Ab Initio EOS for Planetary Matter and Implications for Giant Planets

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Planet Formation and Evolution: The Solar System and Extrasolar Planets
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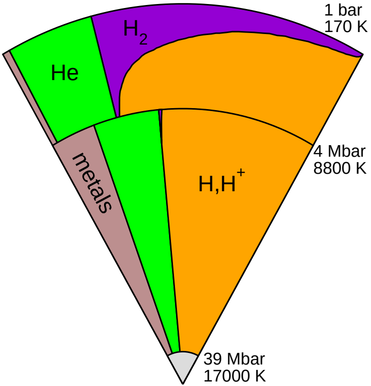
UNIVERSITÄT ROSTOCK
INSTITUT FÜR PHYSIK
SFB 652

Outline

Outline

Model of Jupiter
LM-REOS



Constraints:

- mass, radius
- "surface" temperature
- "surface" helium fraction ($x_{\mathrm{mol}} \approx 7.2\%$)
- mean helium fraction ($x_{\mathrm{mean}} \approx 8.6\%$)
- gravitational moments J_2, J_4

LM-REOS [1]

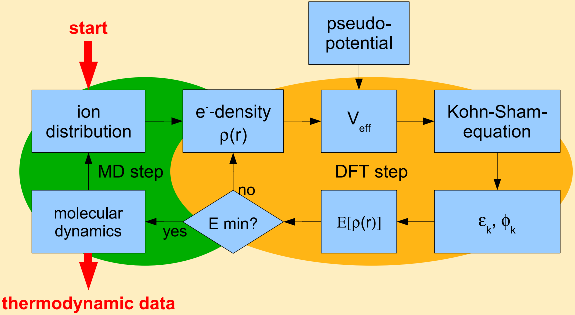
Linear mixing of H, He and H_2O *ab initio* EOS data

[1] N. Nettelmann et al.
Astrophys. J. 683, 1217 (2008)

see also poster P6.8

Finite Temperature Density Functional Theory Molecular Dynamics (FT-DFT-MD)

VASP - Vienna Ab-initio Simulation Package

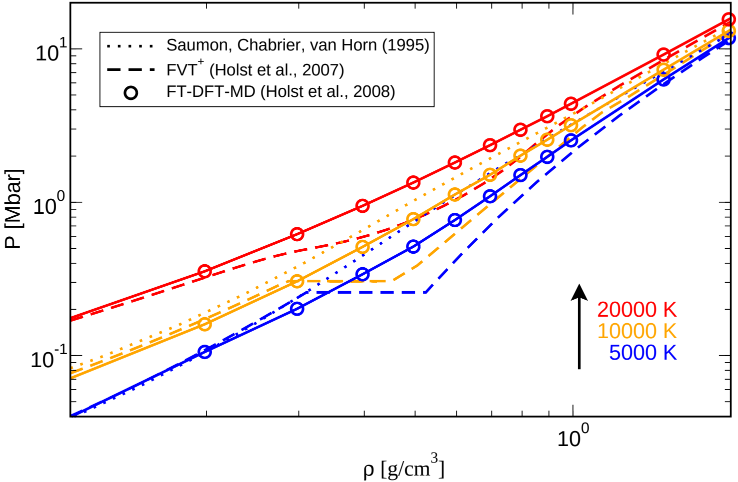


- input: volume, temperature (thermostat)
- output: energy U, pressure P
- also: electrical conductivity, optical reflectivity

Outline

Example: EOS of hydrogen

Also available: helium, water



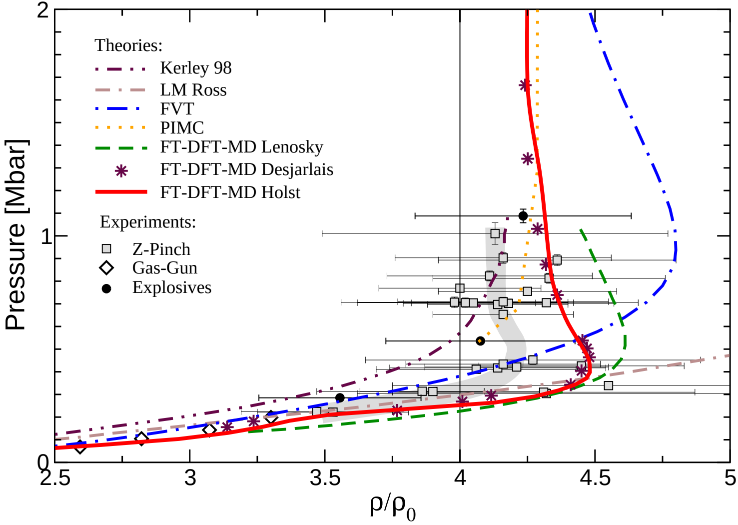
Saumon et al.
ApJS 99, 713 (1995)

B. Holst et al.
Contrib. Plasma Phys. 47, 368 (2007)

B. Holst et al.
Phys. Rev. B 77, 184201 (2008)

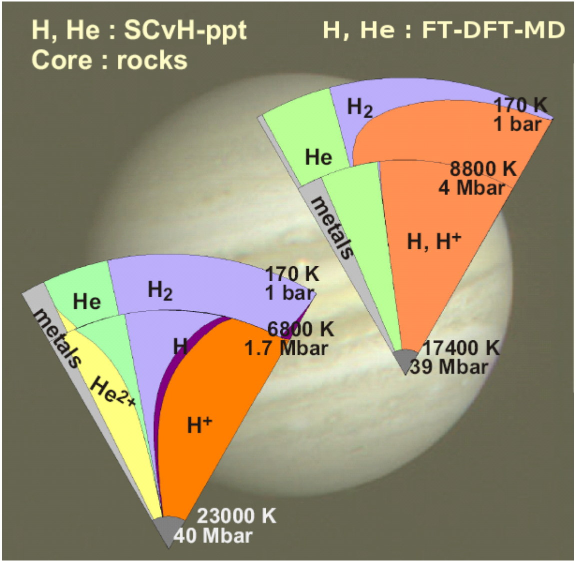
Hugoniot of hydrogen

Benchmark of the method



B. Holst et al.
Phys. Rev. B 77, 184201 (2008)

Implications for Jupiter



Results

- continuous dissociation
- feasible metal distribution
- colder core
- larger P_T

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Excess Gibbs free energy of mixing

Definition

$$\Delta G(x) = G(x) - xG(1) - (1-x)G(0)$$

Helium fraction

$$x = \frac{N_{\mathrm{He}}}{N_{\mathrm{He}} + N_{\mathrm{H}}}$$

$$x = \begin{cases} 0: & \mathrm{H} \\ 1: & \mathrm{He} \end{cases}$$

Contributions to $\Delta G(x)$

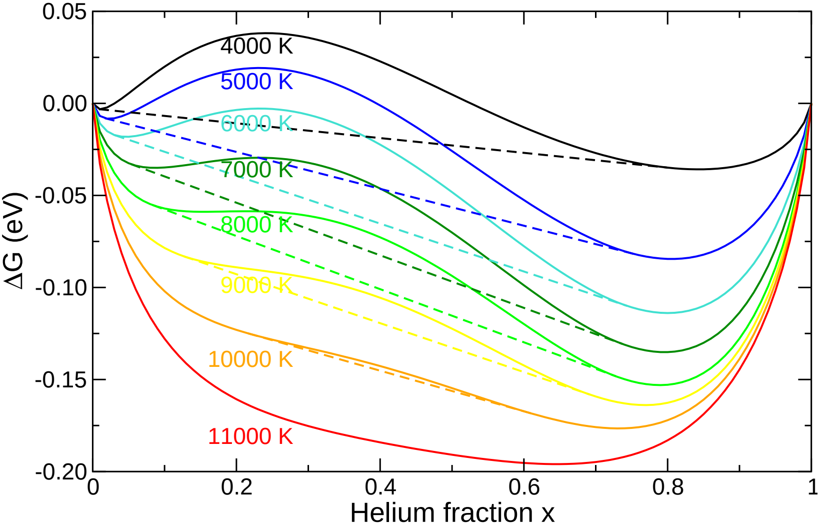
$$\Delta G(x) = \Delta U(x) + p\Delta V(x) - T\Delta S(x)$$

Ideal entropy of mixing

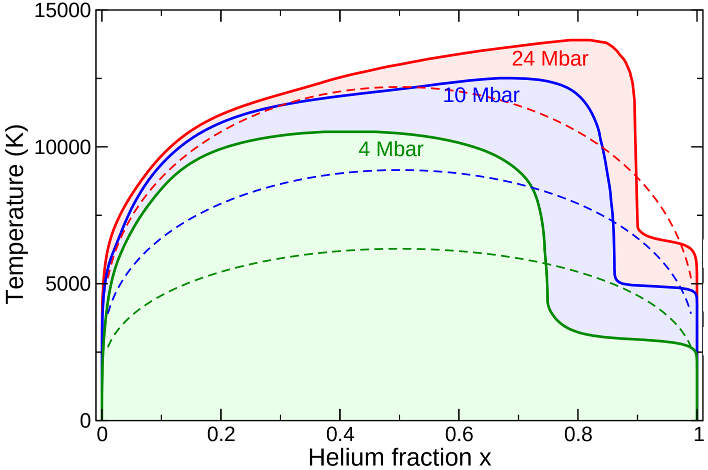
$$\Delta S(x) = -k_B \left[x \ln x + (1-x) \ln (1-x)\right]$$

Excess Gibbs free energy of mixing

Example: 4 Mbar



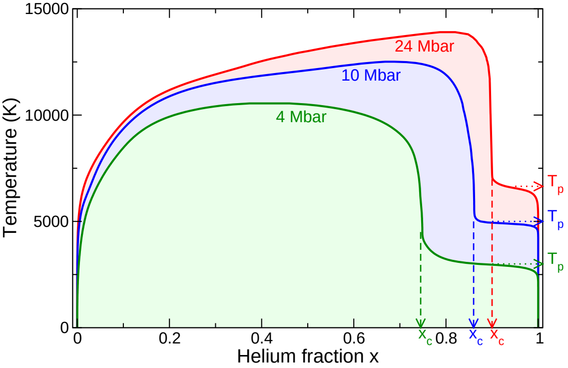
Miscibility gap



— Lorenzen et al.
Phys. Rev. Lett., accepted

– – – Pfaffenzeller et al.
Phys. Rev. Lett. 74, 2599 (1995)

Miscibility gap



plateaus

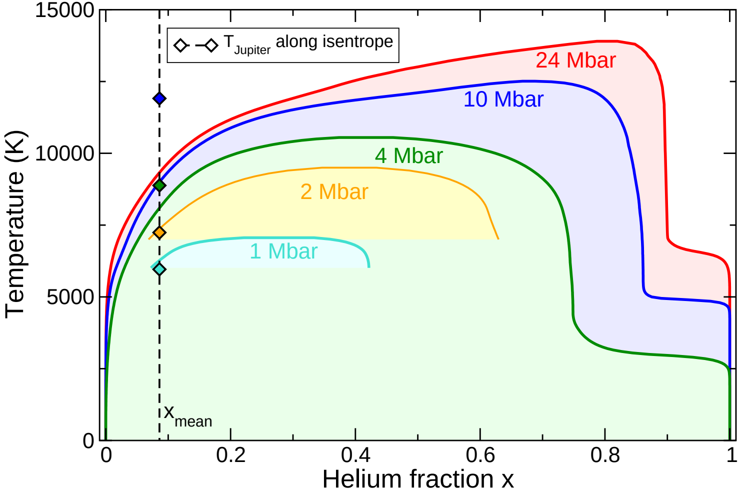
$T_p = T_{melt}$ (He)

critical He fractions

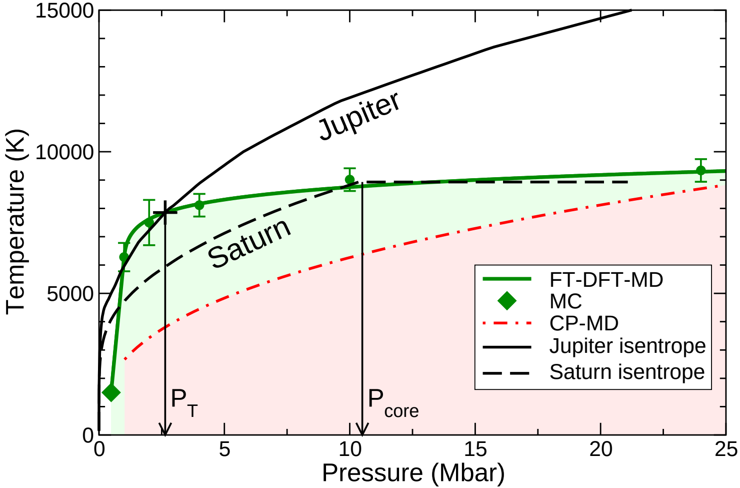
$x_c \Leftrightarrow a_B n_H^{1/3} \approx 0.25$ [Mott-criterion]

N. F. Mott
Metal-Nonmetal Transitions (Second Edition)
Taylor and Francis, London, 1990

Miscibility gap



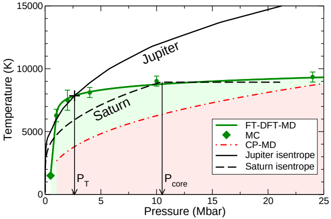
Consequences for Jupiter and Saturn



[CP-MD] Pfaffenzeller et al.
Phys. Rev. Lett. 74, 2599 (1995)

[MC] Schouten et al.
Phys. Rev. B 44, 6630 (1991)

Consequences for Jupiter and Saturn



[1] Fortney and Hubbard
Astrophys. J. 608, 1039 (2004)

Consequences

- three-layer models for Jupiter can be justified by miscibility gap
- transition pressure P_T can be determined
- saturns whole interior is in the demixing region
- this is necessary to reproduce the correct age of Saturn [1]
- miscibility gap might also indicate four layers

Outline

Summary

- FT-DFT-MD gives reliable EOS data for warm dense matter
- simulations for mixtures go beyond linear mixing
- miscibility gap is deeply connected to metallization in hydrogen
- EOS of real mixture should be used as input for planetary models
- phase separation of H and He is relevant for Jovian conditions
- complete phase separation in Saturn yield the correct age for Saturn
- basis for new, advanced planetary models

Appendix

Simulation details

DFT

- finite temperature DFT [1]
- GGA (PBE) [2]
- plane wave basis sets
- Baldereschi mean value point [3]

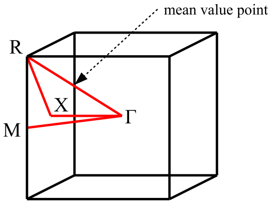
Molecular dynamics

- 64 electrons in a box
- periodic boundary conditions
- ≈ 0.5 fs time steps
- $\approx 1 - 3$ ps simulation time

[1] N. David Mermin
Phys. Rev. 137, 1441 (1965)

[2] John P. Perdew, Kieron Burke, and Matthias Ernzerhof
Phys. Rev. Lett. 77, 3865 (1996)

[3] A. Baldereschi
Phys. Rev. B 7, 5212 (1973)



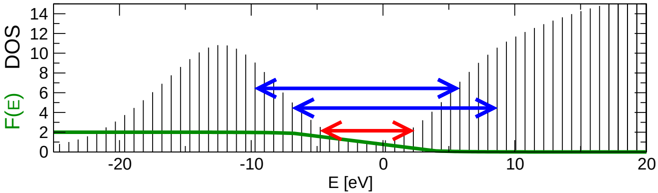
Dynamic conductivity $\sigma(\omega)$

Kubo-Greenwood formula [1, 2]

$$\sigma(\omega) = \frac{2\pi e^2 \hbar^2}{m^2 \omega \Omega} \sum_{\mathbf{k}} W(\mathbf{k}) \sum_{i,j} F_{ij} \, |D_{ij}|^2 \, \delta(\epsilon_{j,\mathbf{k}} - \epsilon_{i,\mathbf{k}} - \hbar\omega)$$

$$D_{ij} = \langle \Psi_{j,\mathbf{k}} | \nabla_\alpha | \Psi_{i,\mathbf{k}} \rangle$$

$$F_{ij} = F(\epsilon_{i,\mathbf{k}}) - F(\epsilon_{j,\mathbf{k}})$$



[1] R. Kubo
J. Phys. Soc. Jpn. 12, 570 (1957)

[2] D. A. Greenwood
Proc. Phys. Soc. London 71, 585 (1958)

Optical properties

Kramers-Kronig relation

$$\sigma_2(\omega) = -\frac{2}{\pi}\ \mathrm{P}\int \frac{\sigma_1(\nu)\omega}{\nu^2-\omega^2} d\nu$$

Dielectric function

$$\epsilon_1(\omega) = 1 - \frac{1}{\epsilon_0\omega}\sigma_2(w)$$
$$\epsilon_2(\omega) = \frac{1}{\epsilon_0\omega}\sigma_1(w)$$

Index of refraction

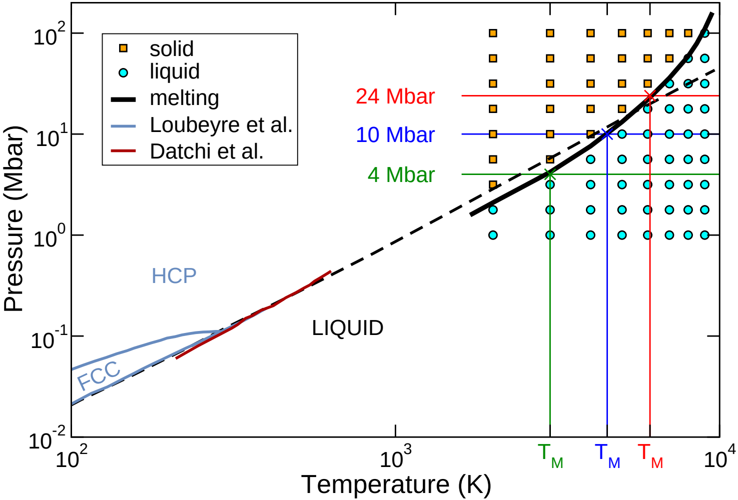
$$n(\omega) = \sqrt{\frac{1}{2}[|\epsilon(\omega)| + \epsilon_1(\omega)]}$$
$$k(\omega) = \sqrt{\frac{1}{2}[|\epsilon(\omega)| - \epsilon_1(\omega)]}$$

Reflectivity

$$r(\omega) = \frac{[1-n(\omega)]^2+k(\omega)^2}{[1+n(\omega)]^2+k(\omega)^2}$$

Explanation for the plateaus

Helium phase diagram

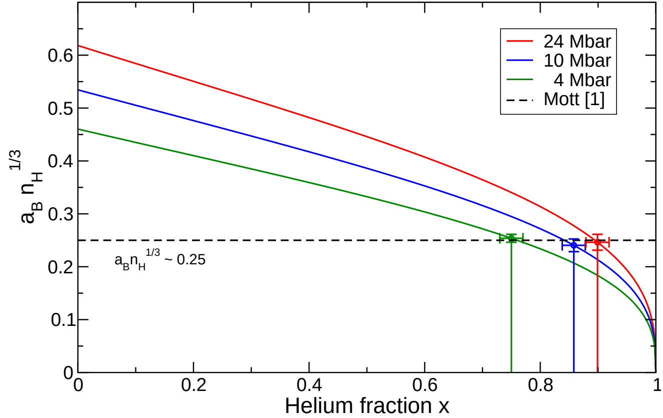


Loubeyre et al.
Phys. Rev. Lett. 71, 2272 (1993)

Datchi et al.
Phys. Rev. B 61, 6535 (2000)

Explanation for the critical He-fractions

The Mott criterion [1]



$$x_c \Leftrightarrow a_B n_H^{1/3} \approx 0.25$$

[1] N. F. Mott
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Planetary modelling