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Precompressed Hugoniots of Hydrogen-Helium Mixtures from Density Functional Theory

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Introduction

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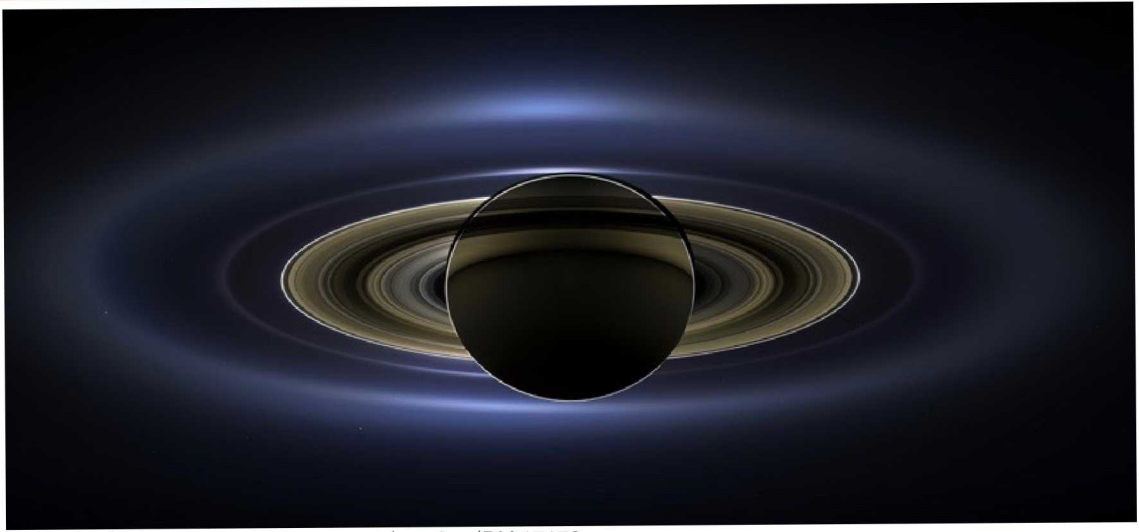
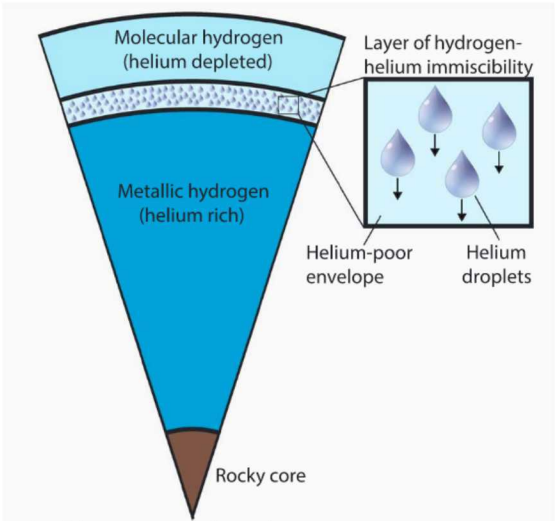


https://photojournal.jpl.nasa.gov/catalog/PIA17172

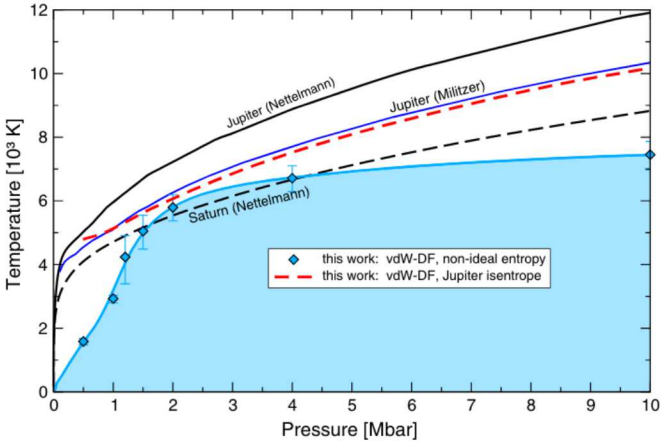
Structure of Jovian Planets

- Jovian planets follow the general schematic at right.
- Hydrogen-Helium demixing explains Saturn's anomalously large IR emission and upper atmospheric depletion of elements.
- Jupiter not expected to experience this process to a large degree.
- That's the intuitive picture. Does this really happen?



Militzer, Burkhard, et al. Journal of Geophysical Research: Planets 121.9 (2016): 1552-1572.

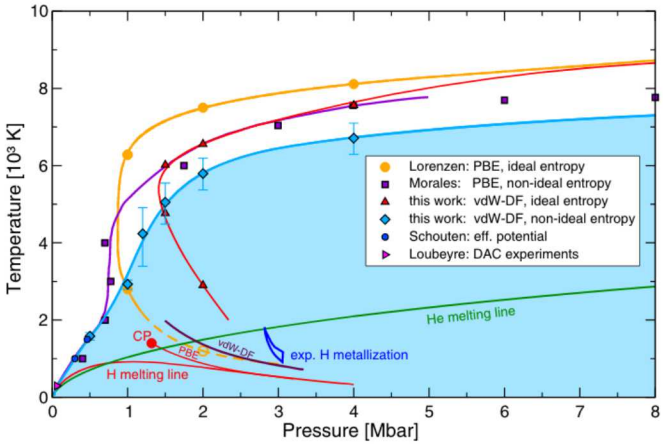
Immisicibility from First-Principles



Schttler, M., & Redmer, R. (2018). PRL, 120(11), 115703

- Figure (left) shows how we can be quantitative.
- Depending on details of Jupiter's and Saturn's adiabats and how they relate to the immiscibility line, could explain current discrepancies and observed differences between Jupiter & Saturn.
- What's the catch?

Immiscibility from First-Principles (Need For Experiment!)



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- Enough uncertainty from theory that it's not predictive for planetary models.
- Need experimental validation. NIF and Z-machine are ideal places to test this.
- This work serves to validate/cross-check a new experimental platform on Z.
- O3.00002: "Shockwave Compression of Pre-Compressed H_2-**He Mixtures**". Ongoing work by Sakun Duwal, Chris Seagle, and Marcus Knudson.

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Rankine-Hugoniot

$$E - E_0 = \frac{1}{2}(P + P_0)[\rho_0^{-1} - \rho^{-1}] \quad (1)$$

- First step of a "shock-ramp" experiment.
- "Easily" and unambiguously measureable with experiment. U_s and u_p directly measured, ρ_0 known.
- E and P can be calculated with *ab initio* thermodynamic sampling.

The Hugoniot is one of the purest objects to cross-validation of theory and experiment

Quantum Molecular Dynamics–Particulars

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System

- 256 electrons, 50-50 molar mixture of H_2 and He.
- Rectlinear density grid. Considered $T = 300, 5000, 10000, 20000K$ isotherms.

Electronic Structure

- Mermin functional with PBE.
- 800eV plane-wave cutoff.
- Single k-point at $(1/4, 1/4, 1/4)$.

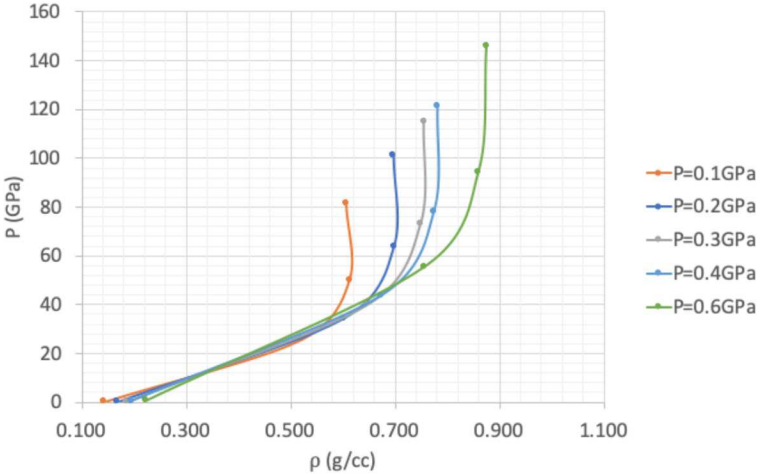
Molecular Dynamics

- Langevin thermostat.
- Time step: $\tau = 0.2fs$
- Equilibrate for Xps, accumulate for Yps.

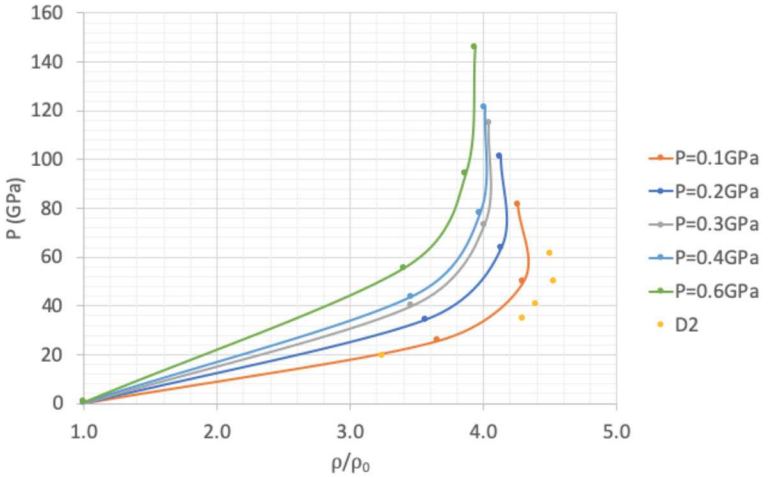
Results: Initial Densities (PBE)

$P_0(GPa)$	ρ_0 (g/cc)
0.1	0.143
0.2	0.169
0.3	0.187
0.4	0.195
0.6	0.222

Results: Precompressed Hugoniots (Absolute)

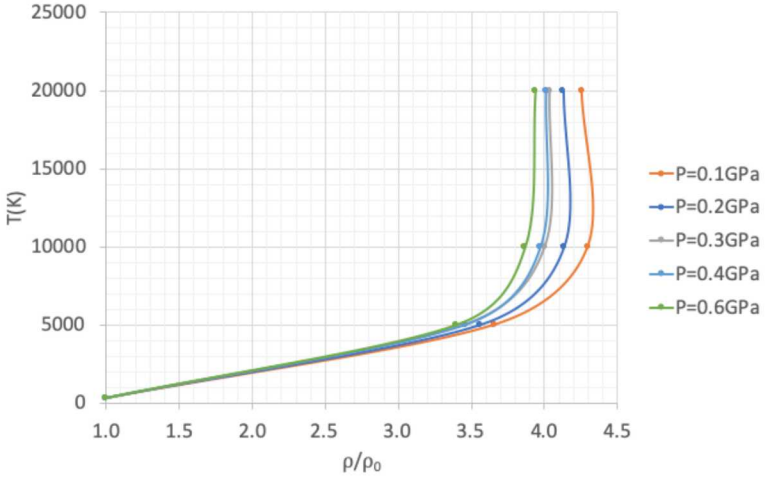


Results: Precompressed Hugoniots (Relative Compression)



- Physics is much more obvious with relative plot.
- H_2 bond breaking dominates qualitative behavior.
- Compares well to D_2 hugoniot.

Results: Precompressed Hugoniots (Temperatures)



Future Work

- Employ vdW-DF functional (In Progress).
- Nuclear quantum corrections for reference point.
- Explore different H+He concentrations.
- **Compare to experiments!!!**