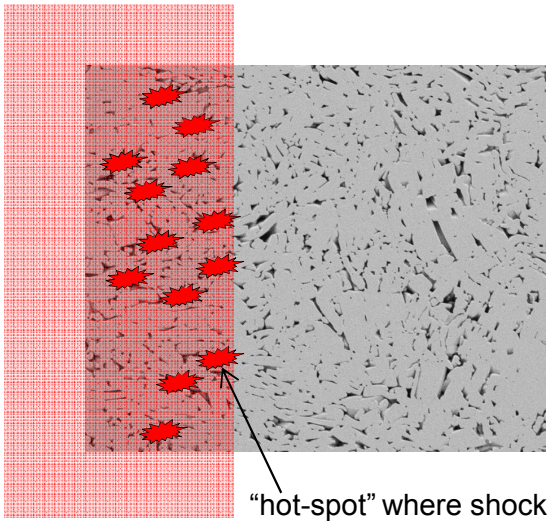
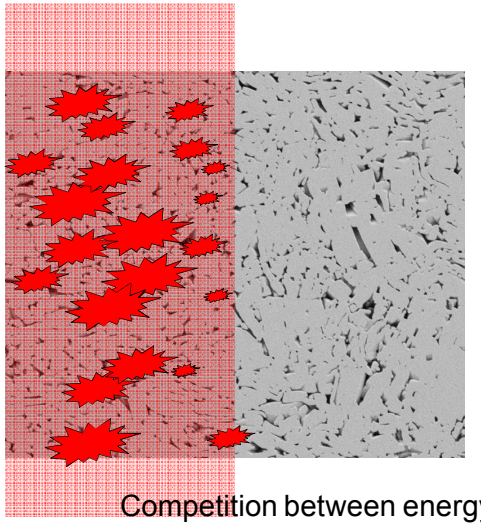
The peoples:

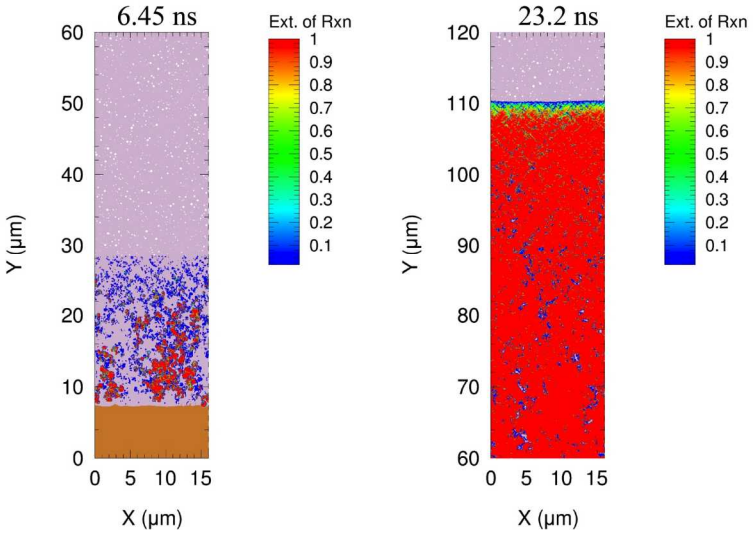

Ann Mattsson (1443)
Thomas Mattsson (1641)
Kyle Cochrane (1641)
Aidan Thompson (1426)
Ray Shan (1425)
David Damm (2554)
Cole Yarrington (1516)
Barry Ritchey (2555)

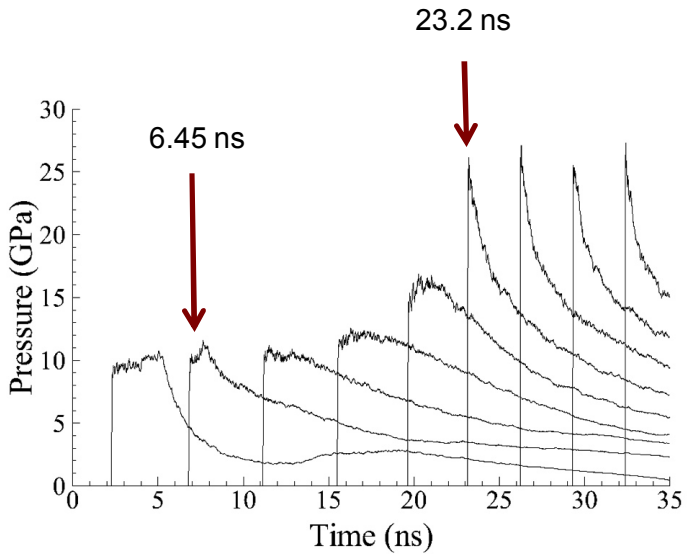
Grain-scale simulations of SDT in HNS







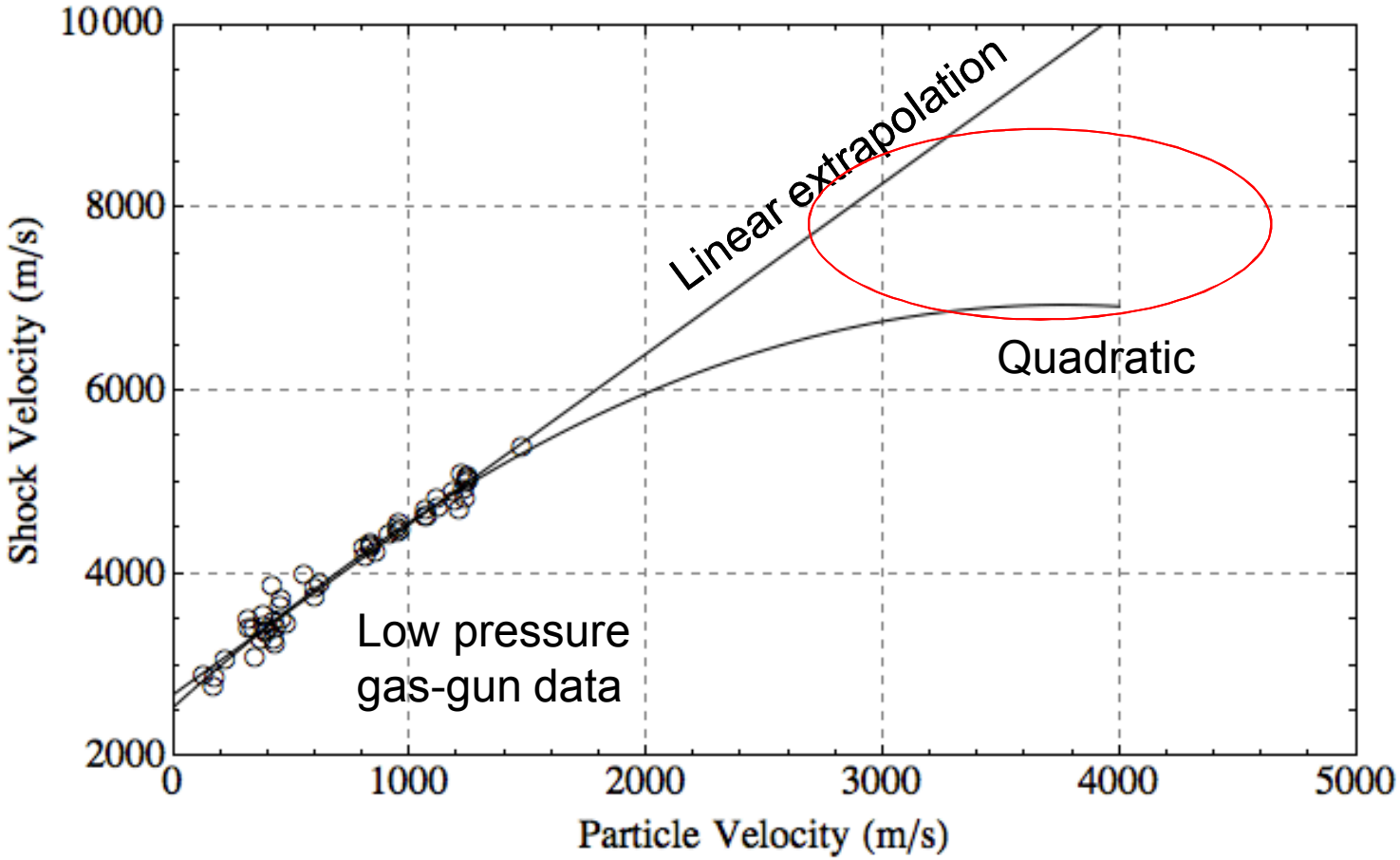




Simulations: Flyer impact at 3.15 km/s, Mean pore size 86 um

Extrapolation = Bad.

#WhyIsMySimulationWrong?



Density Functional Theory (DFT) and XC functionals:

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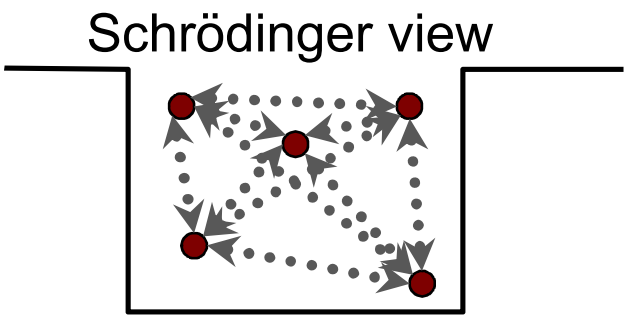
Properties of the system: P,T,V,E on the Hugoniot

Schrodinger Equation SE

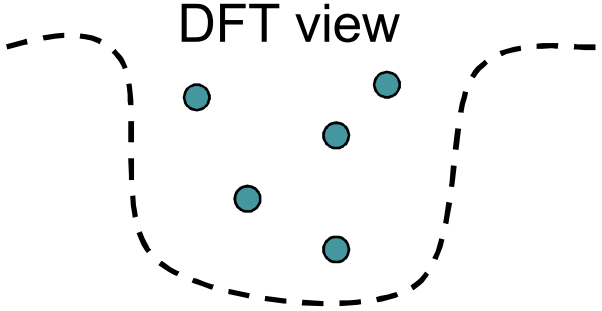
Kohn-Sham Equations KS

Hard problem to solve

"Easy" problem to solve



Formally equivalent



electron
interaction
external potential

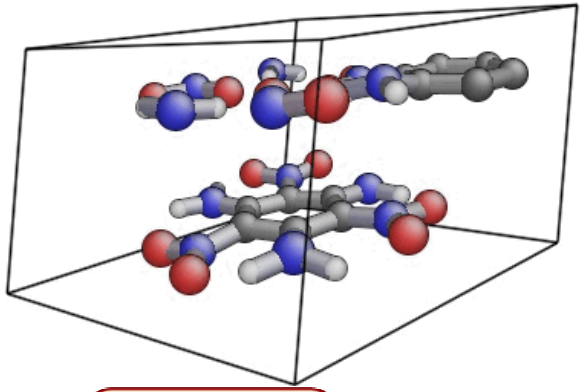
Kohn-Sham particle (non-interacting)
effective potential

$$v_{eff}(\boldsymbol{r}) = v(\boldsymbol{r}) + \int \frac{n(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} d\boldsymbol{r}' + \frac{\delta E_{xc}[n(\boldsymbol{r})]}{\delta n(\boldsymbol{r})}$$

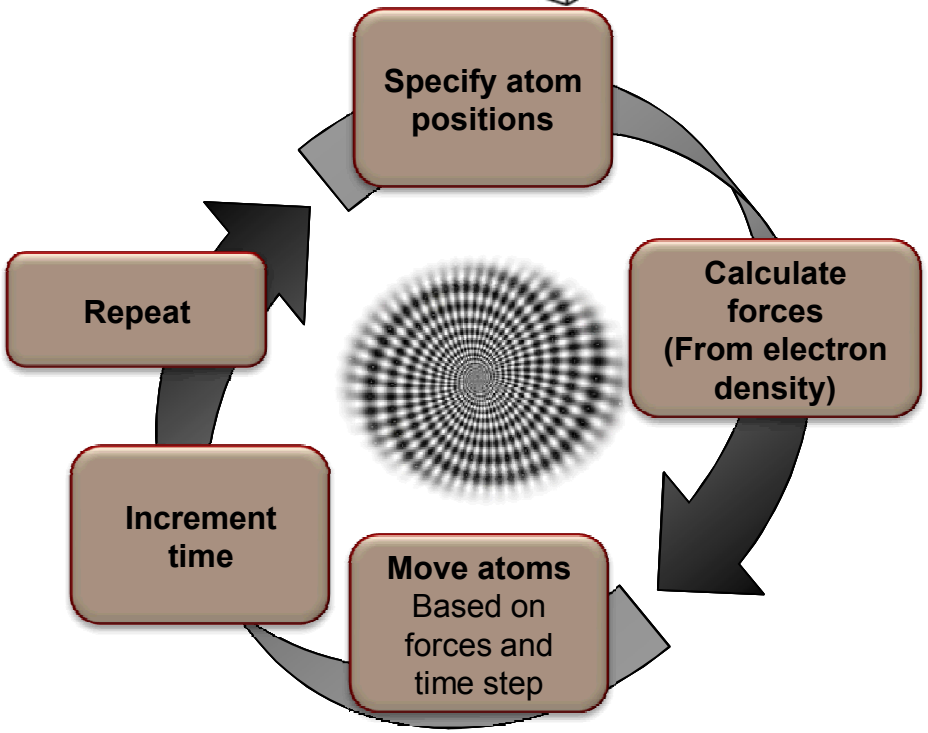
AM05, LDA, GGA, Meta-GGA, Hybrids

Molecular Dynamics (MD):

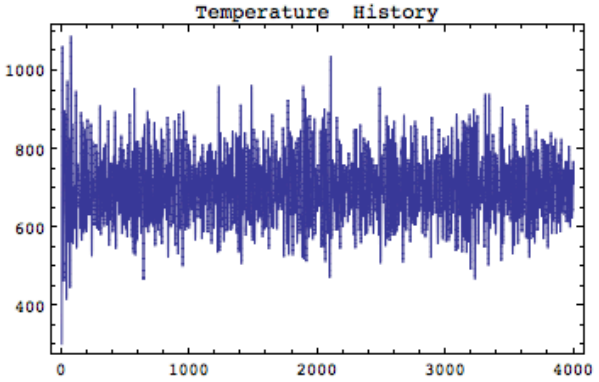
TATB
V/Vo = 0.729
T = 700 K



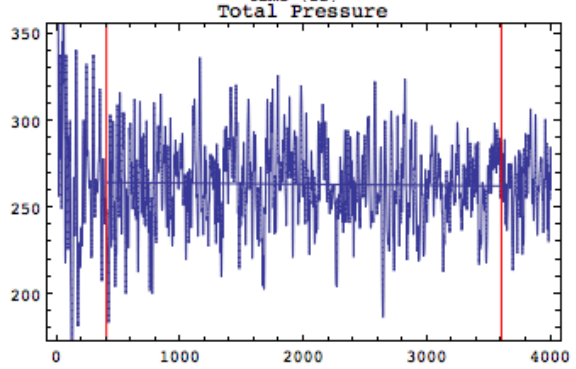
V



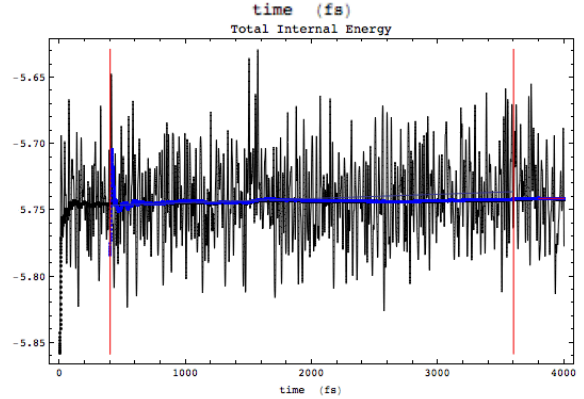
T



P

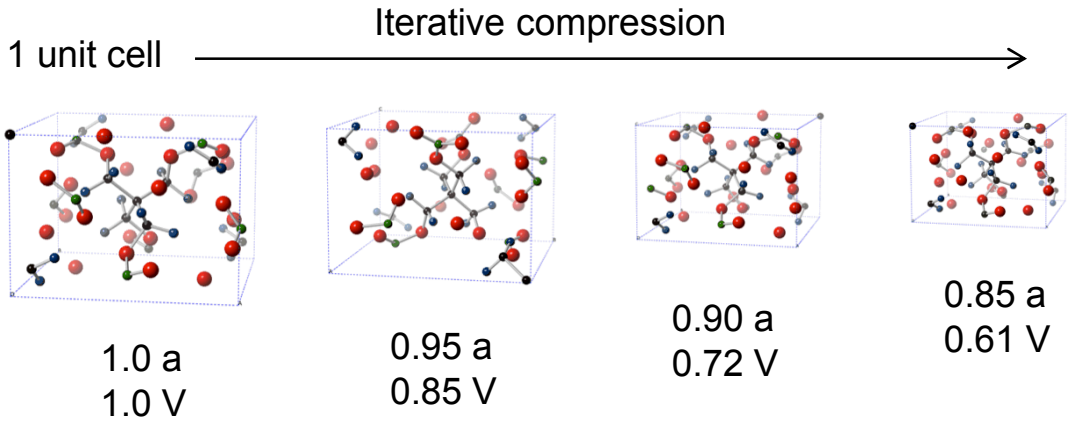


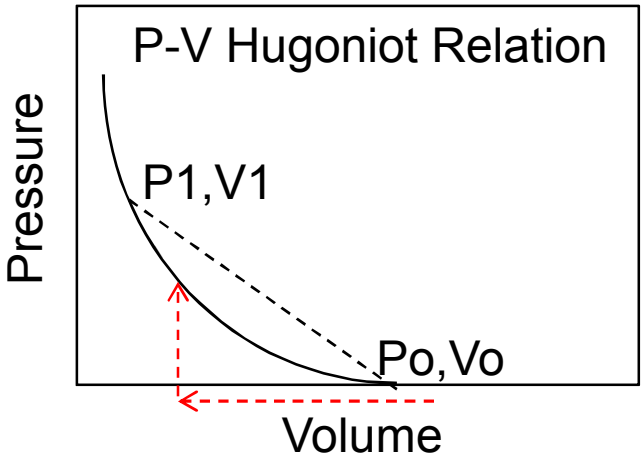
E



10,000 time-steps

Finding the Hugoniot, Iterative compression





Rankine-Hugoniot Relations:

Mass:

$\rho_o D = \rho_1 (D - u_1)$

Momentum:

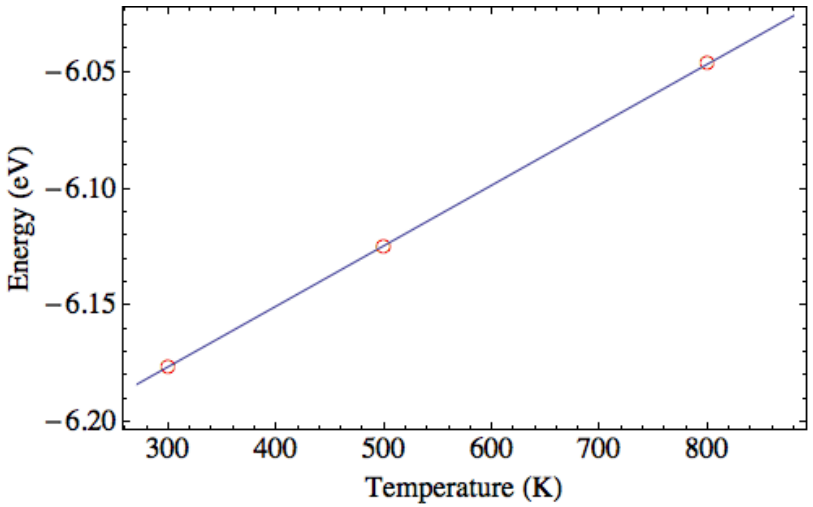
$P_1 = \rho_o D u_1$

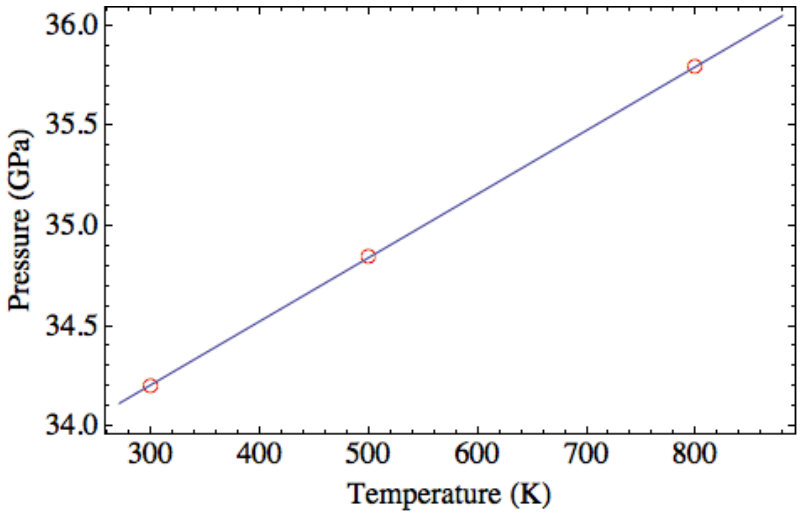
Energy:

$E - Eo = \frac{1}{2}(P + Po)(Vo - V)$

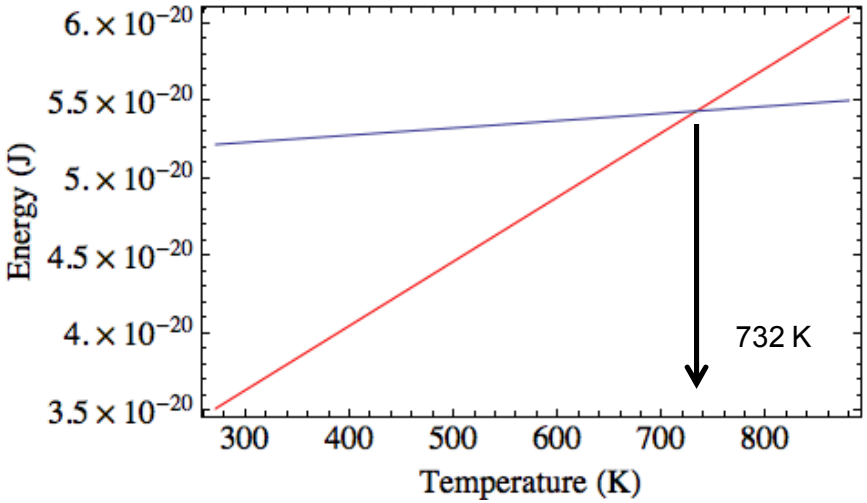
Key Point: jump conditions are only valid on the Hugoniot

Finding the Hugoniot (TATB V=0.85*V_o):





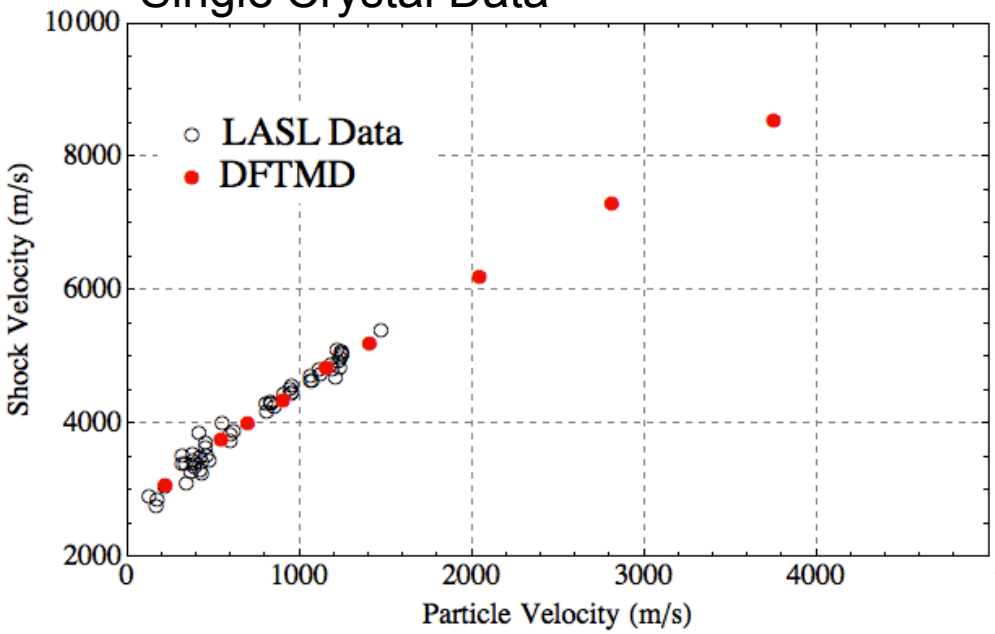
$$E(T) - E_o = \tfrac{1}{2}[P(T) + P_o][V_o - V]$$



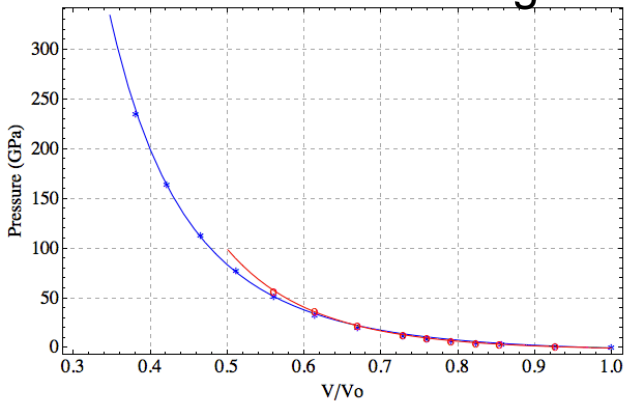
First-principles EoS for PETN

Remarkable Agreement!

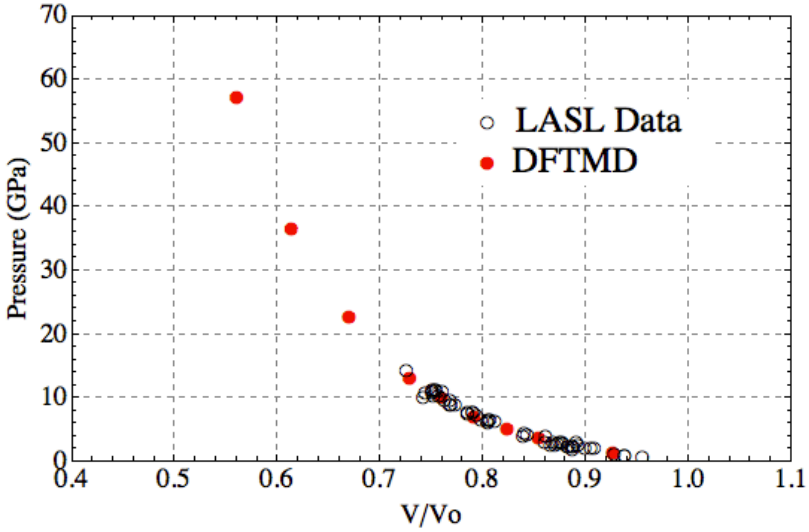
Single Crystal Data



Isotherm and Hugoniot



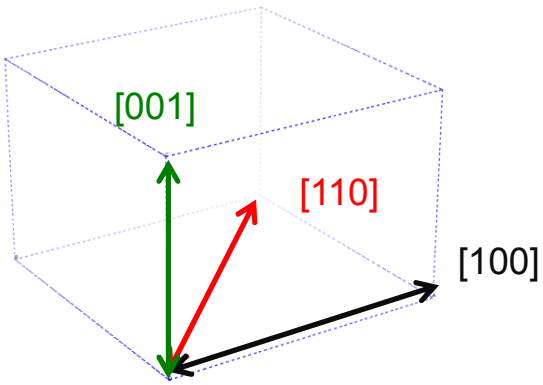
P-V Hugoniot

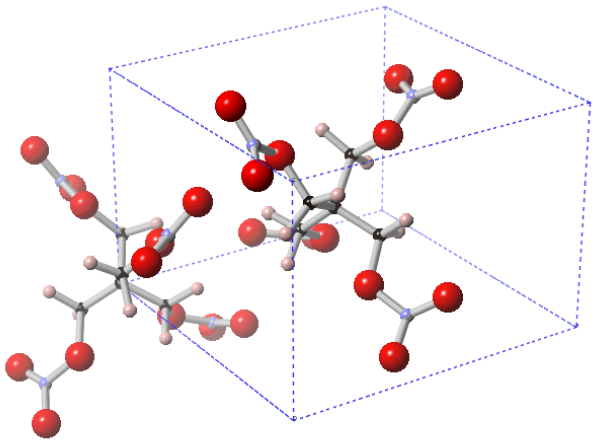


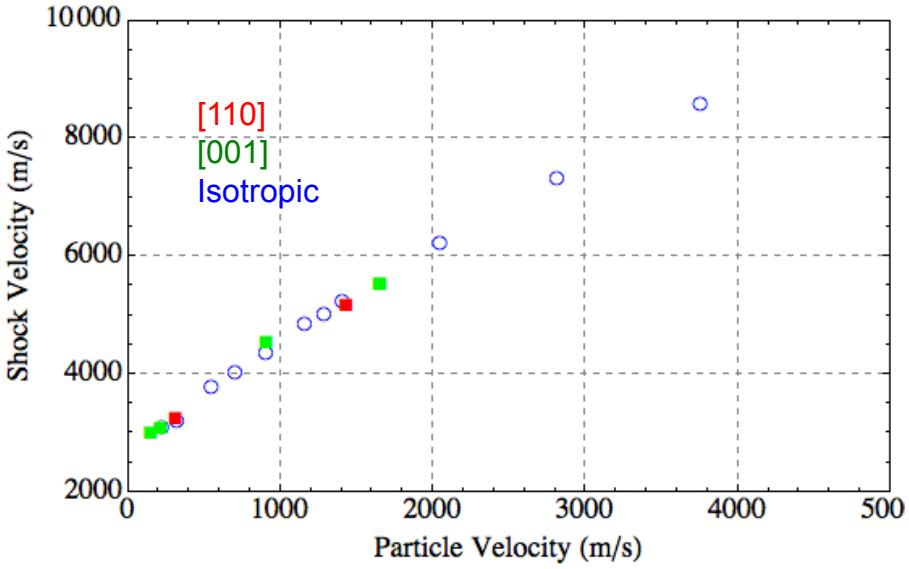
- Uniaxial compression gives similar results (at least for pressure).
- Have all the components necessary to write a tabular EOS.
- Isotherm and Hugoniot are super close in P-V space.

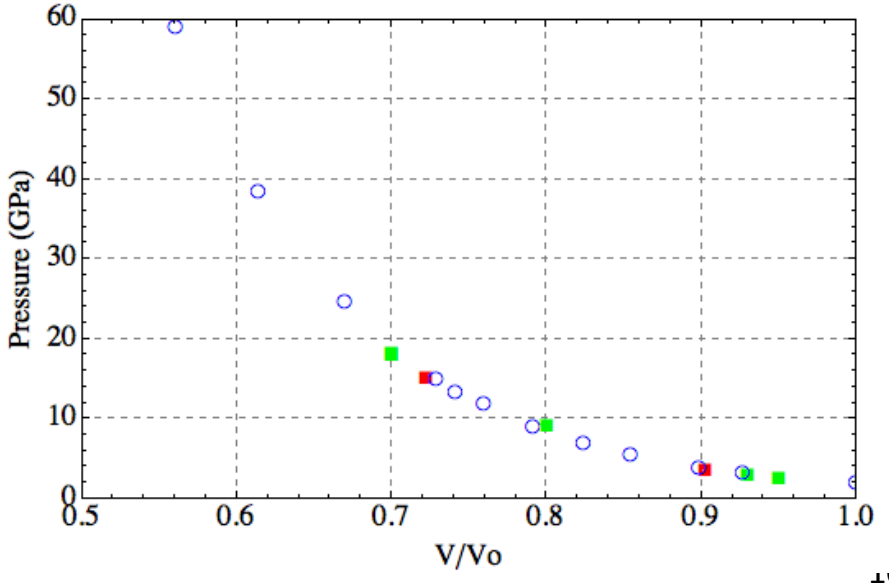
Isotropic vs. Uniaxial shocks in PETN

Lattice Parameters
a = 0.938 nm
b = a
c = 0.671 nm

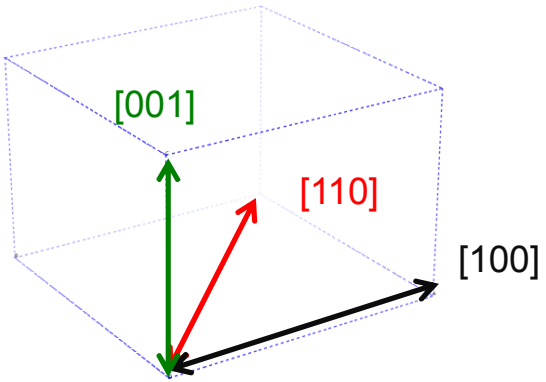


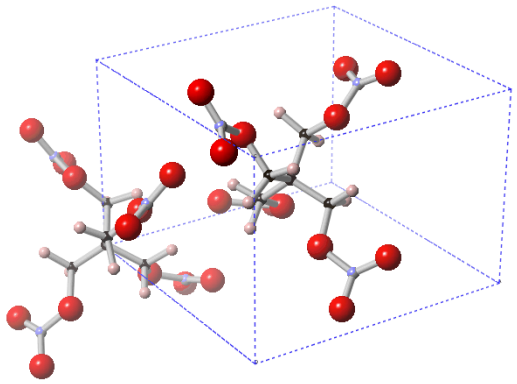


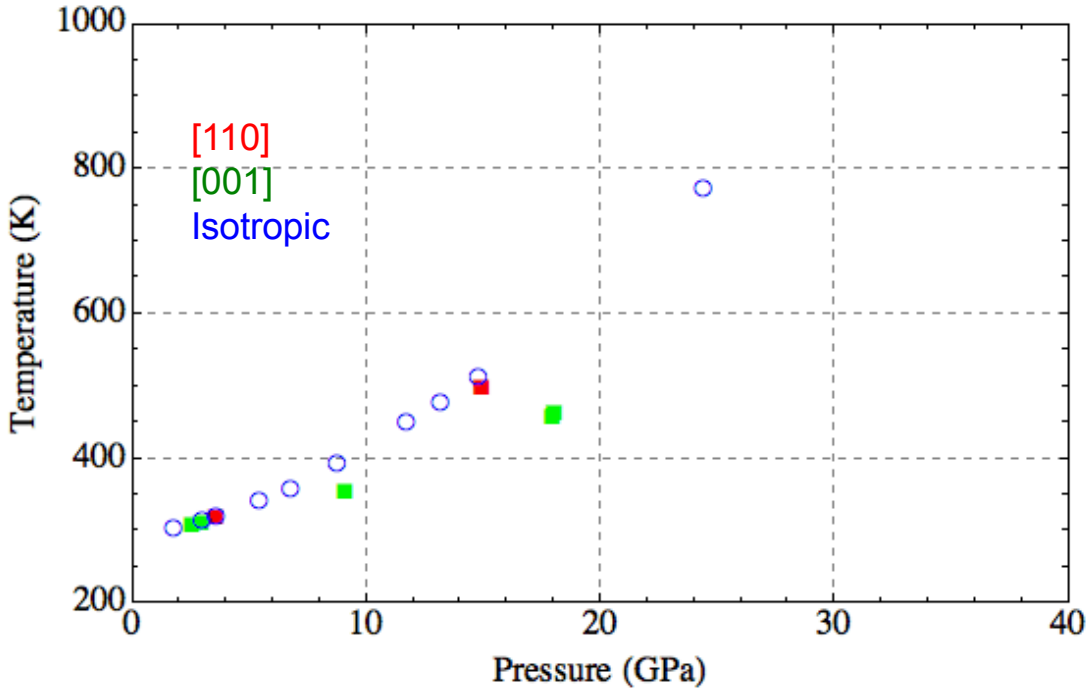




Uniaxial shocks in PETN: Different Temperatures ???

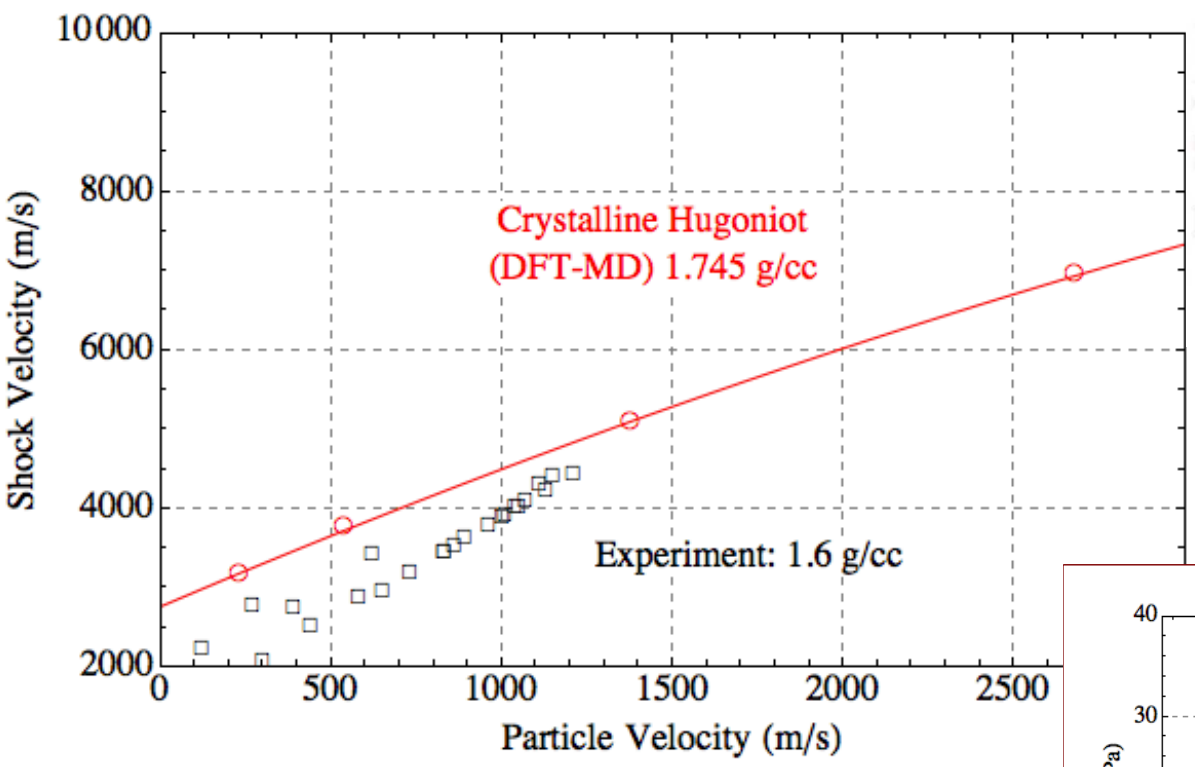


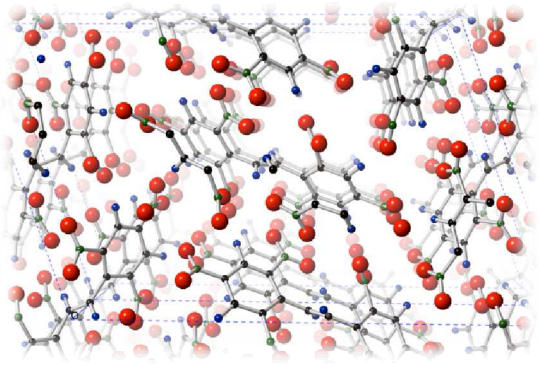


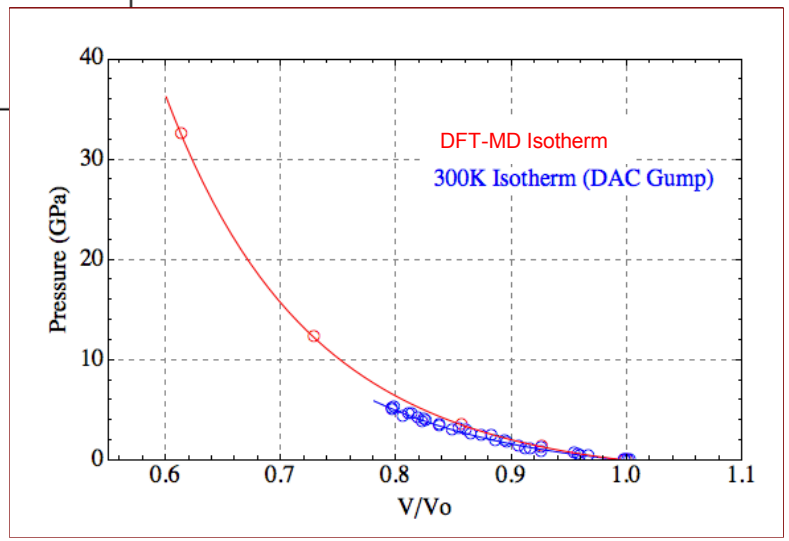


Orientation	Expt.[29]	This work		
	Stress (GPa)	Stress (GPa)	U_s (km/s)	U_p (km/s)
[110]	8.40	12.7	5.0	1.621
[001]	13.3	19.9	6.0	2.118
[100]	31.3	21.1	6.0	2.231

EoS for Hexanitrostilbene (HNS) from DFT-MD







Two issues:

1. No crystalline experimental data.
2. Predicted isotherm doesn't match Gump's DAC data.

Porous Hugoniot from the Crystalline Hugoniot

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[1] $v U_S = v_0 (U_S - u_P)$ Rankine – Hugoniot Relations

[2] $P v_0 = u_P U_S$

[3] $e - e_0 = \frac{1}{2} P (v_0 - v)$

[4] $U_S = C_0 + S_1 u_P + S_2 u_P^2 \ldots$ Polynomial Fit

[5] $\Gamma = v \left(\frac{(P - P_0)}{(e - e_0)} \right)$ Gruneisan Parameter

Assume solid and porous material have the same refernce, $P_0 = P_0^* = 0$ and $e_0 = e_0^*$

[6] $P = \frac{\Gamma}{v} (e - e_0)$ (Solid) $P^* = \frac{\Gamma}{v} (e^* - e_0)$ (Porous*)

[7] $P - P^* = \frac{\Gamma}{v} (e - e^*)$ The two pressures can be related at any shock state, v

[8] $P - P^* = \frac{\Gamma}{v} \left(\frac{1}{2} P (v_0 - v) - \frac{1}{2} P^* (v_0^* - v) \right)$ by substituting [3] into [7]

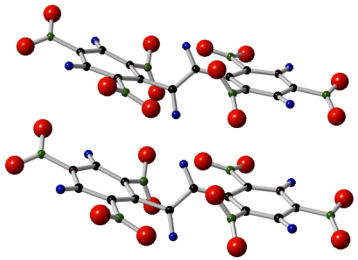
[9] $P^* = P \frac{v_0 - v - \frac{2v}{\Gamma}}{v_0^* - v - \frac{2v}{\Gamma}}$ Where Gamma can be constant or dependent on density $\Gamma = \frac{\Gamma_0 \rho_0}{\rho}$

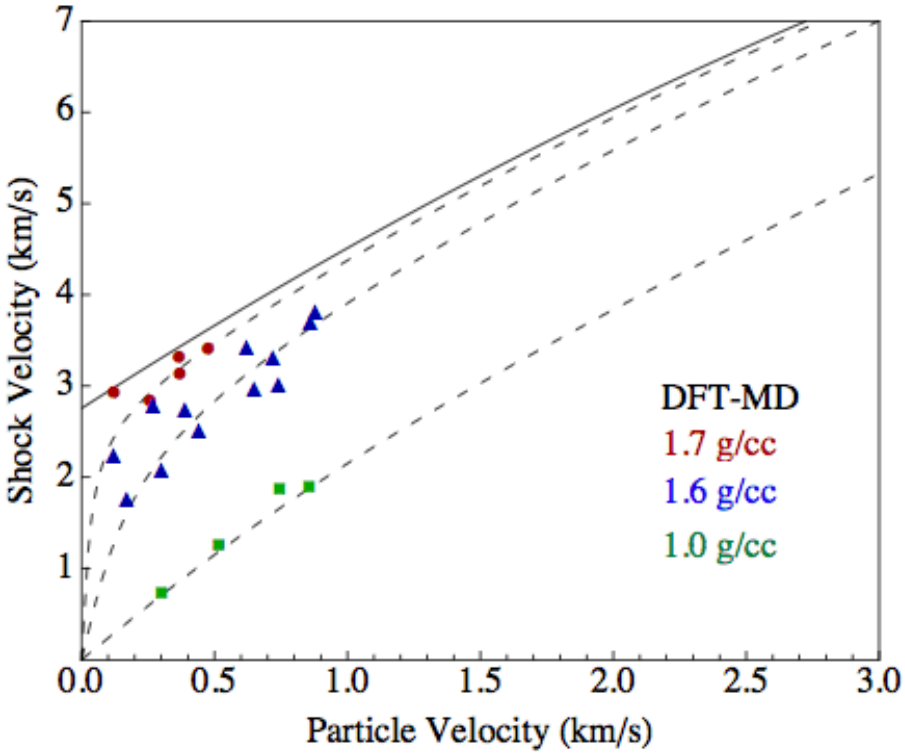
[10] $u_P^* = \frac{U_S^* (v_0^* - v)}{v_0^*}$ by solving [1] for particle velocity

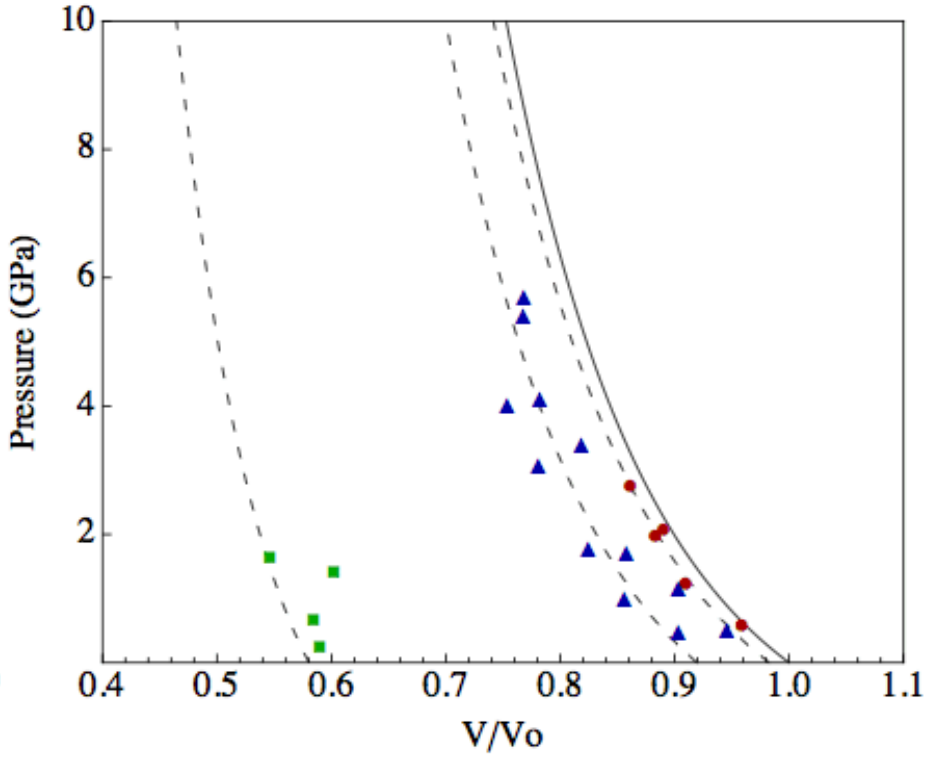
[11] $U_S^* = v_0^* \sqrt{\frac{P^*}{(v_0^* - v)}}$ by substituting [10] into [2]

This does not depend on microstructure, only depends on initial density (... and purity)

Hexanitrostilbene (HNS) Crystalline and Porous Hugoniots



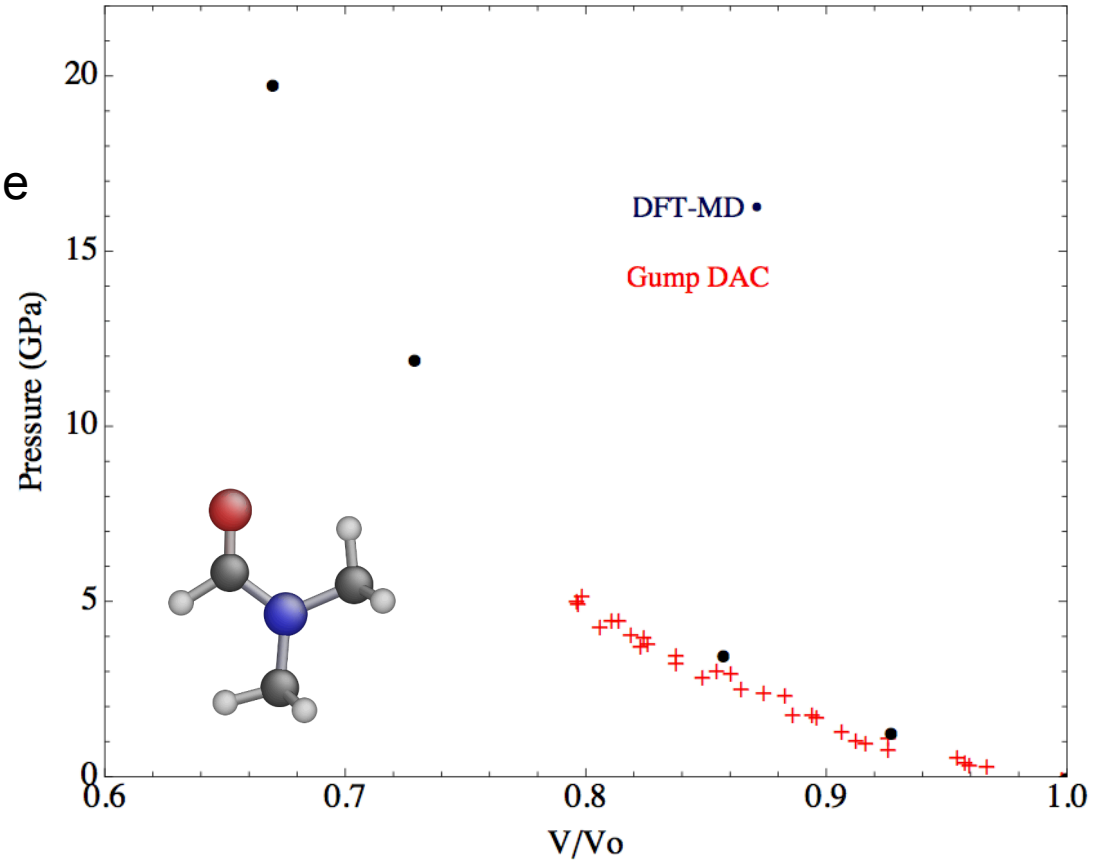




Isotherm of HNS, Validation?

1. Degradation
2. Hydrostatic
3. Polycrystalline
4. Defects

HNS-IV
99.6 % Pure



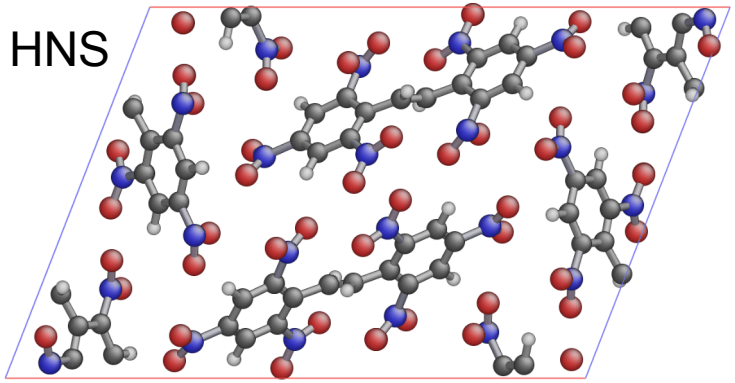
EQUATIONS OF STATE OF HEXANITROSTILBENE (HNS)

Jared C. Gump, Chad A. Stoltz, Brian P. Mason and Emily M. Heim[1]

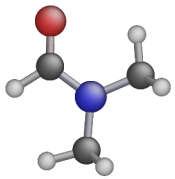
Naval Surface Warfare Center, Indian Head Division, Indian Head, MD 20640
[1]Naval Research Enterprise Intern Program

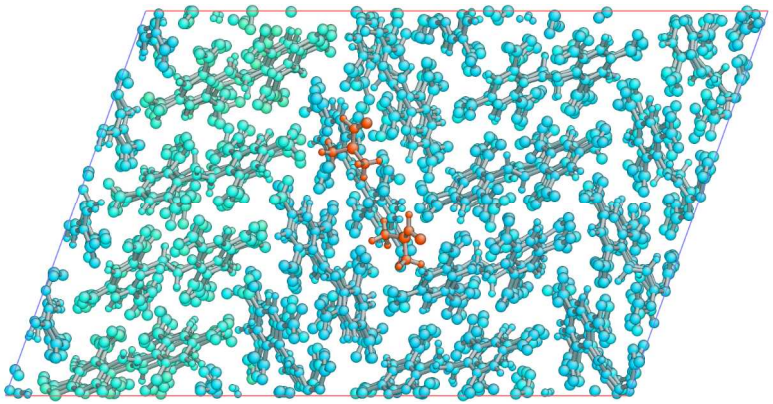
ReaxFF MD, Isotherm of HNS w/ DMF

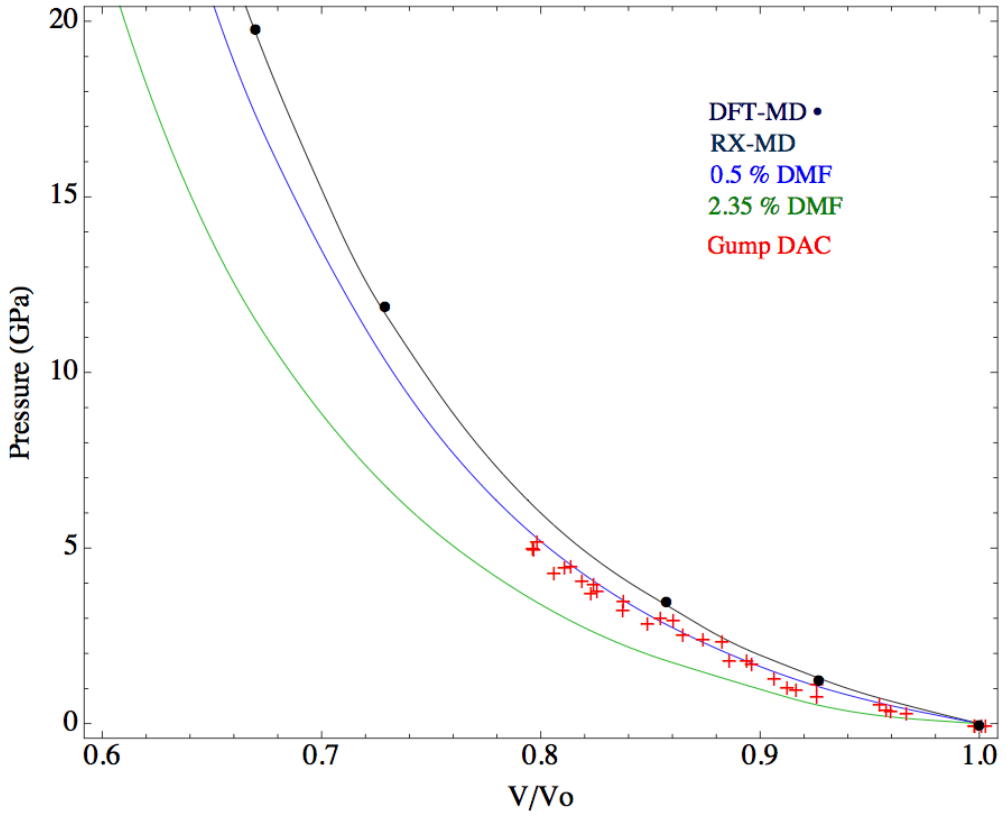
HNS



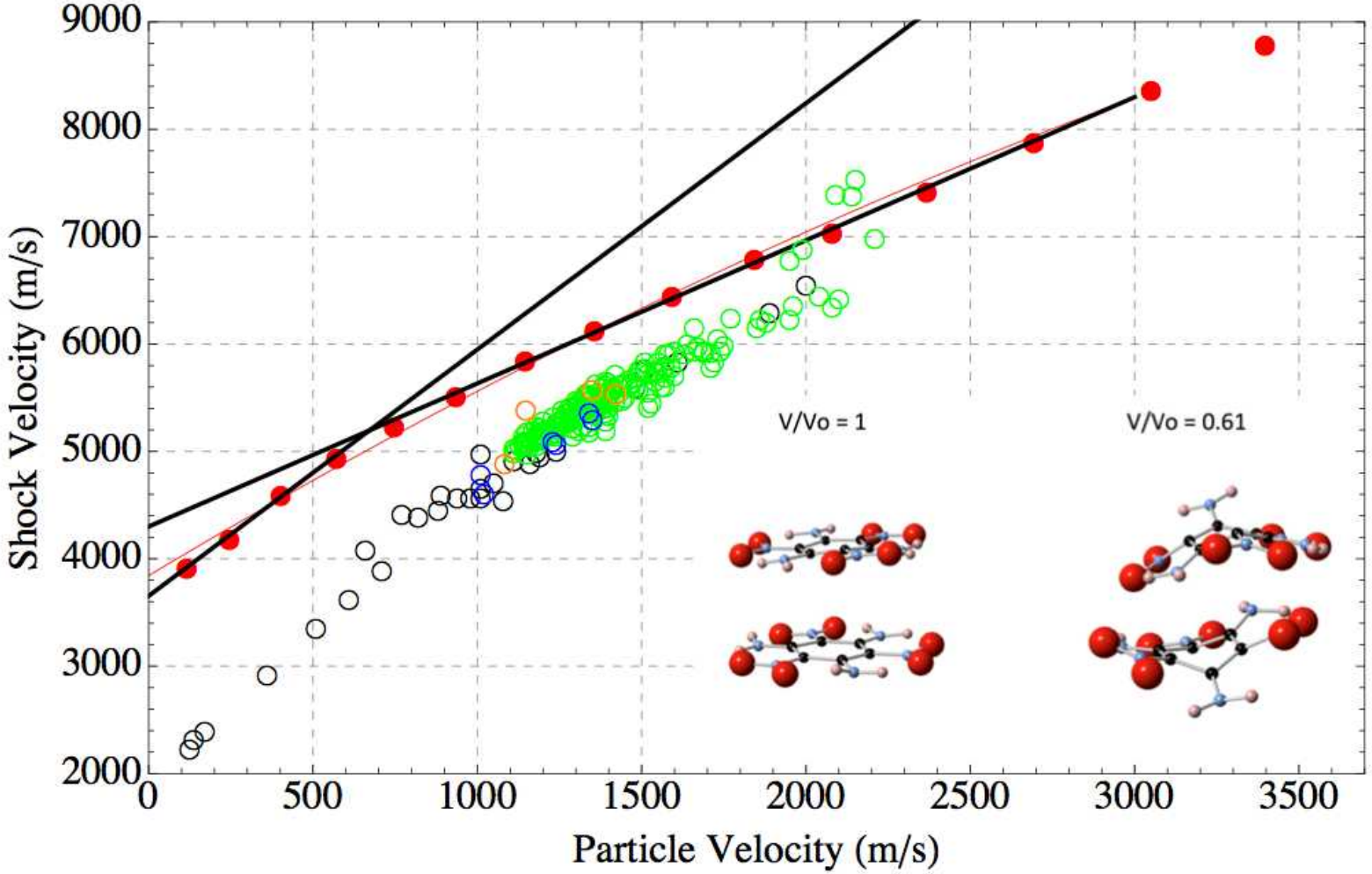
DMF



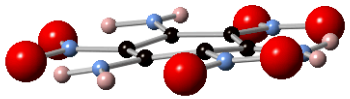


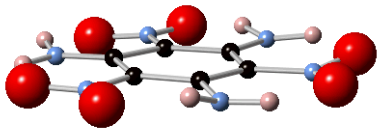


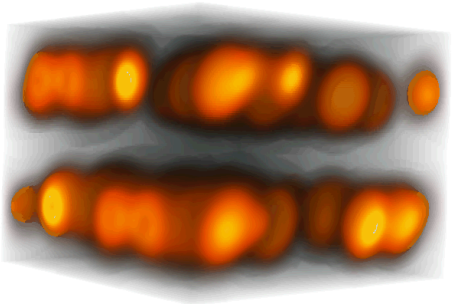
DFT-MD Hugoniot of TATB and data for PBX-5902

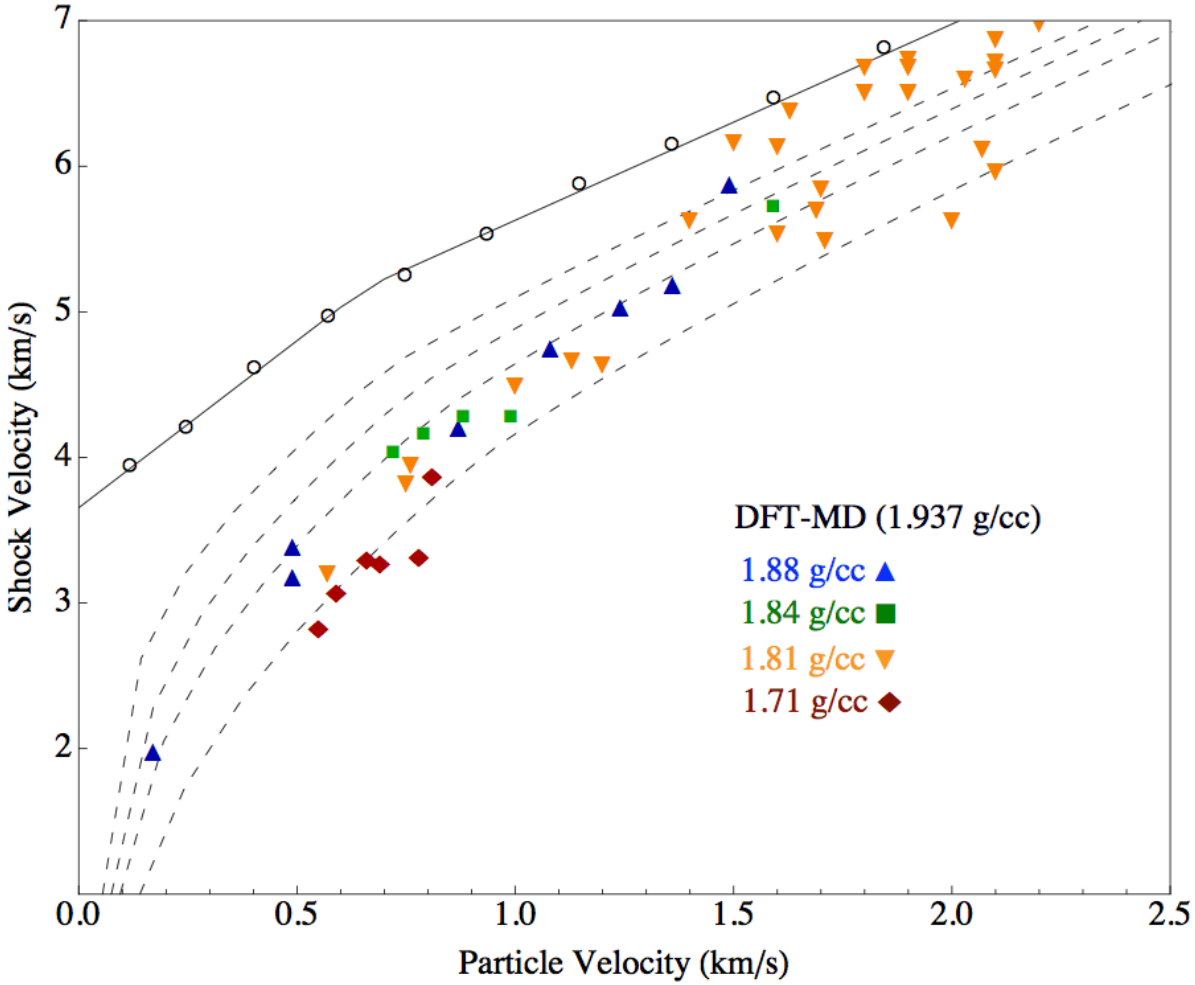


TATB Crystalline and Porous Hugoniots

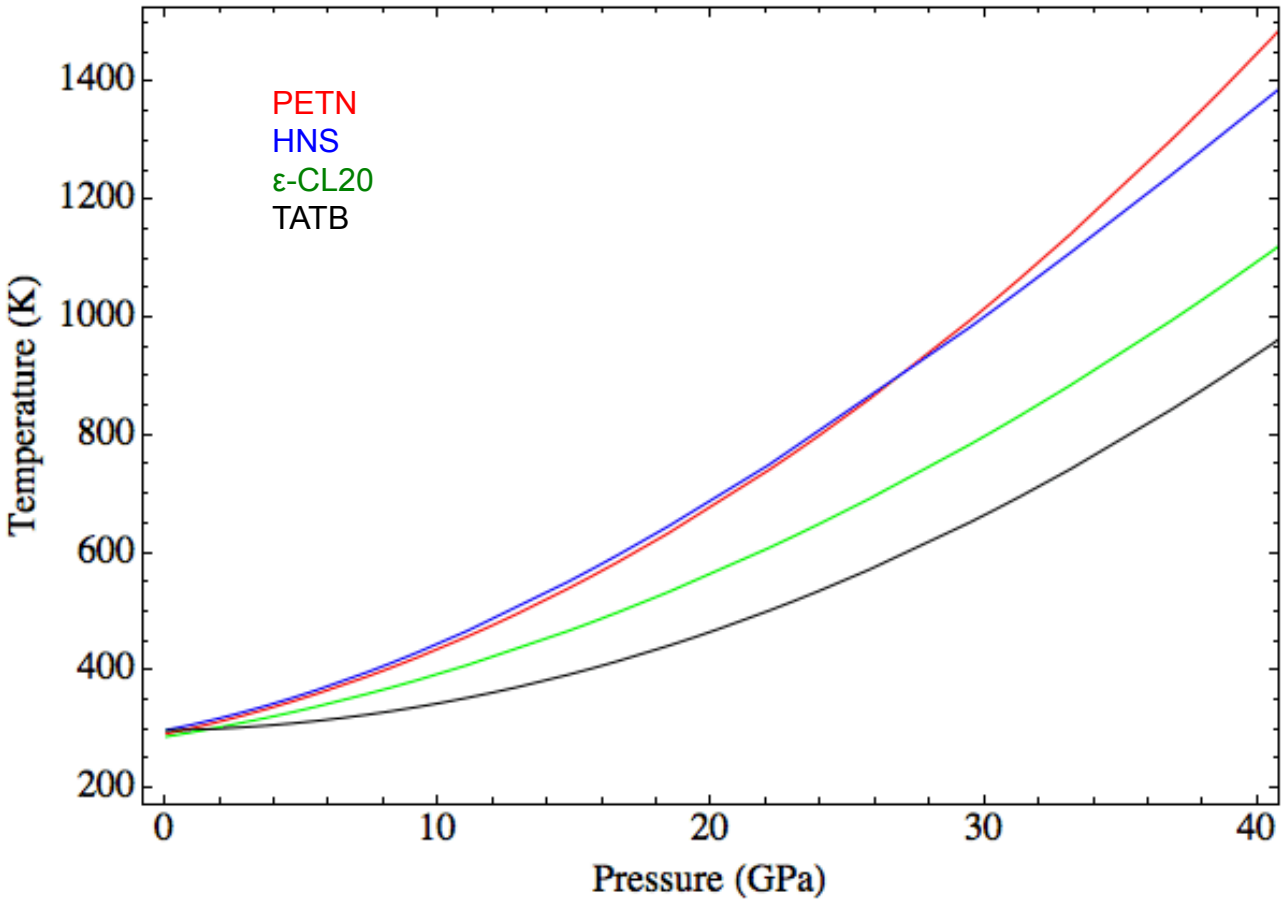








Comparison of shock temperature: Implications for sensitivity?



Conclusions / Future Work

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1. We can predict EoS data using DFT-MD and ReaxFF

2. We should make a tabular EoS and remove the need for making approximations to C_v and Gamma. Temperatures are predicted… need to be validated.

3. Impurities (solvent, defects) changes the EoS. How much? We can predict it and account for it.

4. Shock temperature could be linked to sensitivity.

5. Working to incorporate DFT-MD EoS with microstructural characterization and reactive process to build a predictive grain-scale simulation of shock initiation.

Extras:

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