

# 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

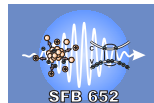
5.3.2009



UNIVERSITÄT ROSTOCK



INSTITUT FÜR PHYSIK



SFB 652

# Outline

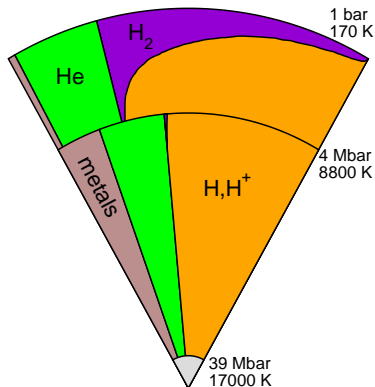
- 1 Introduction
- 2 Ab initio EOS and its implications
- 3 H-He phase separation and its implications
- 4 Conclusion

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# Model of Jupiter

## LM-REOS



### Constraints:

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

### LM-REOS [1]

Linear mixing of H, He and H<sub>2</sub>O *ab initio* EOS data



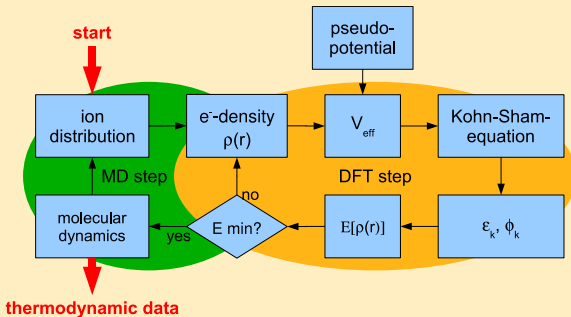
[1] N. Nettelmann et al.  
Astrophys. J. 683, 1217 (2008)



see also poster P6.8

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

## VASP - Vienna Ab-initio Simulation Package



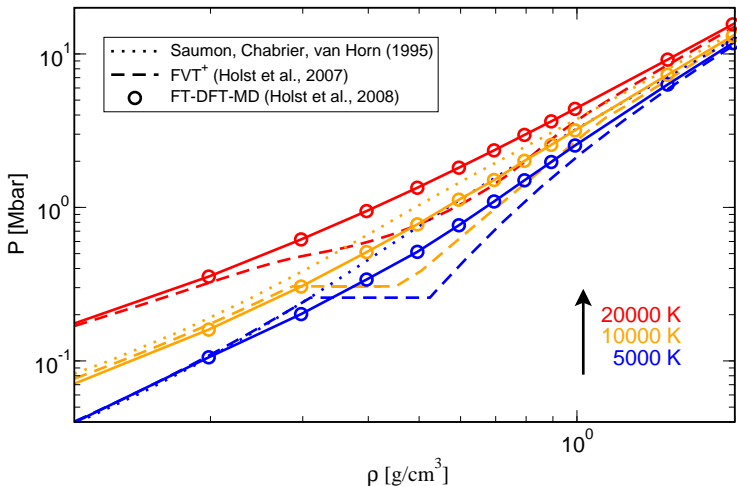
- input: volume, temperature (thermostat)
- output: energy  $U$ , pressure  $P$
- also: electrical conductivity, optical reflectivity

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# Example: EOS of hydrogen

Also available: helium, water



Saumon et al.  
ApJS 99, 713 (1995)



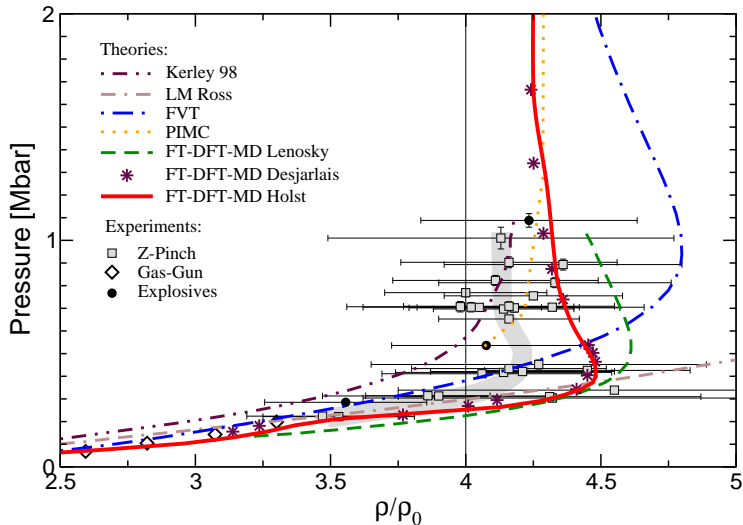
B. Holst et al.  
Contrib. Plasma Phys. 47, 368 (2007)



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

# Hugoniot of hydrogen

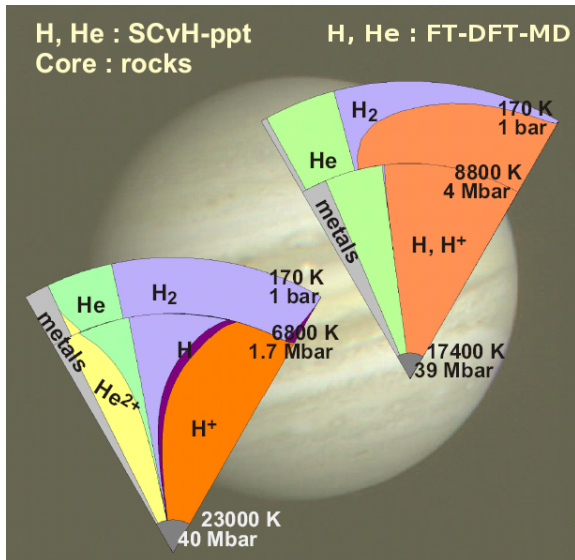
## Benchmark of the method



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

$$x = \frac{N_{\text{He}}}{N_{\text{He}} + N_{\text{H}}}$$
$$x = \begin{cases} 0 : \text{H} \\ 1 : \text{He} \end{cases}$$

## Contributions to $\Delta G(x)$

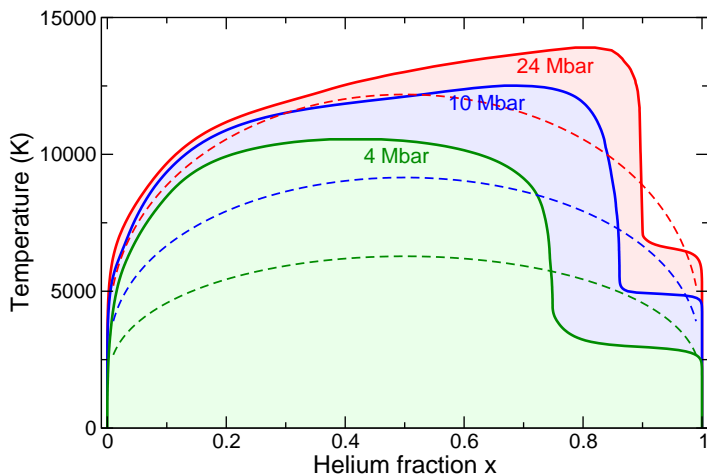
$$\Delta G(x) = \Delta U(x) + p\Delta V(x) - T\Delta S(x)$$

## Ideal entropy of mixing

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



# Miscibility gap

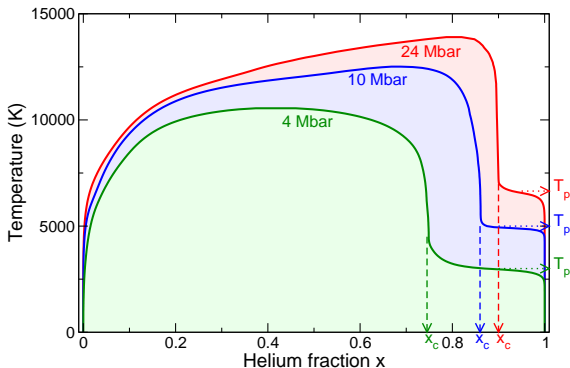


— Lorenzen et al.  
Phys. Rev. Lett., accepted



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

# Miscibility gap



plateaus

$$T_p = T_{melt}(\text{He})$$

critical He fractions

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

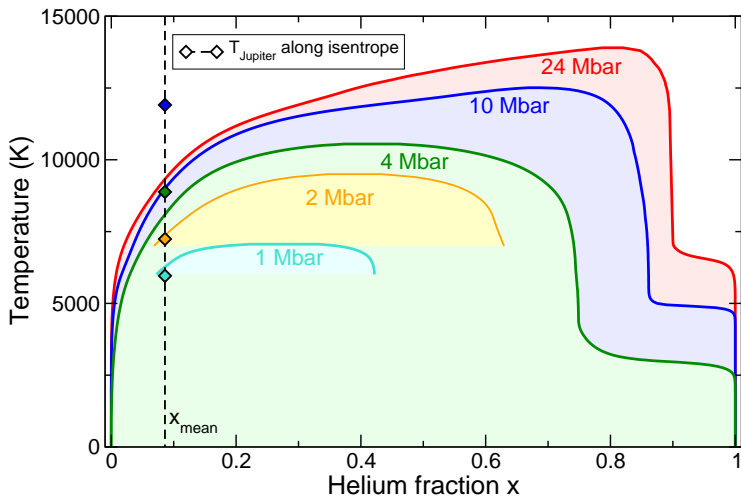
[Mott-criterion]



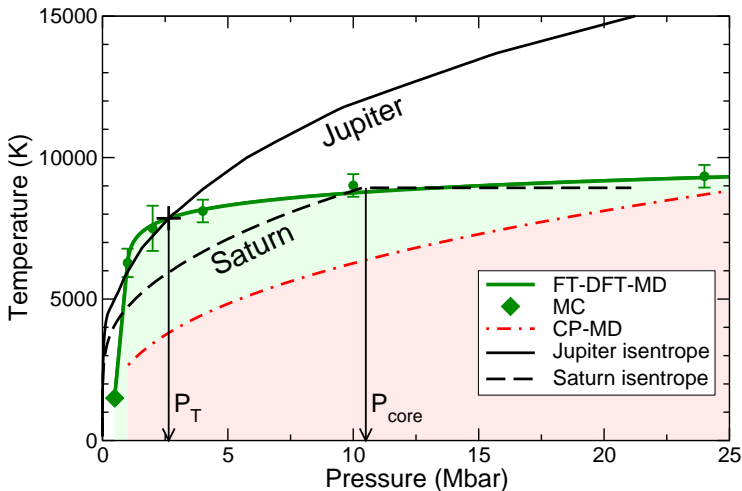
N. F. Mott

Metal-Nonmetal Transitions (Second Edition)  
Taylor and Francis, London, 1990

# Miscibility gap



# Consequences for Jupiter and Saturn

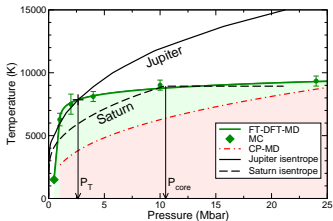


[CP-MD] Pfaffenzeller et al.  
Phys. Rev. Lett. 74, 2599 (1995)



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

# Consequences for Jupiter and Saturn



## 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



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

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# 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

- 5 FT-DFT-MD
- 6 Explanation of miscibility gap
- 7 Planetary modelling

# Simulation details

## DFT

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



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



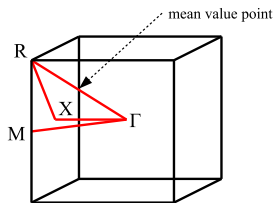
[2] John P. Perdew, Kieron Burke, and Matthias Ernzerhof  
Phys. Rev. Lett. 77, 3865 (1996)



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

## Molecular dynamics

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



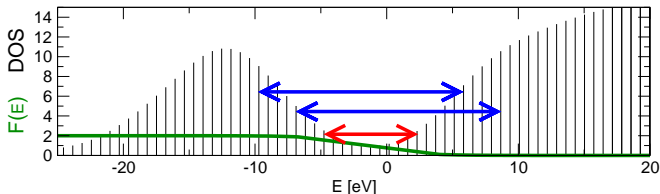
# Dynamic conductivity $\sigma(\omega)$

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

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

## Dielectric function

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

$$\epsilon_2(\omega) = \frac{1}{\epsilon_0\omega} \sigma_1(\omega)$$

## Index of refraction

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

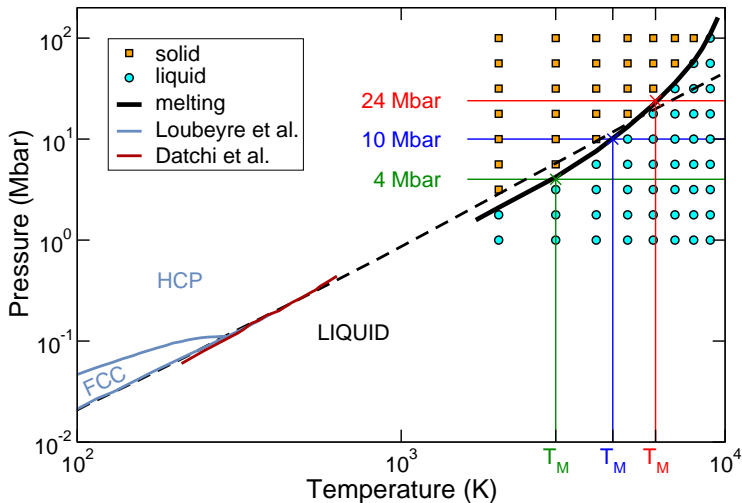
$$k(\omega) = \sqrt{\frac{1}{2}[|\epsilon(\omega)| - \epsilon_1(\omega)]}$$

## 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



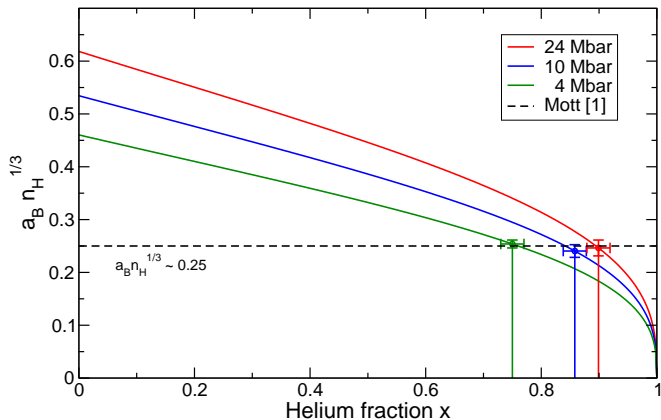
Loubeyre et al.  
Phys. Rev. Lett. 71, 2272 (1993)



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

# Explanation for the critical He-fractions

The Mott criterion [1]



[1] N. F. Mott

Metal-Nonmetal Transitions (Second Edition)  
Taylor and Francis, London, 1990

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

# Planetary modelling

