

Deuterium Principal Hugoniot by Coupled Electron-Ion Monte Carlo: revisited results

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The deuterium Hugoniot

- Shockwave experiments: Hugoniot curves
- Hugoniot – Rankine relation

$$H(v, T) = E(v, T) - E_0 + \frac{1}{2}(v - v_0)(P(v, T) + P_0) = 0$$

Reference state: $T = 22$ K, $P_0 = 1.24 \cdot 10^{-4}$ GPa, $\rho_0 = 0.167$ g/cm³

- Theoretical description:
 - DFT: good agreement, independent on XC functional
 - QMC: greater compressibility than experiments

New QMC calculation of Hugoniot ¹

¹MR, M. Holzmann, D.M. Ceperley and C. Pierleoni, arXiv:2008.00269

Simulation protocol

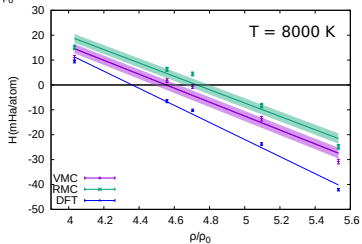
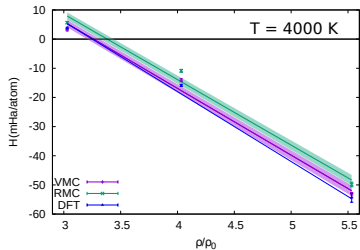
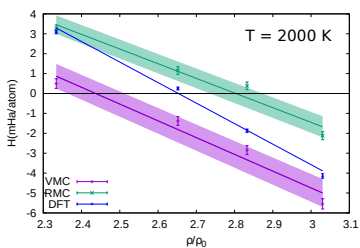
We generate atomic configurations and run electronic QMC simulations

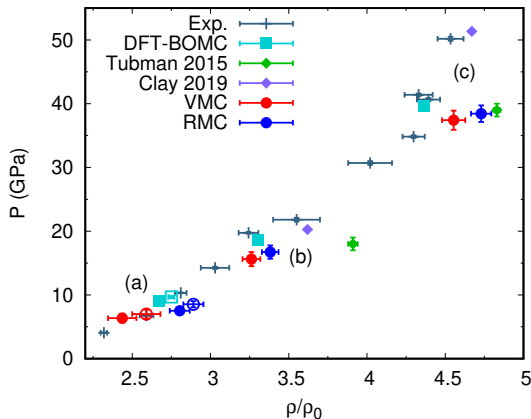
- Configurations generation:
 - Reference state: PIMC, Silvera – Goldman, Kolos – Wolniewicz potentials
 - $T = 2000, 4000$ and 8000 K: CEIMC
- For each configuration:
 - Wave function optimization
 - Variational Monte Carlo and Reptation Monte Carlo computation of energy and pressure $\rightarrow H(v, T)$
- Results are averaged, $H(v, T) = 0$ from linear interpolation

Warning!

- Electronic thermal effects: negligible for $T < 10000$ K (DFT study)
- Nuclear quantum effects: only relevant for $T = 2000$ K
- Reference state: great accuracy is required

Results





Knudson et al., PRL 118, 035501 (2017) and Science 348, 1455 (2015)

Tubman et al., PRL 115, 045301 (2015)

Clay et al., PRB 100, 075103 (2019)

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