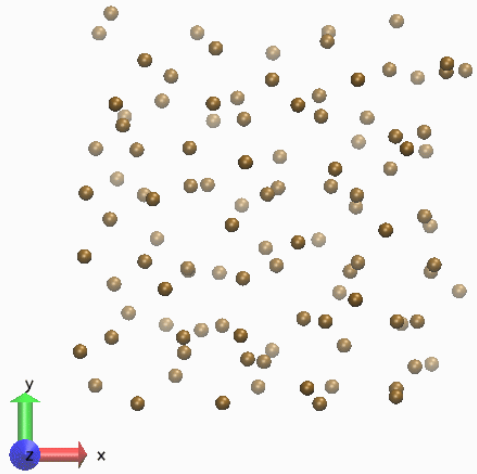
Compression Isentrope of Deuterium by Quantum Molecular Dynamics

Alexey Chentsov, Pavel Levashov

Joint Institute for High Temperatures, Russian Academy of Sciences



Non-ideal Plasma Research, November 23-24 2011, Moscow

Why?

- Previous calculations by Reactive Monte Carlo (classical potentials from Juranek & Redmer, JCP, 2000; accurate account of dissociation)
- This region is difficult for PIMC (low temperatures)

Isentrope Reconstruction

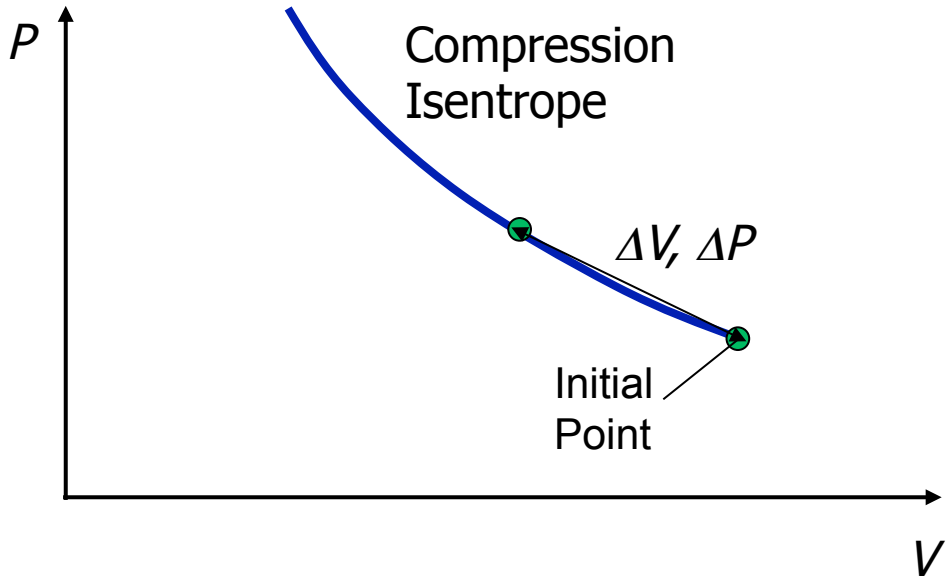
- Zel'dovich method (Zel'dovich, 1957):

$$\frac{dT}{dV} = -\frac{T}{\left(\partial E/\partial P\right)_V}$$

- **Global isentrope reconstruction:** interpolate $P(T, V)$ and $E(T, V)$ on the mesh of isotherms and isochors

$$\left(\frac{\partial E}{\partial P}\right)_V = \left(\frac{\partial E}{\partial T}\right)_V \Big/ \left(\frac{\partial P}{\partial T}\right)_V$$

  - Integration with any step on V
  - Isentrope can be improved by mesh refinement



Grid parameters:

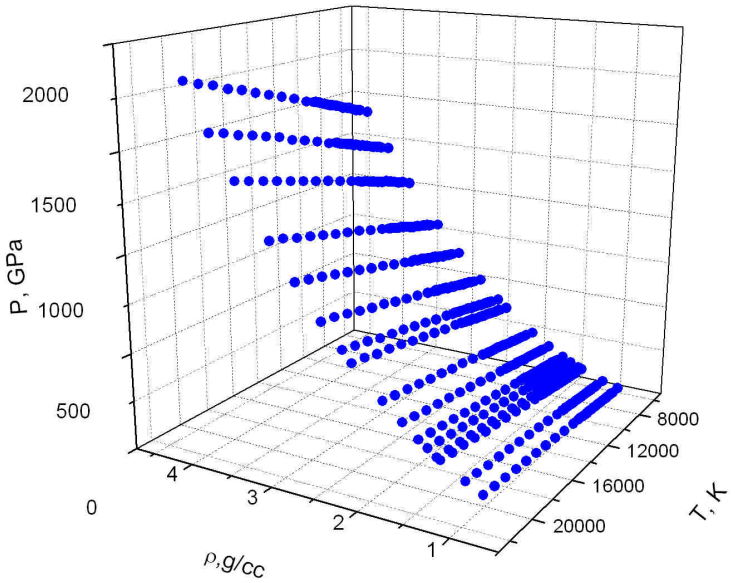
23 isotherms, 6.5 - 21 kK
16 isochors, 0.9 – 4.3 g/cm^3

Isentrope Reconstruction

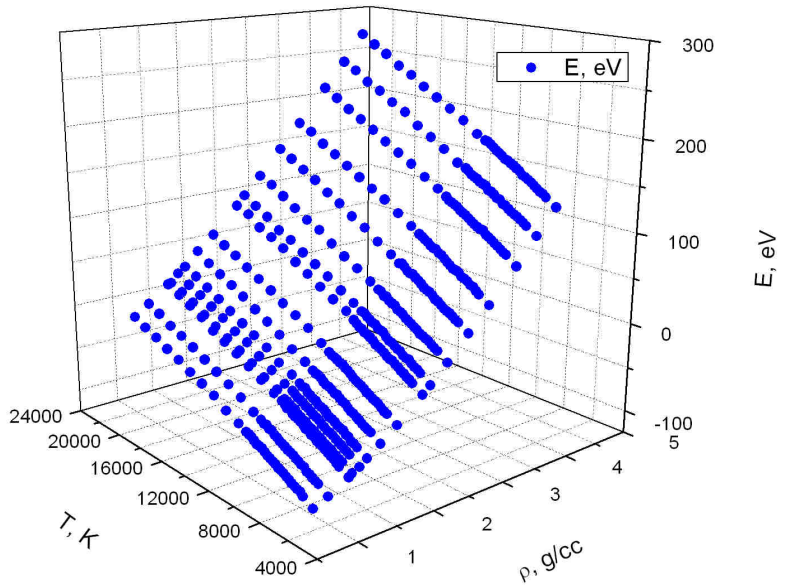
- To construct the compression isentrope the data grids of $E(V, T)$ and $P(V, T)$ were obtained by means of quantum molecular dynamics code VASP[1].
- ρ = 0.9 - 4.3 g/cm^3 and P = 48 -1800 GPa.
- N_{atoms} = 64 in a supercell with periodic boundary conditions.
- First 1000 steps with E_{cut} = 250 eV without pressure calculation.
- Next 1000 steps with E_{cut} = 1250 eV to obtain results.
- One step of a simulation = 0.2 fs.

- Isentrope can be improved by grid refinement.

Pressure

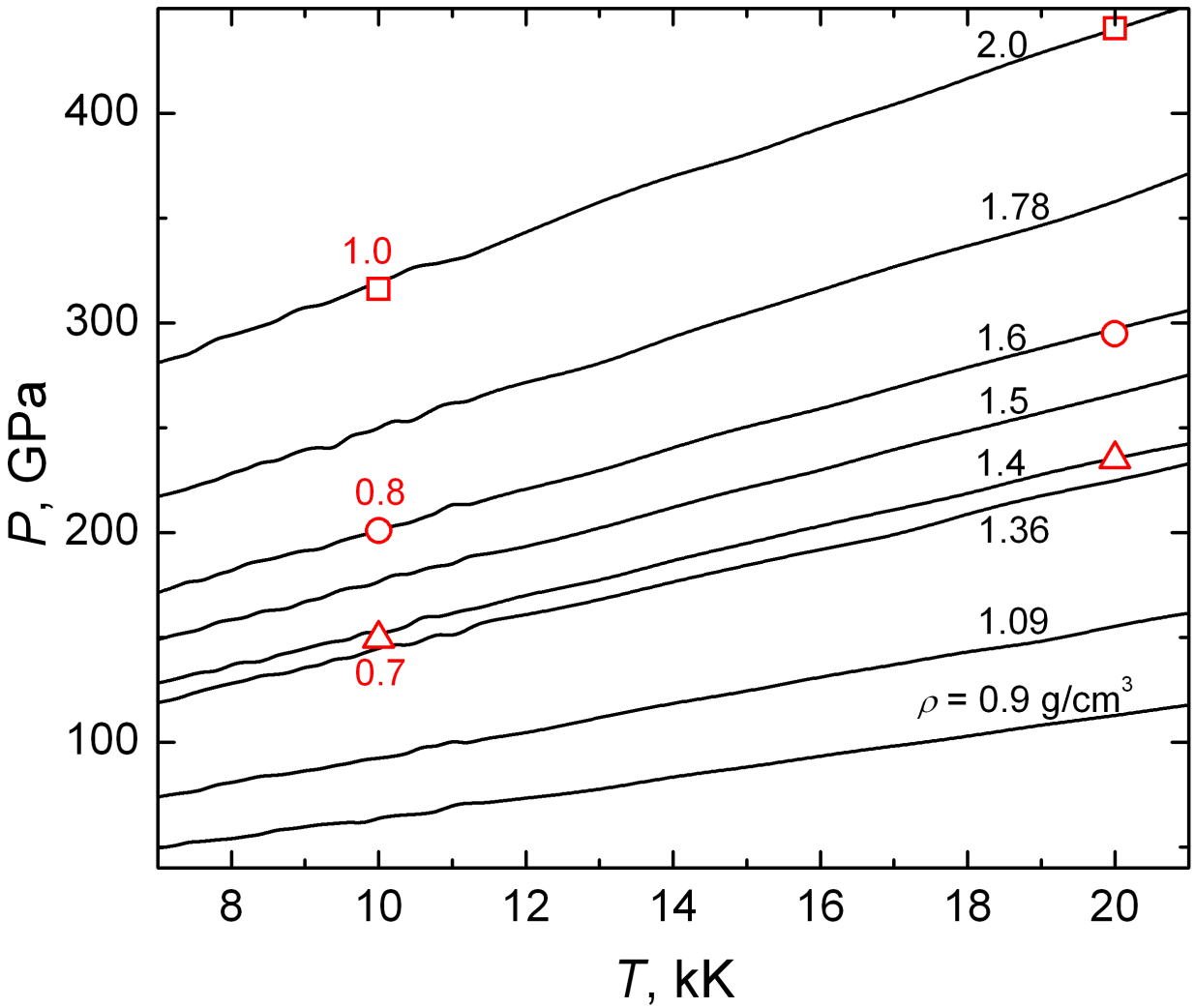


Energy



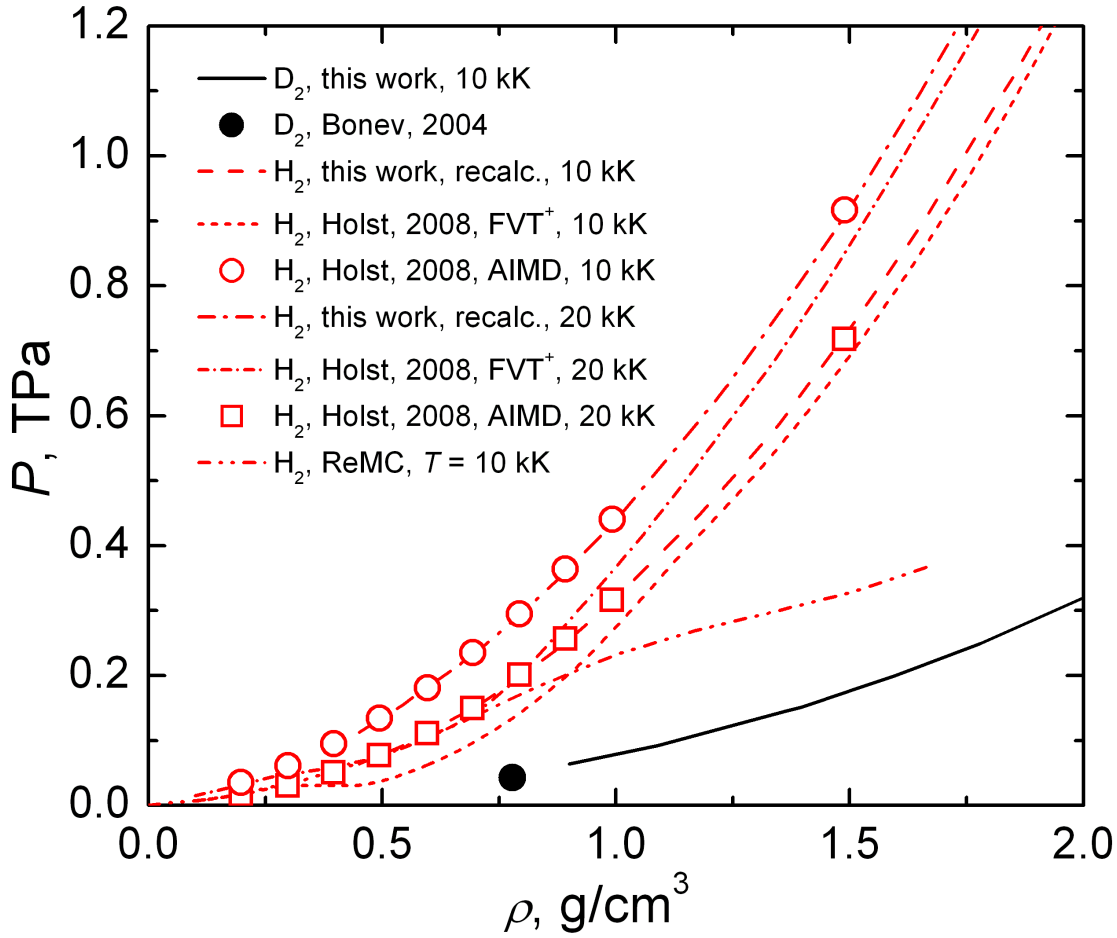
G. Kresse, J. Hafner, Phys. Rev. B. 1993, 47, 558; Ibid. 1994, 49, 14251.

AIMD Isochors for hydrogen and deuterium



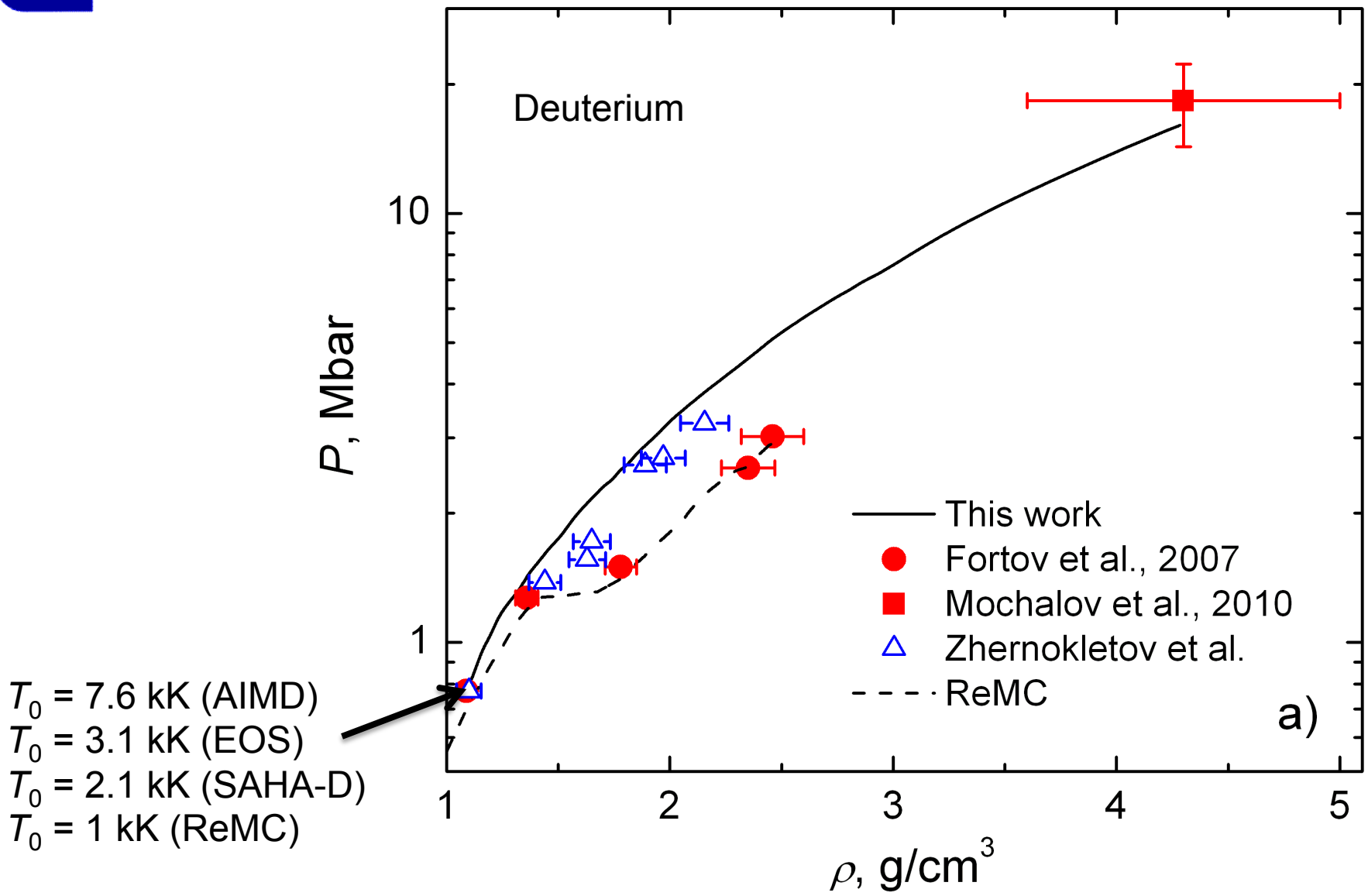
Holst B., Redmer R., Desjarlais M., PRB **77**, 184201 (2008)

AIMD isotherms for hydrogen and deuterium

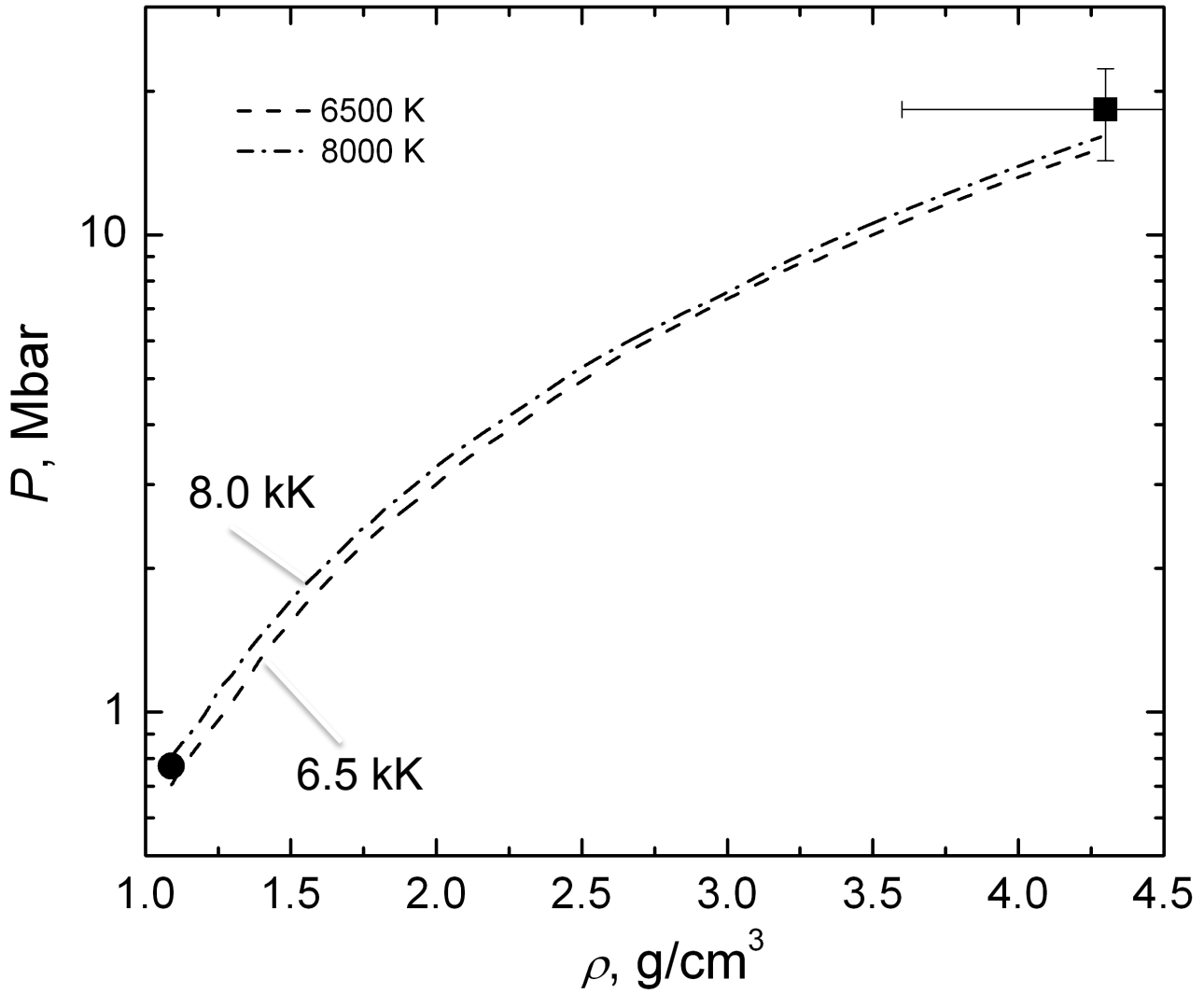


Bonev S.A., Militzer B., Galli G., PRB **69**, 014101 (2004)
Bezkrovniy V. et al., PRE **69**, 061204 (2004)
Holst B., Redmer R., Desjarlais M., PRB **77**, 184201 (2008)
B. Holst, N. Nettleman, and R. Redmer, Contrib. Plasma Phys. **47**, 368–374 (2007)

Compression isentrope

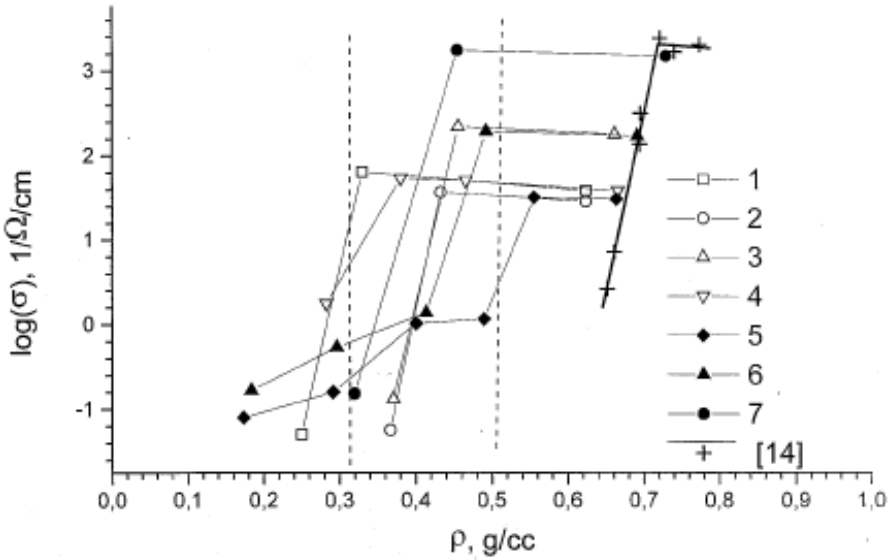


Influence of Initial Point



Ionization and Mean Ion Charge

Conductivity rise in hydrogen under multiple shock compression

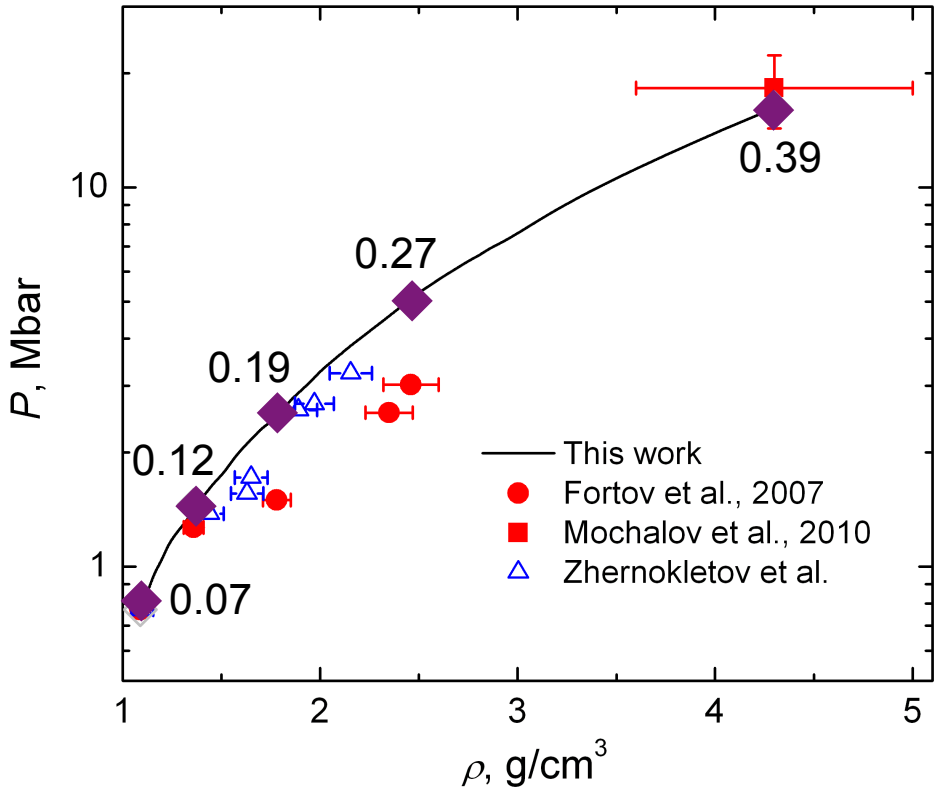


Ternovoi V.Ya. et al., Phys. B **265**, 6 (1999)

$$\langle Z \rangle (T_e) = \frac{m_e^{3/2}}{\sqrt{2}\pi^2\hbar^3 n_i} \int_0^\infty g f_e(\varepsilon, \mu_e, T_e) \sqrt{\varepsilon} d\varepsilon,$$

Loboda et al., HEDP **7**, 361 (2011)

Mean ion charge along the isentrope



Conclusion

- The AIMD compression isentrope of deuterium is smooth
- The isentrope should be calculated from the experimental conditions
- Dissociation effects under pressure should be investigated