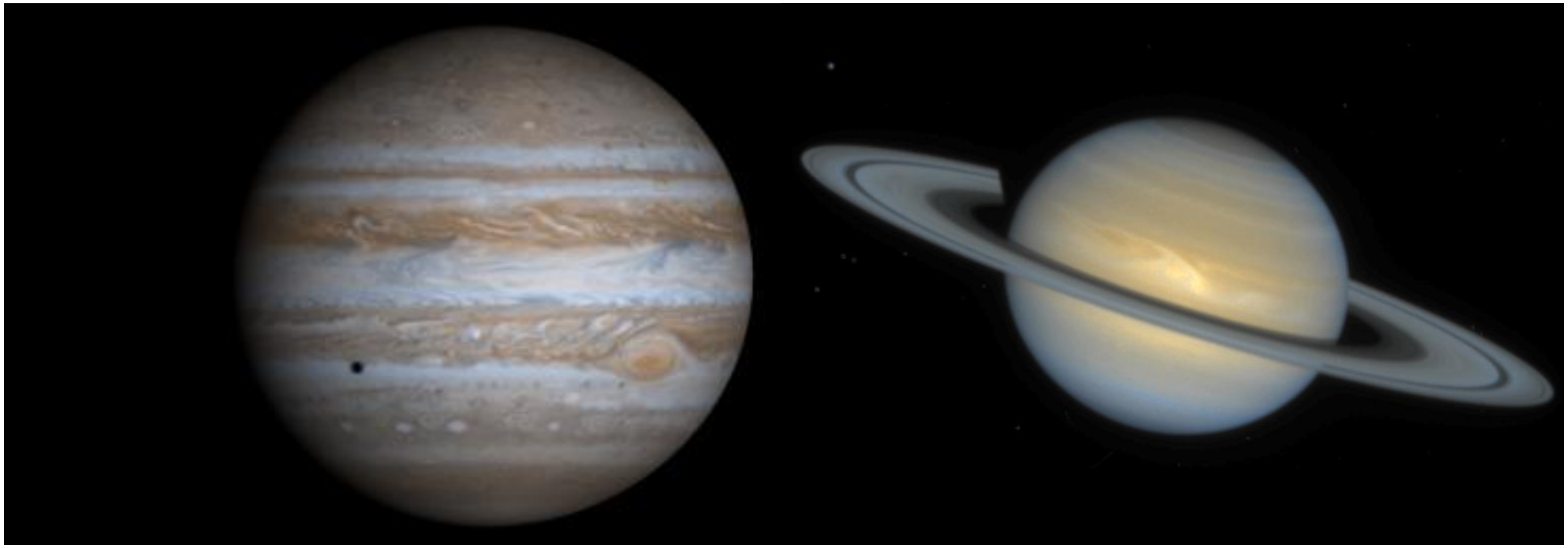
IPAM Workshop IV: Computational Challenges in WDM
May 21-25, 2012

Warm Dense Matter and the Interior of (Solar and Extrasolar) Giant Planets



Ronald Redmer
Universität Rostock, Institut für Physik
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THEORY GROUP AT U ROSTOCK

Ab initio simulations:

Martin French, Winfried Lorenzen, Mandy Bethkenhagen, Daniel Cebulla, Bastian Holst (CEA Paris)

Planetary physics:

Nadine Nettelmann, Andreas Becker, Ulrike Kramm, Robert Püstow

X-ray Thomson scattering:

Philipp Sperling, Kai-Uwe Plagemann, Richard Bredow, Thomas Bornath, Robert Thiele (CFEL Hamburg)

SUPPORTED BY

DFG via SFB 652 Strong Correlations in Radiation Fields
DFG via SPP 1488 PlanetMag and SPP 1385 Young Planets
DFG via grant RE 882/11
Supercomputing Center North (HLRN)
BMBF FSP-301 FLASH

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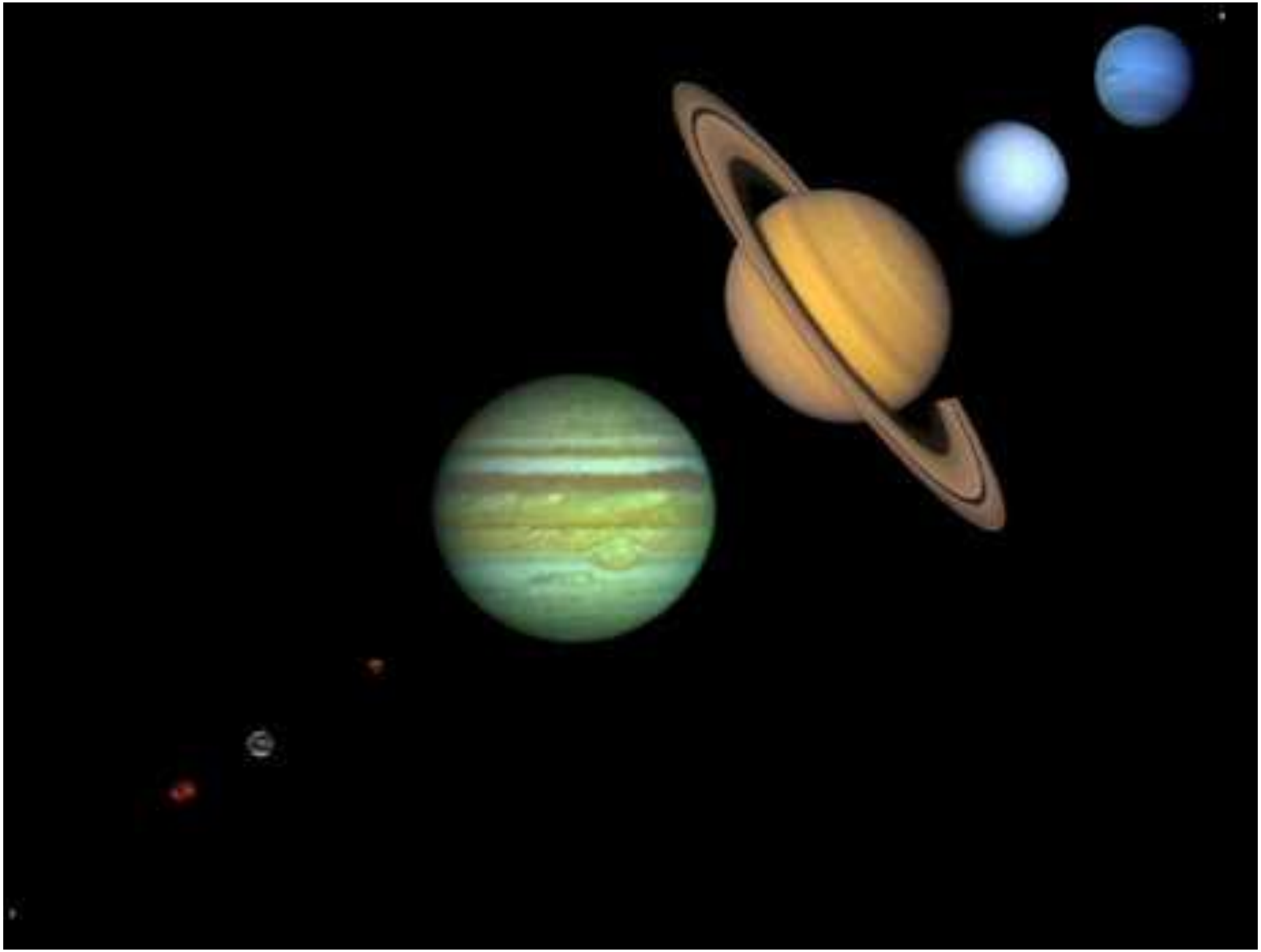
1. **Introduction:**
    - **Matter under extreme conditions** M. Desjarlais
    - **Problems in planetary physics**
2. **Fundamental properties:**
    - **Ab initio molecular dynamics simulations**
    - **H, H-He mixtures, H2O - EOS and MIT**
3. **Application in astrophysics:**
    - **Modeling solar and extrasolar giant planets**
    - **Material properties for the deep interior**
4. **Summary**

Solar system: Eight planets*



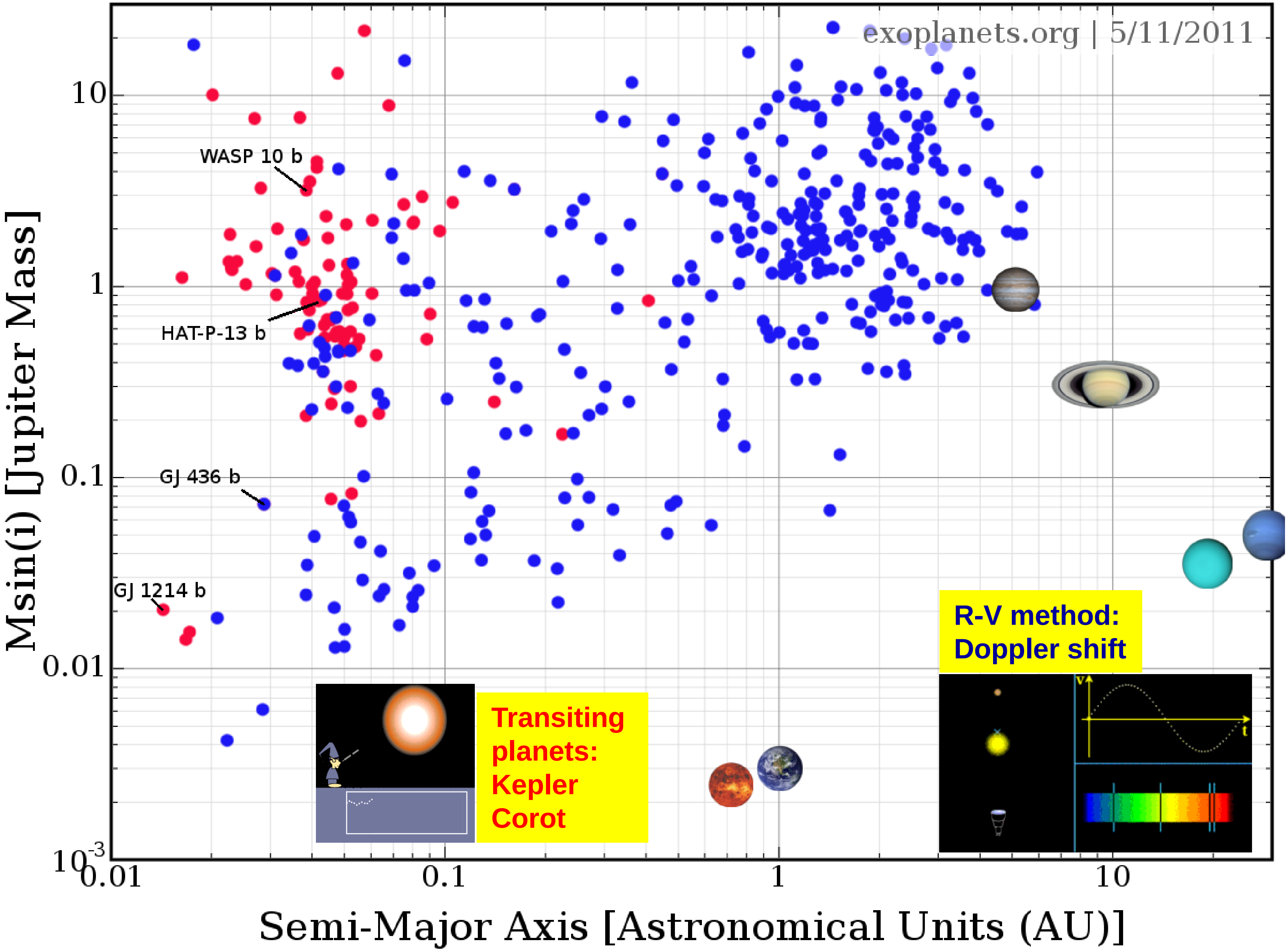
*IAU Meeting Prague 24.08.2006: Pluto is considered as „Dwarf Planet“

Solar system: Eight planets*

Brown Dwarfs with $13M_J<M_{BD}<75M_J$
White Dwarfs (final state of >95% of all stars)

*IAU Meeting Prague 24.08.2006: Pluto is considered as „Dwarf Planet“

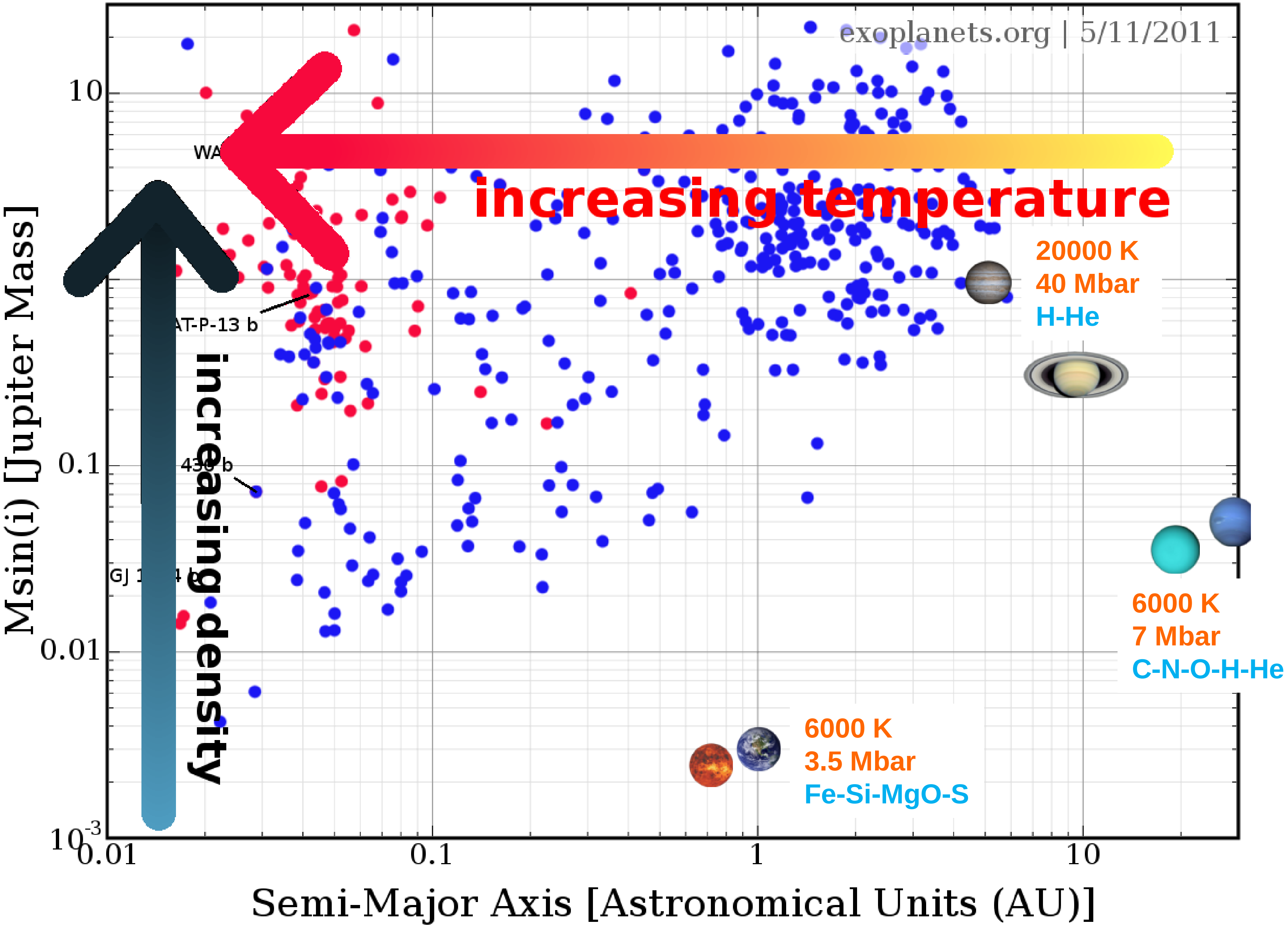
Exoplanets – strange new worlds



Transiting planets: Kepler Corot

R-V method: Doppler shift

Exoplanets – probe the n-T plane



increasing temperature

increasing density

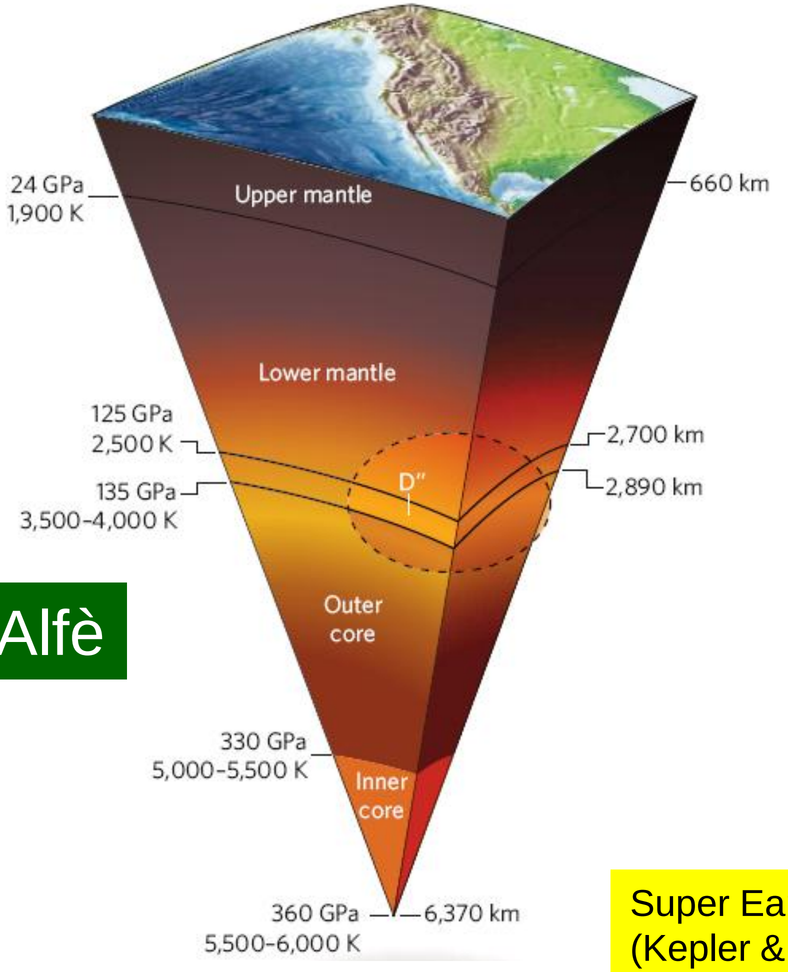
20000 K
40 Mbar
H-He

6000 K
7 Mbar
C-N-O-H-He

6000 K
3.5 Mbar
Fe-Si-MgO-S

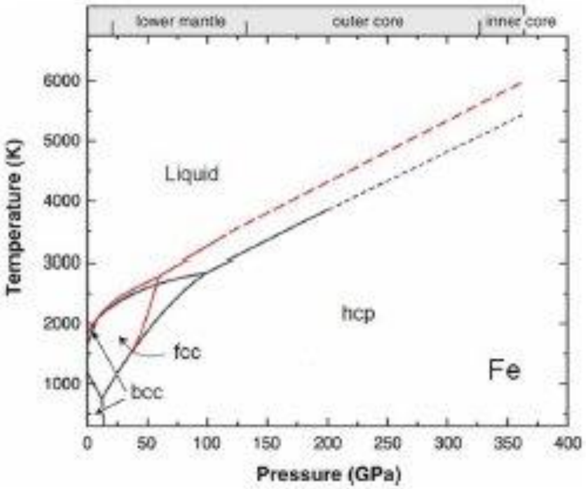
(Super) Earth(s) - mineralogy at the extreme

Upper mantle: olivine $(Mg,Mn,Fe)_2[SiO_4]$
Lower mantle: perovskite $MgSiO_3$, ppv and p-ppv
Core: (Fe,Ni)[Si,O,S,C…] – melting line, dynamo

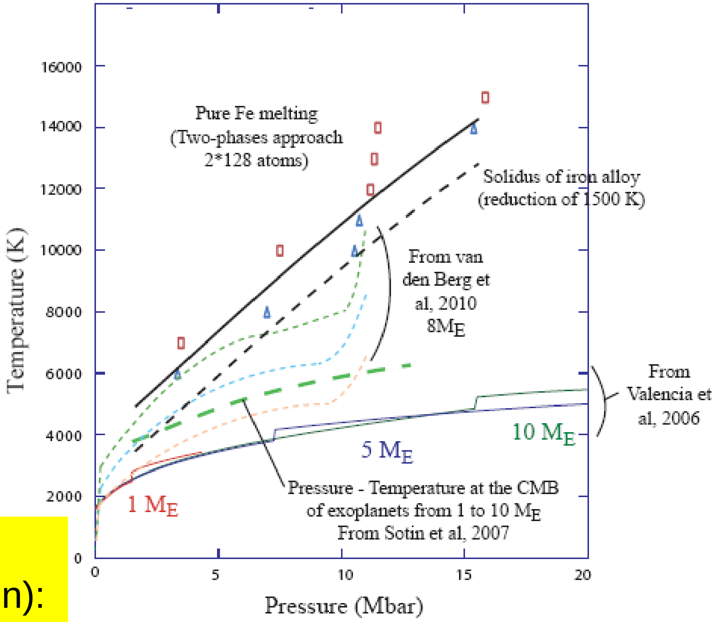


D. Alfè

T.S. Duffy, Nature **451**, 269 **(**2008)



Fe phase diagram (exp.): Boehler et al. 1993, Hemley & Mao 2001, Ma et al. 2004.



Super Earths 1-10 M_E
(Kepler & Corot mission):
Completely different?

G. Morard, HEDP **7**, 141 **(**2011)

Planetary physics – fundamental problems

What is the composition of planets?
→ planetary materials and element abundancies
→ H, He **(gases)** – C-N-O **(ices)** – Fe-Si-Mg-O-S **(rocks)**
→ gas giants (J, S) – ice giants (U, N) – rocky planets (Me, V, E, Ma)

What is the structure of planets?
→ various layers – but how many?
→ Composition of the layers? Origin and stability of the layer boundaries?
→ Do they have a (solid) core? Of what size is it (has it to be)?

How do planets form and develop?
→ Via core accretion or gravitational instability?
→ Cooling behavior and age? → accurate **M-R[P(r),T(r));t]** relations needed!
→ Radiation transport and sources of internal (excess) luminosity?

Can we understand the diversity of their magnetic fields?
→ Dynamo simulations: solve magnetohydrodynamic equations
→ Magnetization processes and magnetic materials
→ material properties (thermal coefficients, conductivities, viscosity)

J.J. Fortney, N. Nettelmann, Space Sci. Rev. **152**, 423 (2010)
I. Baraffe, G. Chabrier, T. Barman, Rep. Prog. Phys. **73**, 016901 (2010)
J. Wicht, A. Tilgner, Space Sci. Rev. **152**, 501 (2010)

Planetary physics – fundamental problems

What is the composition of planets?
→ planetary materials and element abundancies
→ H, He (gases) – C,N,O (ices) – Fe,Si,Mg,O,S (rocks)
→ gas g

What is
→ variou
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→ Do th

How do
→ Via co
→ Cooli !
→ Radia

Can we
→ Dyna
→ Magn
→ mater

Focus here is on the

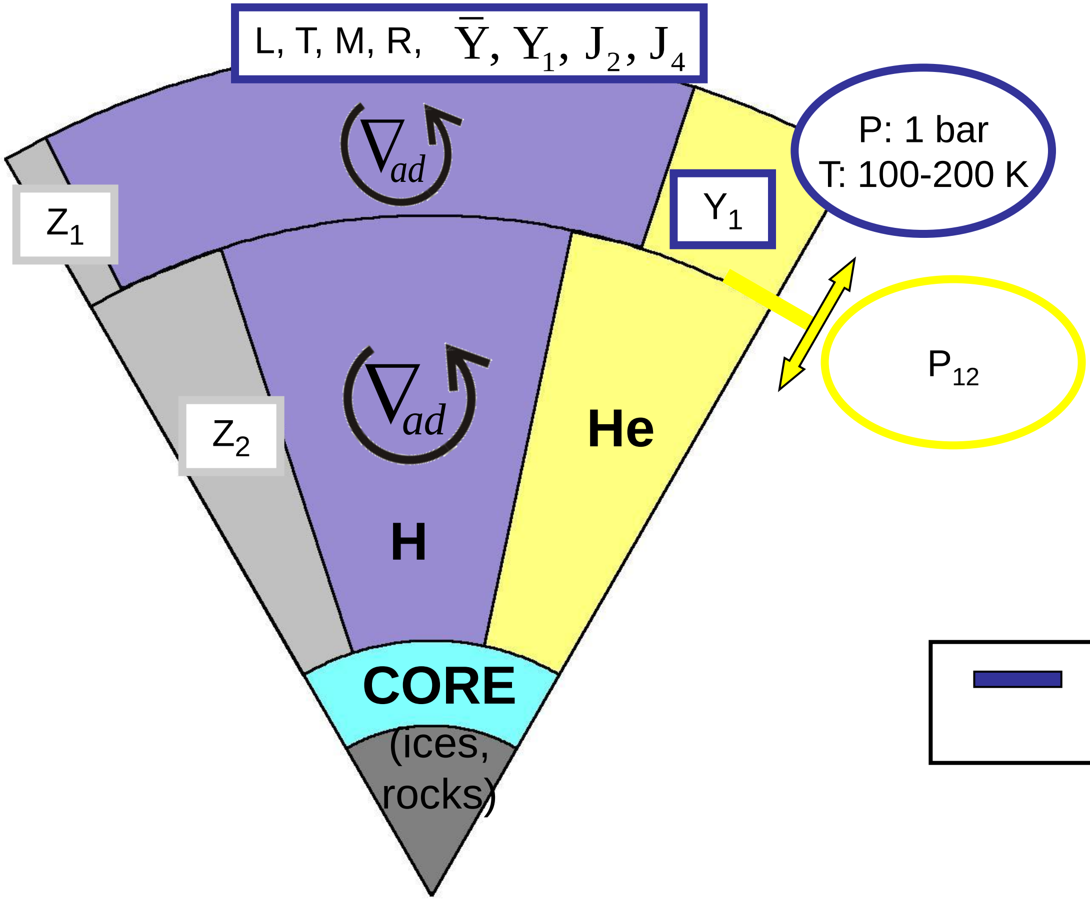
→ EOS and phase diagram
→ demixing phenomena
→ nonmetal-to-metal transitions

in the warm dense matter region
T ~ (1-10) eV and P ~ (1-100) Mbar
as relevant for planetary interiors

J.J. Fortney, N. Nettelmann, Space Sci. Rev. **152**, 423 (2010)
I. Baraffe, G. Chabrier, T. Barman, Rep. Prog. Phys. **73**, 016901 (2010)
J. Wicht, A. Tilgner, Space Sci. Rev. **152**, 501 (2010)

Assume an interior structure for solar GPs:

Standard three-layer model



Y: fraction of He

Z: fraction of metals

J_2, J_4: gravitational moments

Physical origin and location of the layer boundary…
→ NM-M-T (PPT)
→ H-He demixing

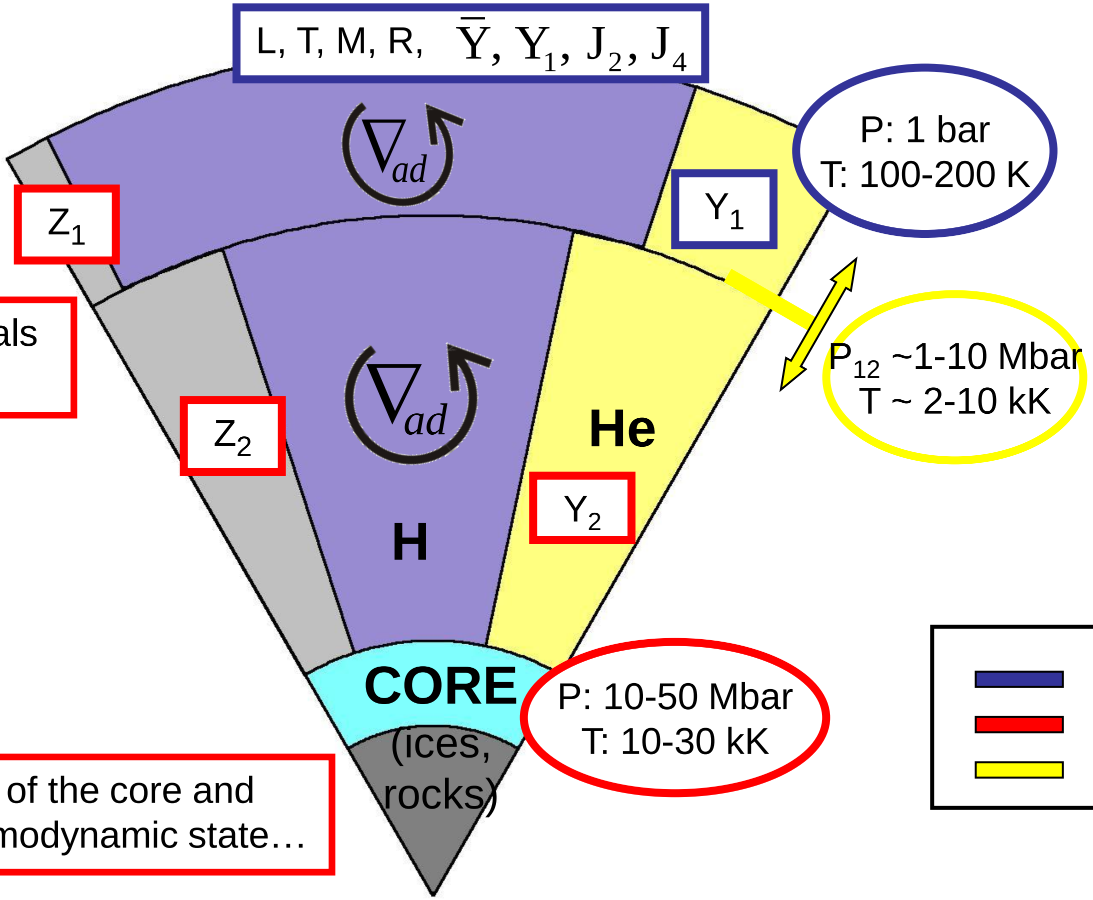
▬ constraints

Interior structure models of this type are uniquely defined by the observables, except P_{12}.

See e.g. D.J. Stevenson (1982), T. Guillot (1999), N. Nettelmann et al. (2008, 2012)

Determine the interior structure for solar GPs:

Standard three-layer model



Fraction of metals in the layers…

Size of the core and thermodynamic state…

Y: fraction of He

Z: fraction of metals

J_2, J_4: gravitational moments

Physical origin and location of the layer boundary…
→ NM-M-T (PPT)
→ H-He demixing

🟦 constraints
🟥 results from modeling
🟨 free parameter

Interior structure models of this type are uniquely defined by the observables, except P_{12}. Accurate EOS data for warm dense H, He and the representative of metals (H_2O) is the most important input.

See e.g. D.J. Stevenson (1982), T. Guillot (1999), N. Nettelmann et al. (2008, 2012)

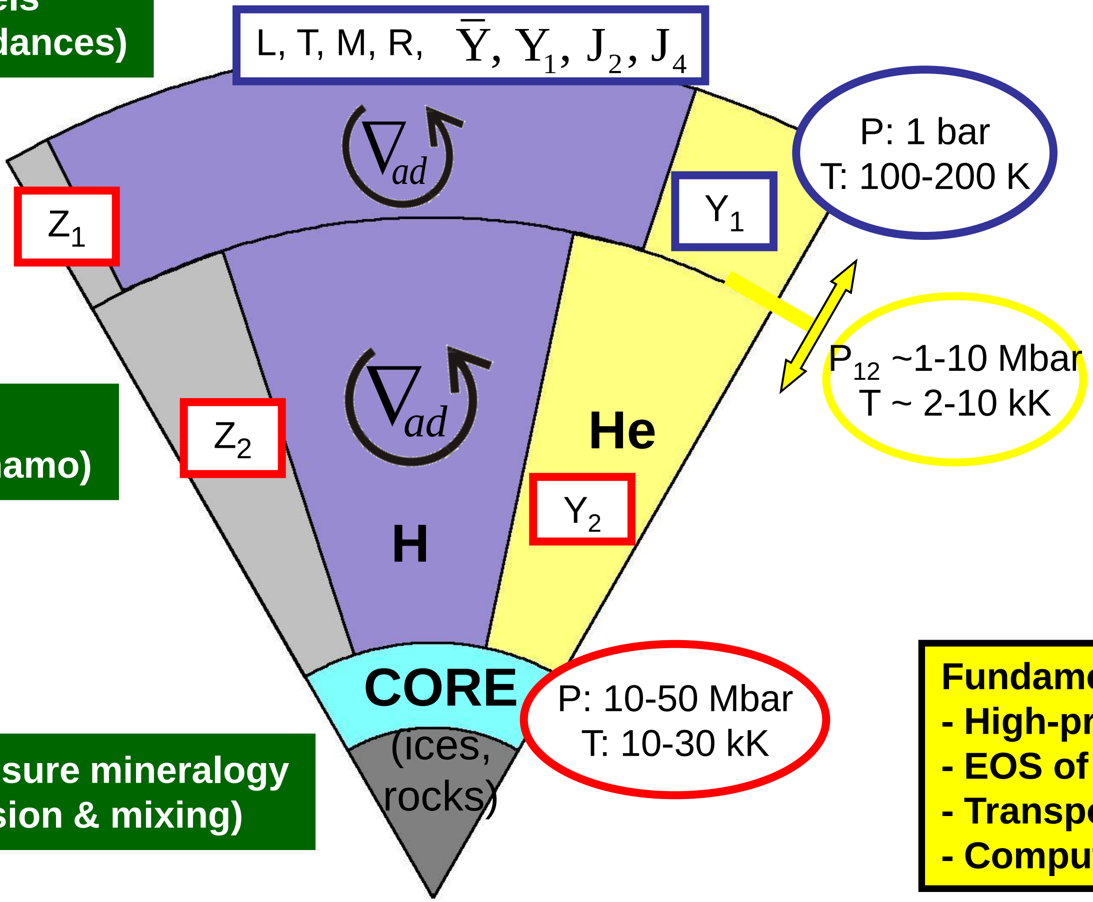
Progress in interior modeling:

Further input and constraints

Atmosphere models (luminosity, abundances)

Magnetic field generation (dynamo)

High-pressure mineralogy (core erosion & mixing)



🟦 constraints
🟥 results from modeling
🟨 free parameter

Future missions to Jupiter (Juno) and S, U, N and observations

Physical origin and location of the layer boundary…
→ NM-M-T (PPT)
→ H-He demixing

↕

Fundamental physical problems
- **High-pressure phase diagram**
- **EOS of complex mixtures**
- **Transport coefficients**
- **Computational methods**

↕

GOAL OF THE IPAM PROGRAM

Basic equations for planetary modeling

mass conservation:

$$dm = 4\pi r^2 \rho(r)\, dr$$

hydrostatic equation of motion:

$$\frac{1}{\rho}\frac{dP}{dr} = \frac{dU}{dr} \ , \qquad U = V + Q$$

gravitational potential:

$$V(\vec{r}) = -G \int_{V_0} d^3r' \frac{\rho(r')}{\left|\vec{r} - \vec{r}\,'\right|}$$

expansion into Legendre polynomials:

$$V(r,\theta) = -\frac{GM}{r(\theta)}\left(1 - \sum_{i=1}^{\infty}\left(\frac{R_{eq}}{r(\theta)}\right)^{2i} J_{2i} P_{2i}\left(\cos\theta\right)\right)$$

gravitational moments:

$$J_{2i} = -\frac{1}{MR_{eq}^{2i}} \int d^3r'\, \rho(r'(\theta'))\, r'^{2i}\, P_{2i}(\cos\theta')$$

Calculations via theory of figures (Zharkov & Trubitsyn) with boundary conditions $M_p(R_p)$, Y_1, $\bar{Y}$, P and T at 1 bar.

Mass distribution along (piecewise) isentropes according to ab initio EOS data for a H-He-H_2O mixture (LM-REOS).

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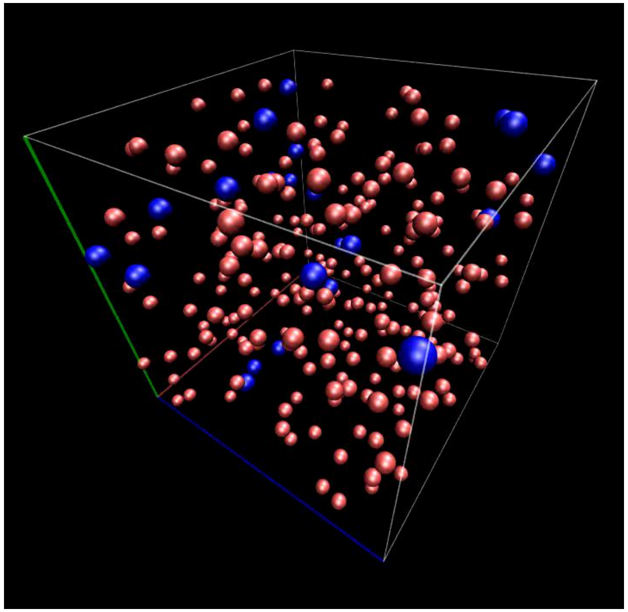
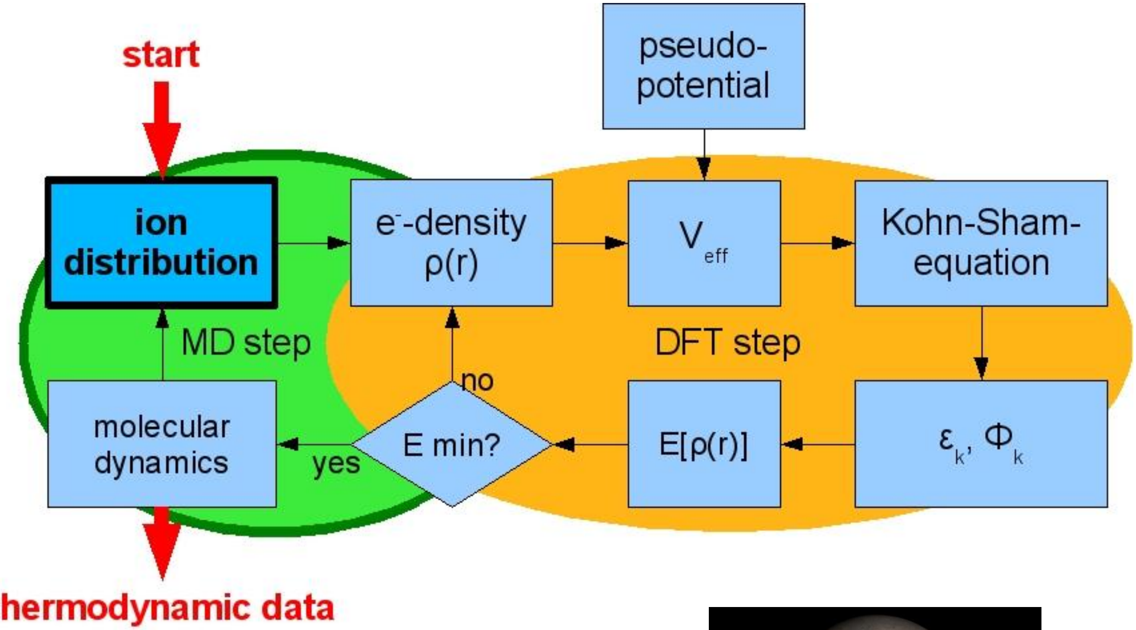
Ab initio MD (AIMD) simulations

Born-Oppenheimer approximation: combination of (quantum) DFT and (classical) MD
Warm Dense Matter: finite-temperature DFT-MD simulations based on
N.D. Mermin, Phys. Rev. **137,** A1441 (1965)
Implemented e.g. in the Vienna Ab-initio Simulation Package (VASP)
G. Kresse and J. Hafner, PRB **47**, 558 (1993), ibid. **49**, 14251 (1994)
G. Kresse and J. Furthmüller, Comput. Mat. Sci. **6**, 15 (1996), PRB **54**, 11169 (1996)

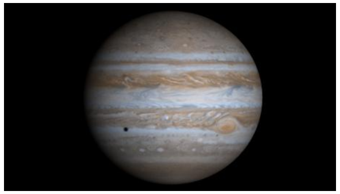


H-He (8.6%) @ 1 Mbar, 4000 K

box length ~ 10^{-9} m



high-pressure phase diagram
pair correlation functions
electrical & thermal conductivity
diffusion coefficient
viscosity, opacity



GP size ~ 10^8 m

Some details of the AIMD simulations

VASP: G. Kresse et al., Phys. Rev. B **47**, 558 (1993)

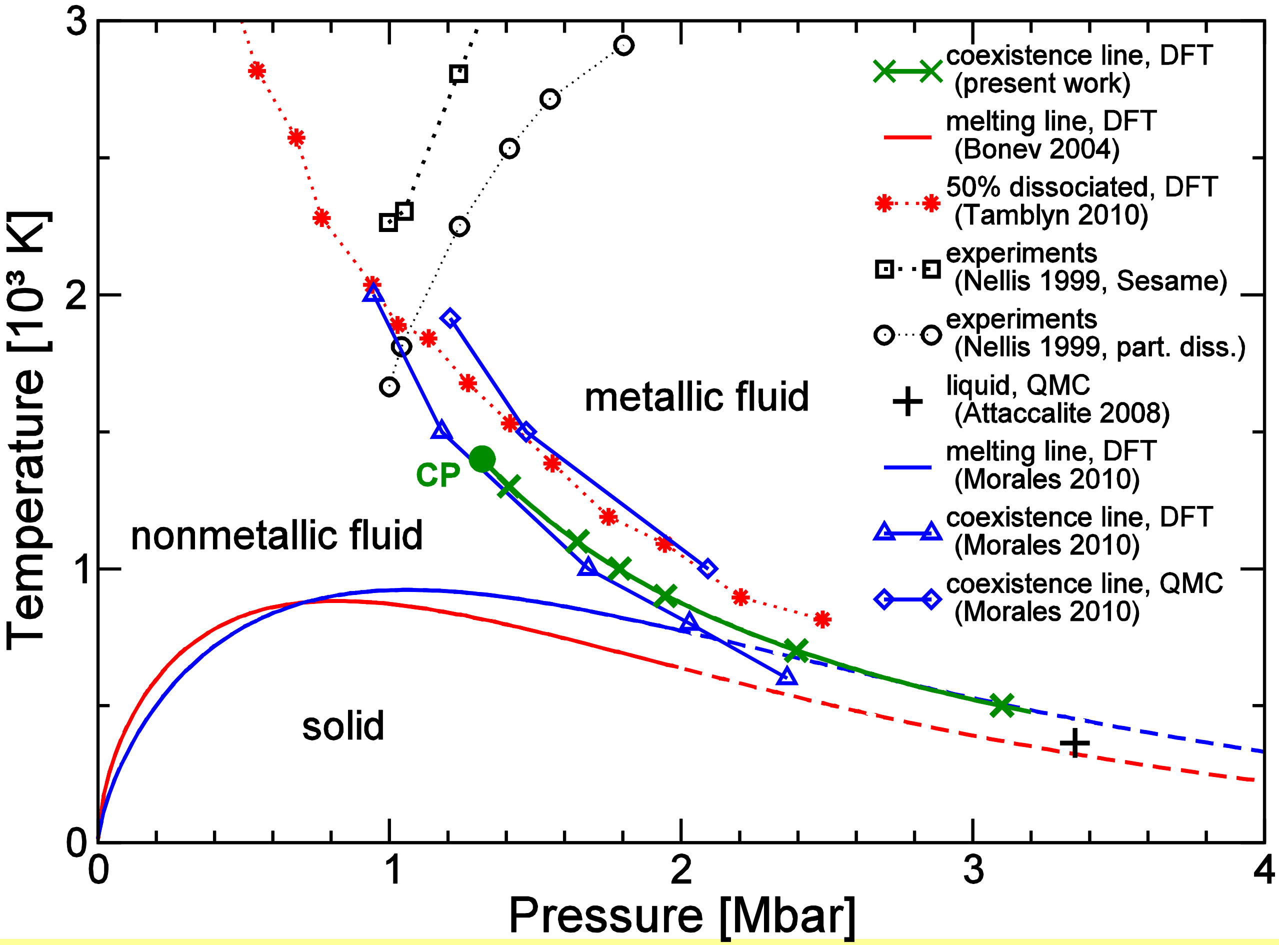
- VASP uses plane wave basis sets, energy cut-off at about 1 keV
- Exchange-correlation functional: usually GGA [1], some HSE [2]
- PAW pseudo-potentials [3]: 1 e/H, 2 e/He, 6(8) e/O
- Ion temperature control by Nosé thermostat [4]
- Evaluation of electronic states in BZ at (few) special points (EOS)
- Higher k-point sets are needed for σ, 10-20 snapshots
- $N \leq 2000$ electrons in a box of volume V at temperature T
- Simulation time: up to 20 ps with several 10^3-10^4 time steps
- Check convergence with respect to E_{cut}, k-points, N, Δt …

Rostock Group: Martin French, Winfried Lorenzen, Andreas Becker, Kai-Uwe Plagemann, Mandy Bethkenhagen, Daniel Cebulla

[1] J.P. Perdew, K. Burke, M. Ernzerhof, PRL **77**, 3865 (1996)
[2] J. Heyd et al., JCP **118**, 8207 (2003); **124**, 219906 (2006)
[3] P.E. Blöchl, PRB **50**, 17953 (1994), G. Kresse, J. Joubert, PRB **59**, 1758 (1999)
[4] S. Nosé, J. Chem. Phys. **81**, 511 (1984)

H phase diagram at high pressure

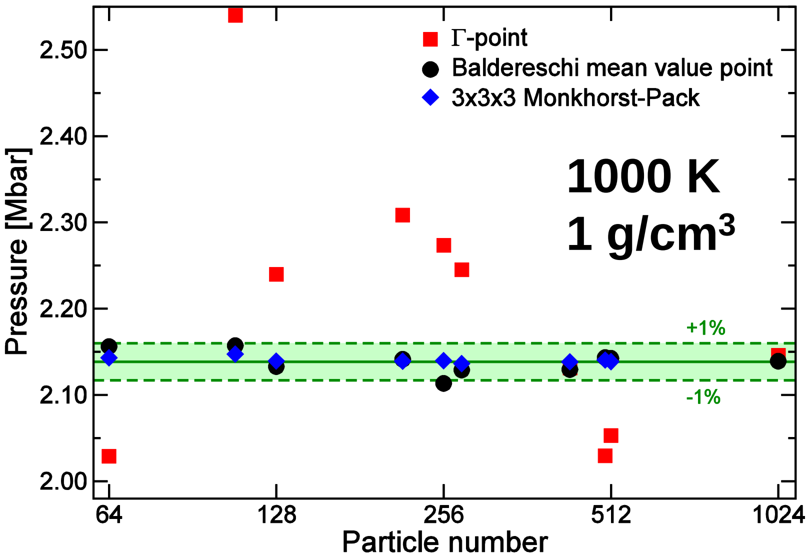
M.A. Morales et al., PNAS 107, 12799 (2010)
W. Lorenzen, B. Holst, R. Redmer, PRB **82**, 195107 (2010)

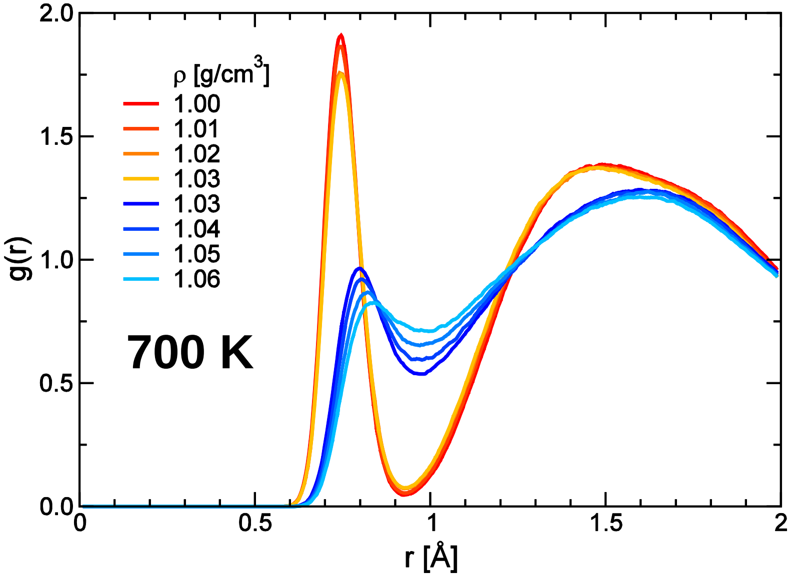


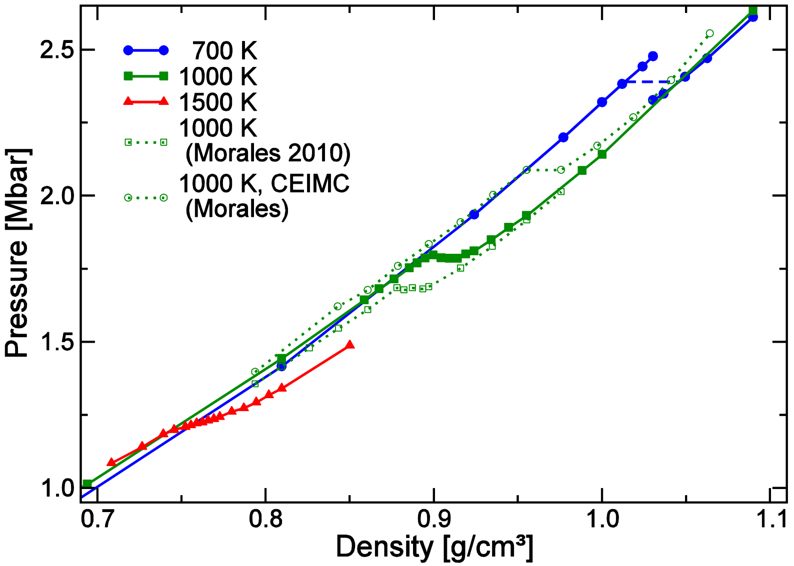
see also I. Tamblyn, S.A. Bonev, PRL **104**, 065702 (2010), critical point located at about 1500 K, 0.82 g/ccm, 1.4 Mbar

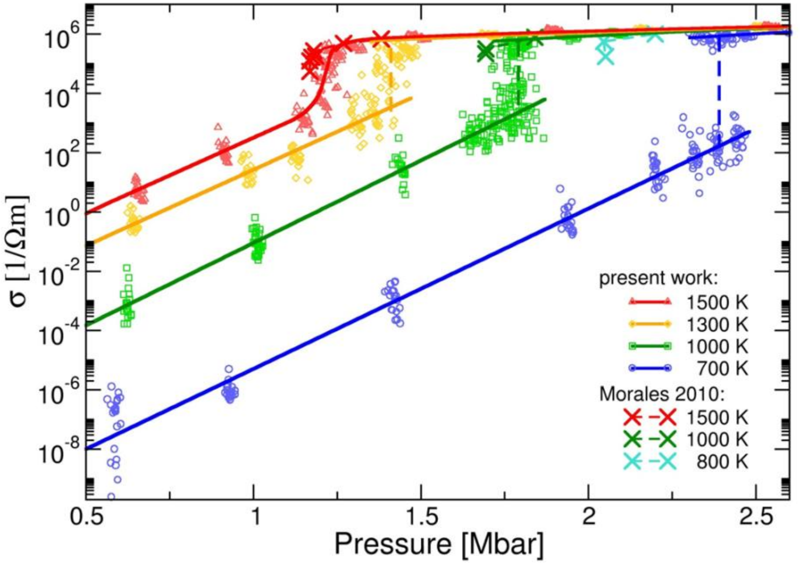
H phase diagram at high pressure

W. Lorenzen, B. Holst, R. Redmer, PRB **82**, 195107 (2010)



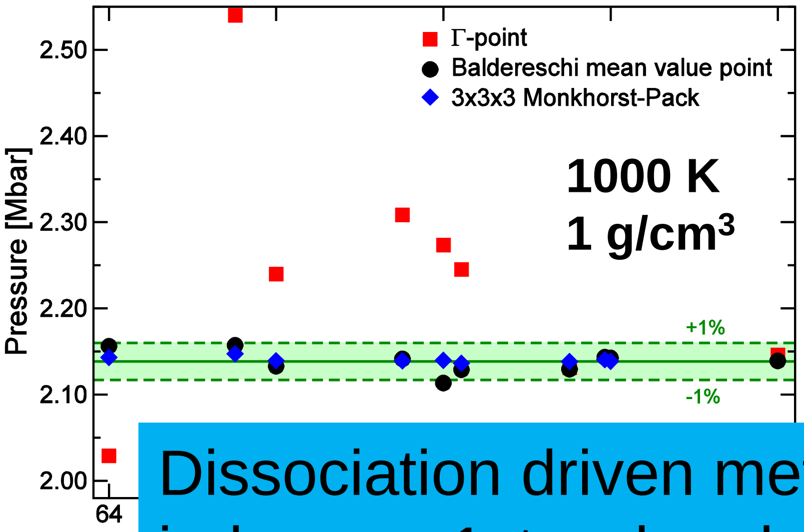


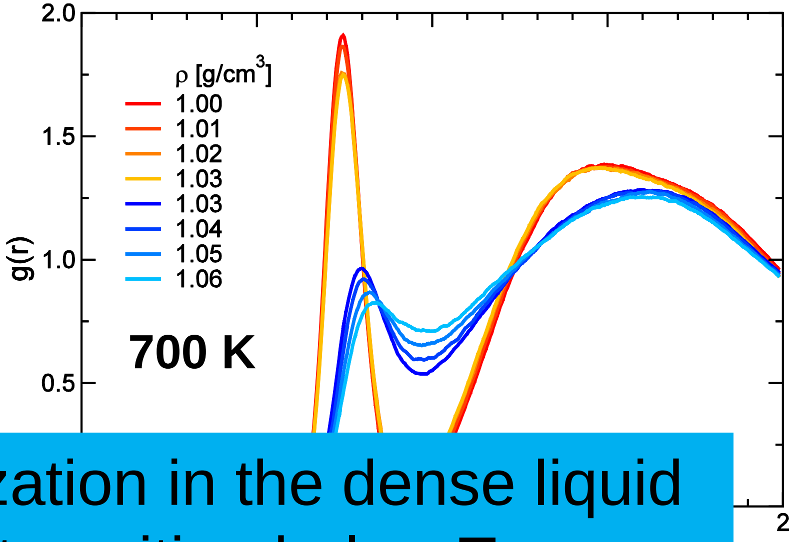


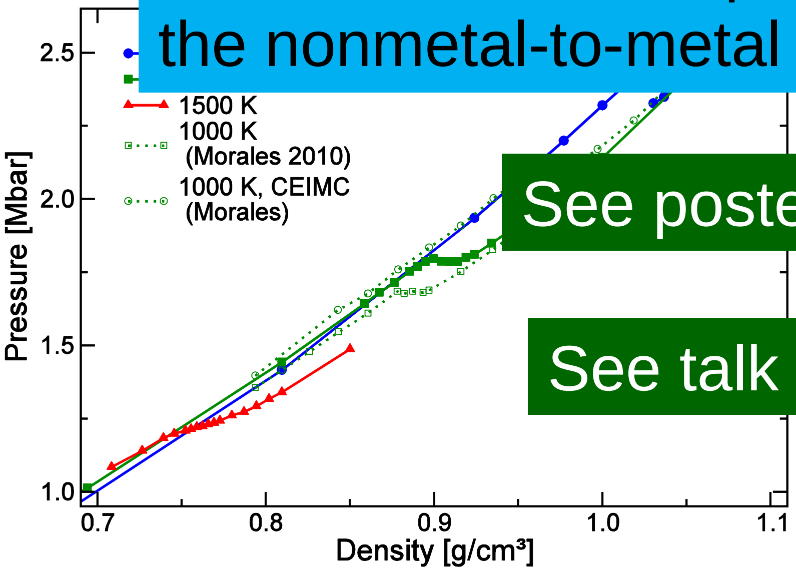


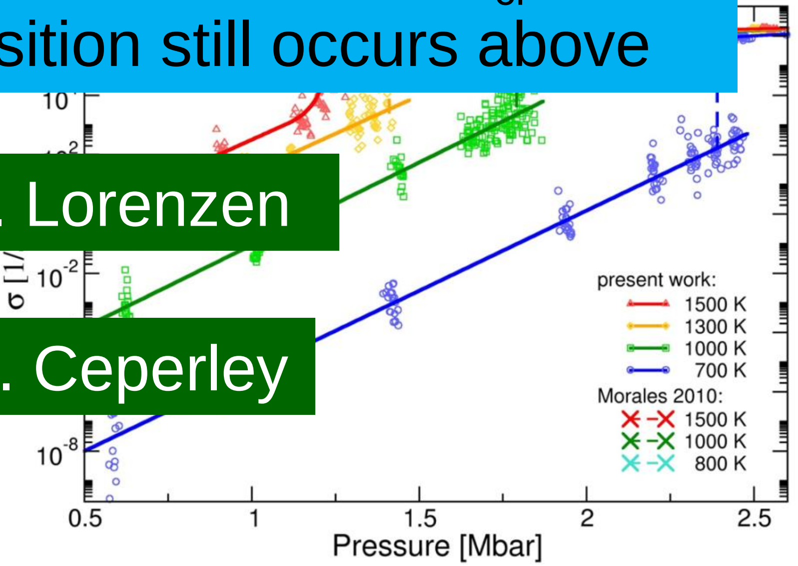
H phase diagram at high pressure

W. Lorenzen, B. Holst, R. Redmer, PRB **82**, 195107 (2010)









Dissociation driven metallization in the dense liquid induces a 1st-order phase transition below T_{cr} – the nonmetal-to-metal transition still occurs above

See poster W. Lorenzen

See talk of D. Ceperley

H phase diagram and GPs

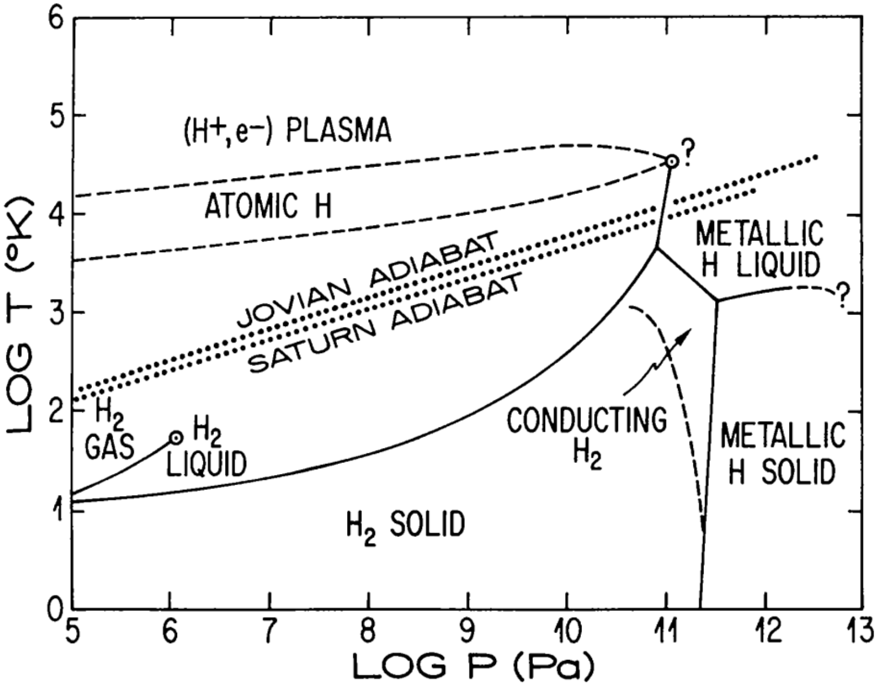
1st-order phase transition relevant for Jupiter & Saturn?

PPT predicted by chemical models extends to much higher temperatures!

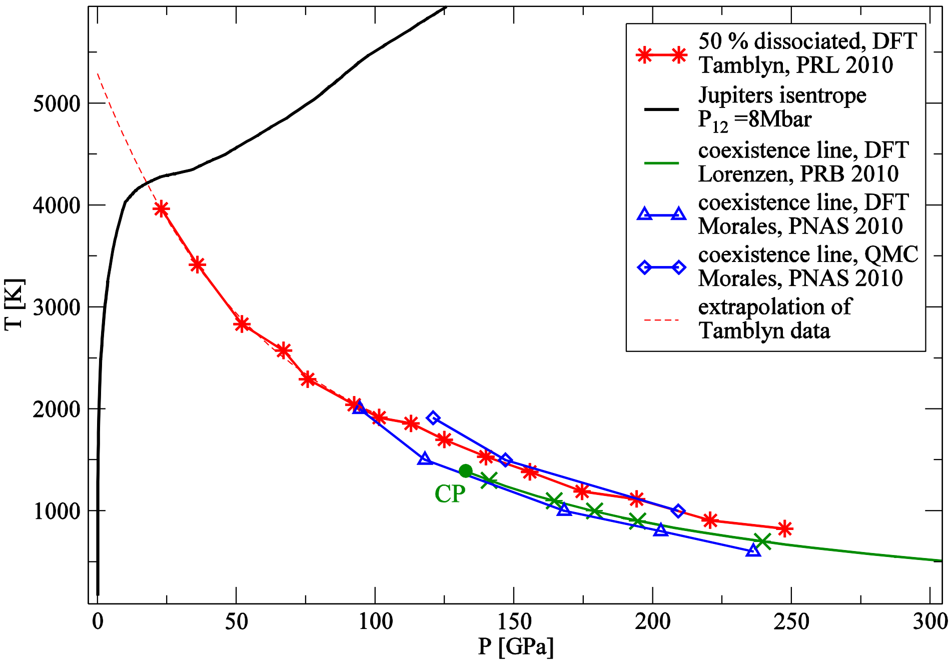
→ reason for a boundary between two fluid envelopes?

→ locate the conducting zone in gas giants (σ along radius)

→ input into dynamo simulations (magnetic field structure)



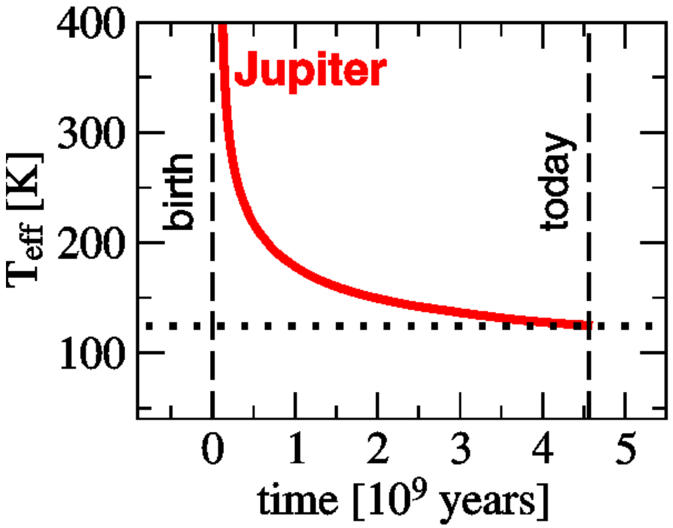
D.J. Stevenson, Ann. Rev. Earth Planet. Sci. **10**, 257 (1982)

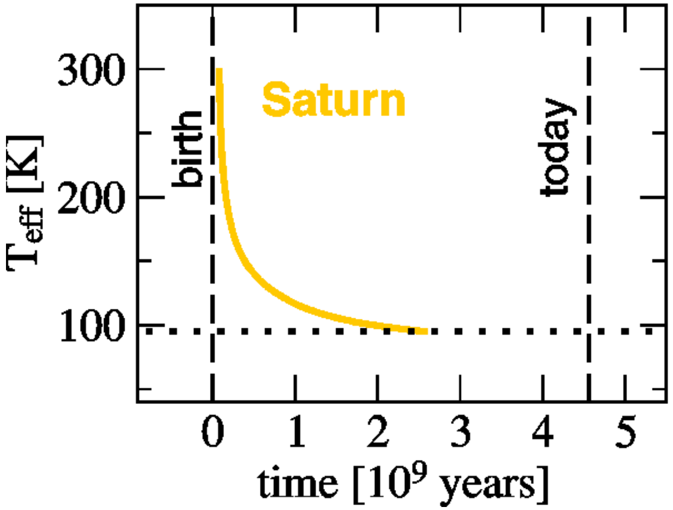


M. French et al. (2012)

Experimental verification? Location of the PPT in H-He?

H-He and thermal evolution of GPs





Formation out of the protosolar cloud:

1. Same age of 4.5×10^9 a
2. Similar composition/abundance, especially He-H ratio of Y=27.5%

Facts:

1. Evolution models yield correct age of Jupiter but too young Saturn with about 2.5×10^9 a – additional internal heat source: He rain?
2. He is depleted in the outer layer of Jupiter (~23%) and Saturn (~18%)!

H-He demixing at high pressure?

D.J. Stevenson, E.B. Salpeter 1977
J.J. Fortney, W.B. Hubbard, 2003
W. Lorenzen et al., 2009, 2011: AIMD
M.A. Morales et al., 2009: AIMD

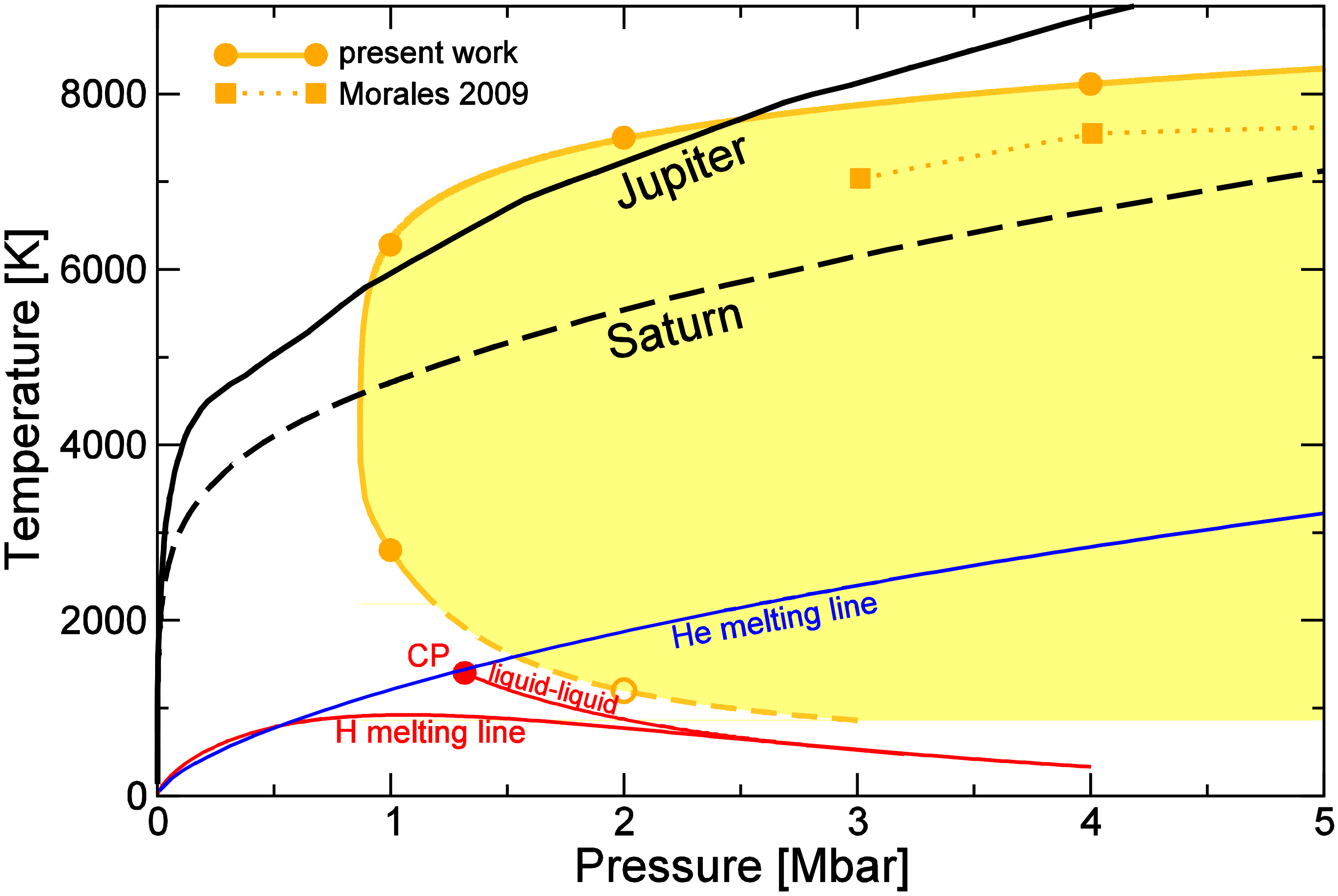
H-He demixing in GPs

Relevant for Jupiter (?) and Saturn (!)

Calculation of modified cooling curves: in progress.

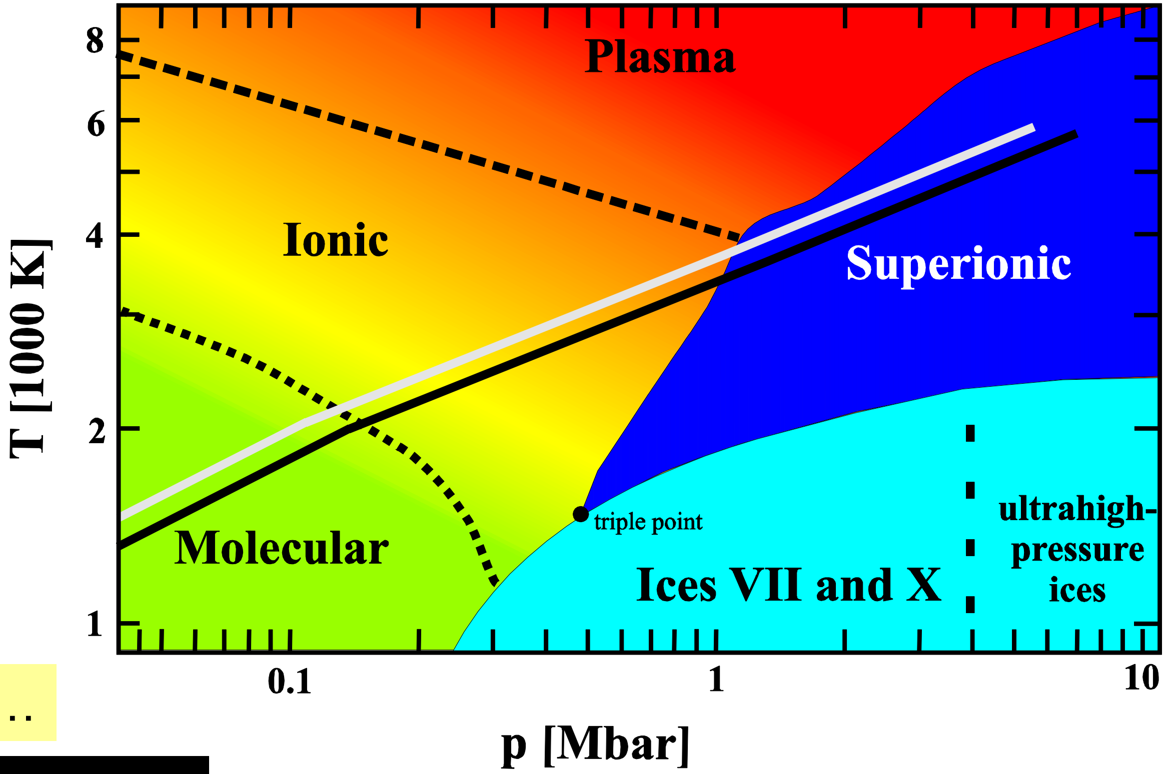
May yield stable stratification → thus **B** field perfectly axisymmetric?

W. Lorenzen et al., PRB **84**, 235109 (2011)



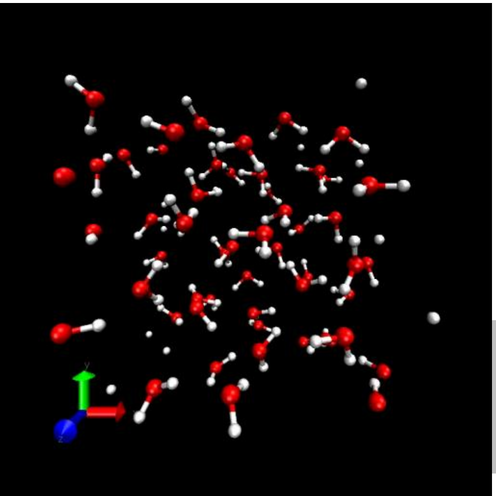
Similar results by M.A. Morales et al., PNAS **106**, 1324 (2009) based on DFT-MD.

Water phase diagram at ultra-high pressures

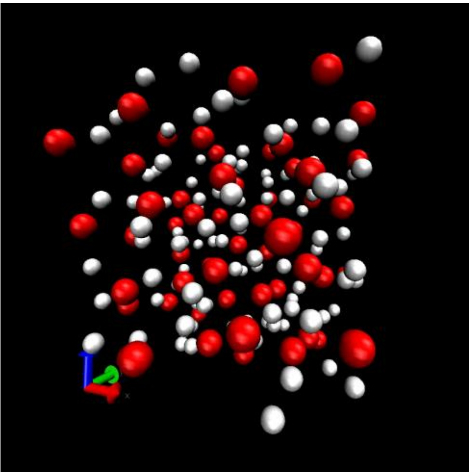


Relevant for the interiors of Neptune (black) and Uranus (white)

Normal ice…



… and superionic water at 7 g/cm^3 and 6000 K



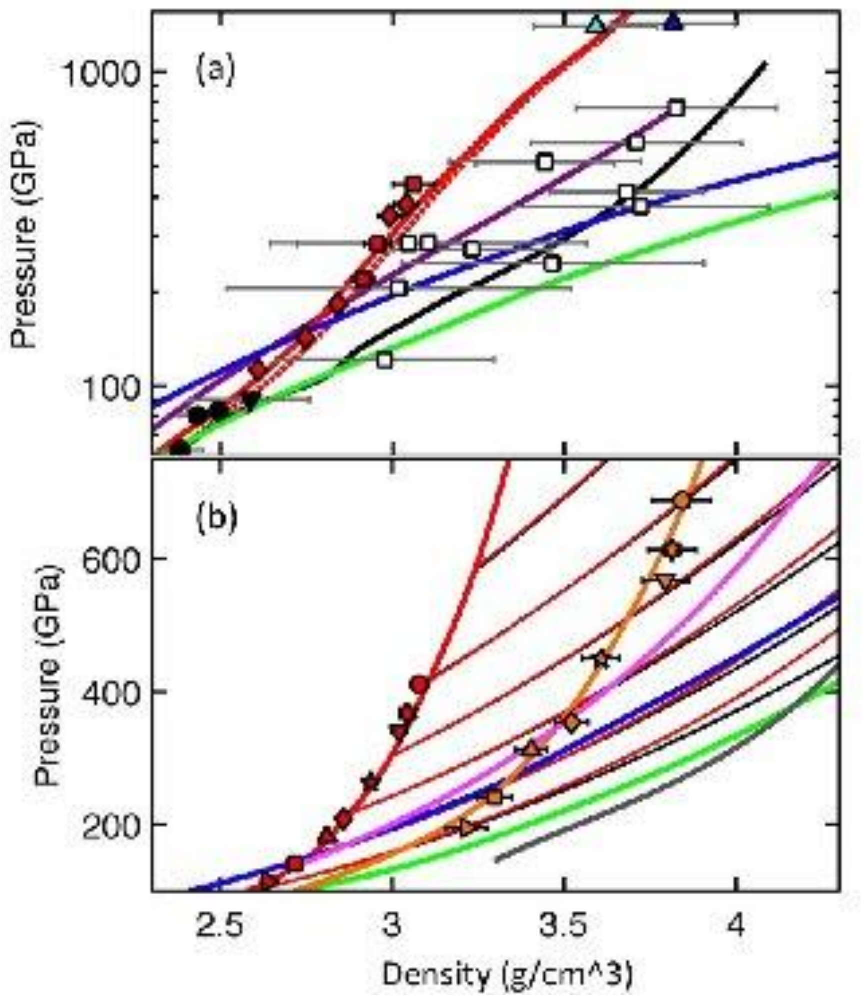
EOS and phase diagram:
M. French et al., PRB **79**, 054107 (2009),
Transport properties (diffusion, conductivity):
M. French et al., PRB **82**, 174108 (2010)

see also C. Cavazzoni et al., Science **283**, 44 (1999),
T.R. Mattsson, M.P. Desjarlais, PRL **97**, 017801 (2006),
E. Schwegler et al., PNAS **105**, 14779 (2008)

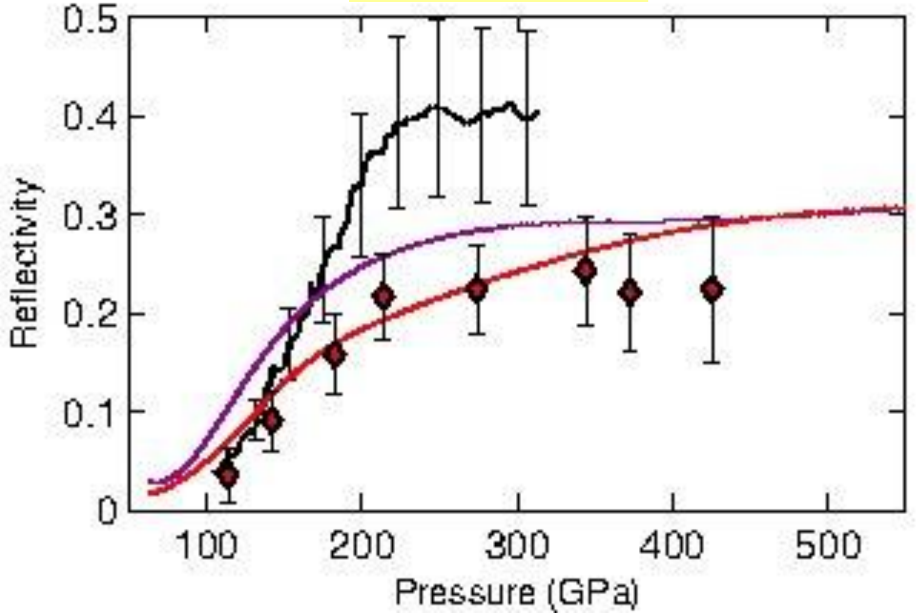
H2O: AIMD results and new Z experiments

M.D. Knudson et al., PRL **108**, 091102 (2012)

Hugoniot curve



Reflectivity



Theory:
Red: AIMD
Black: Sesame
Magenta: ANEOS
Neptune adiabat
GJ 436b adiabat

Data:
Red ◊ □ : Sandia Z
Open □ : Laser shocks
Black ●: Gas gun
Blue ▲: Nuclear expl.
Orange: reshock data (Z and AIMD)

Excellent agreement – AIMD high-pressure EOS for water will be used for icy planets!

Dynamic (optical) conductivity via AIMD

- Dynamic conductivity $\sigma(\omega) = \sigma_1(\omega) + i\sigma_2(\omega)$
- Kubo-Greenwood formula:

$$\sigma(\omega) = \frac{2\pi e^2\hbar^2}{3m^2\omega\Omega}\sum_{\mathbf{k}} W(\mathbf{k})\sum_{j=1}^{N}\sum_{i=1}^{N}\sum_{\alpha=1}^{3}[F(\epsilon_{i,\mathbf{k}}) - F(\epsilon_{j,\mathbf{k}})]$$

$$\times|\langle\Psi_{j,\mathbf{k}}|\nabla_\alpha|\Psi_{i,\mathbf{k}}\rangle|^2\delta(\epsilon_{j,\mathbf{k}} - \epsilon_{i,\mathbf{k}} - \hbar\omega),$$

- Dielectric function:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) = 1 - \frac{1}{\varepsilon_0\omega}\sigma_2(\omega) + i\frac{1}{\varepsilon_0\omega}\sigma_1(\omega)$$

- Kramers-Kronig relation: $\sigma_2(\omega) = \frac{2}{\pi}P\int\frac{\sigma_1(\nu)\omega}{(\nu^2 - \omega^2)}.d\nu$
- Index of refraction:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) = [n(\omega) + ik(\omega)]^2$$

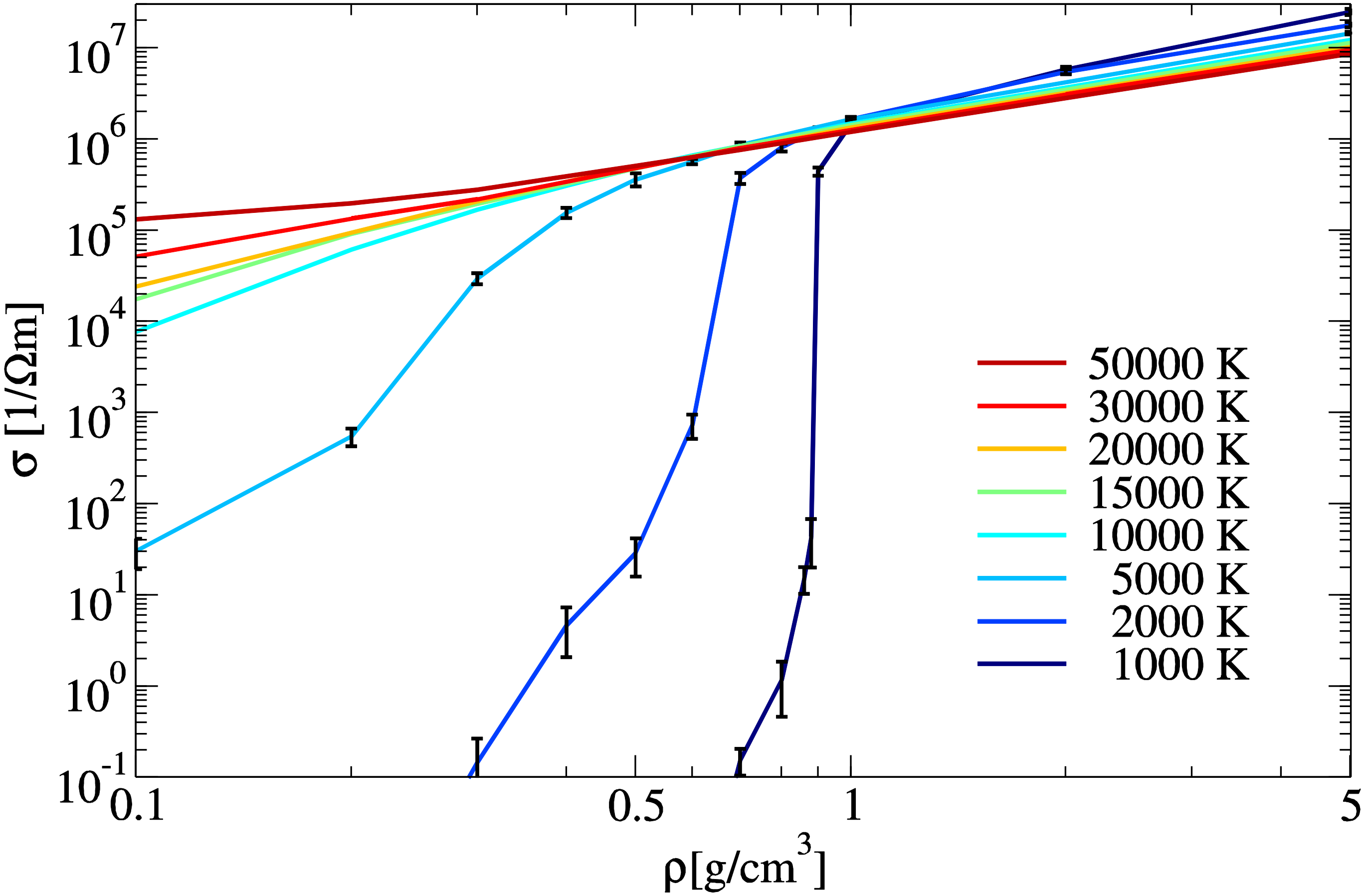
See M.P. Desjarlais, J.D. Kress, L.A. Collins, PRE **66**, 025401(R) (2002)

Electrical conductvity in warm dense H –

based on generalized Kubo-Greenwood formula for L_{ik}

$$L_{mn}(\omega) = \frac{2\pi q^{4-m-n}}{3V m_e^2 \omega} \sum_{\mathbf{k}\nu\mu} \langle \mathbf{k}\nu|\hat{\mathbf{p}}|\mathbf{k}\mu\rangle \cdot \langle \mathbf{k}\mu|\hat{\mathbf{p}}|\mathbf{k}\nu\rangle$$

$$\times \epsilon_{\mathbf{k}\nu \mathbf{k}\mu}^{m+n-2} \left(f_{\mathbf{k}\nu} - f_{\mathbf{k}\mu}\right) \delta\left(E_{\mathbf{k}\mu} - E_{\mathbf{k}\nu} - \hbar\omega\right)$$



B. Holst, M. French, R. Redmer, Phys. Rev. B **83**, 235120 (2011)

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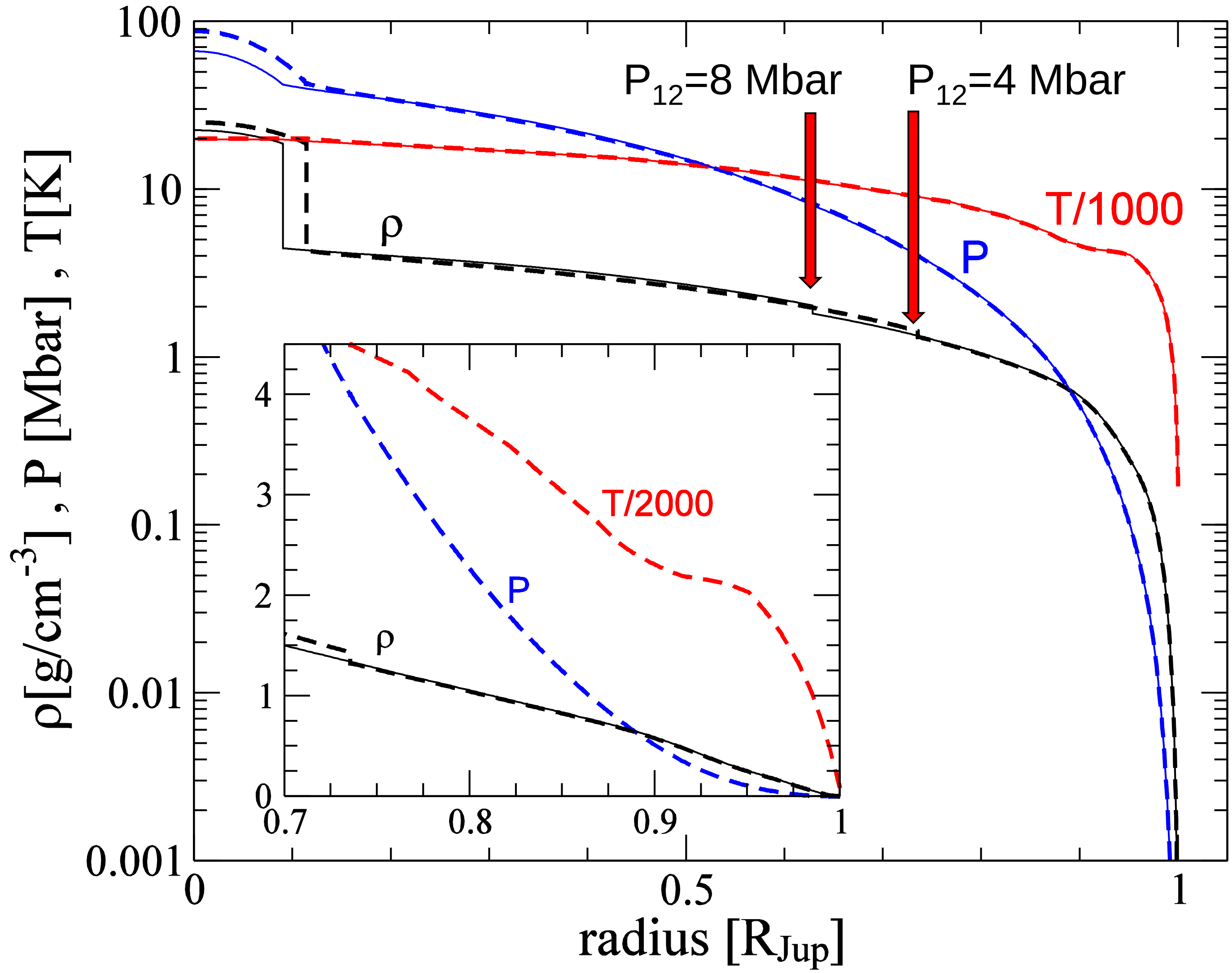
    - Problems in planetary physics
2. Fundamental properties:
    - Ab initio molecular dynamics simulations
    - H, H-He mixtures, H2O - EOS and MIT
3. **Application in astrophysics:**
    - **Modeling solar and extrasolar giant planets**
    - **Material properties for the deep interior**
4. Summary

Interior of Jupiter with LM-REOS

M. French et al. (2012)

See poster A. Becker

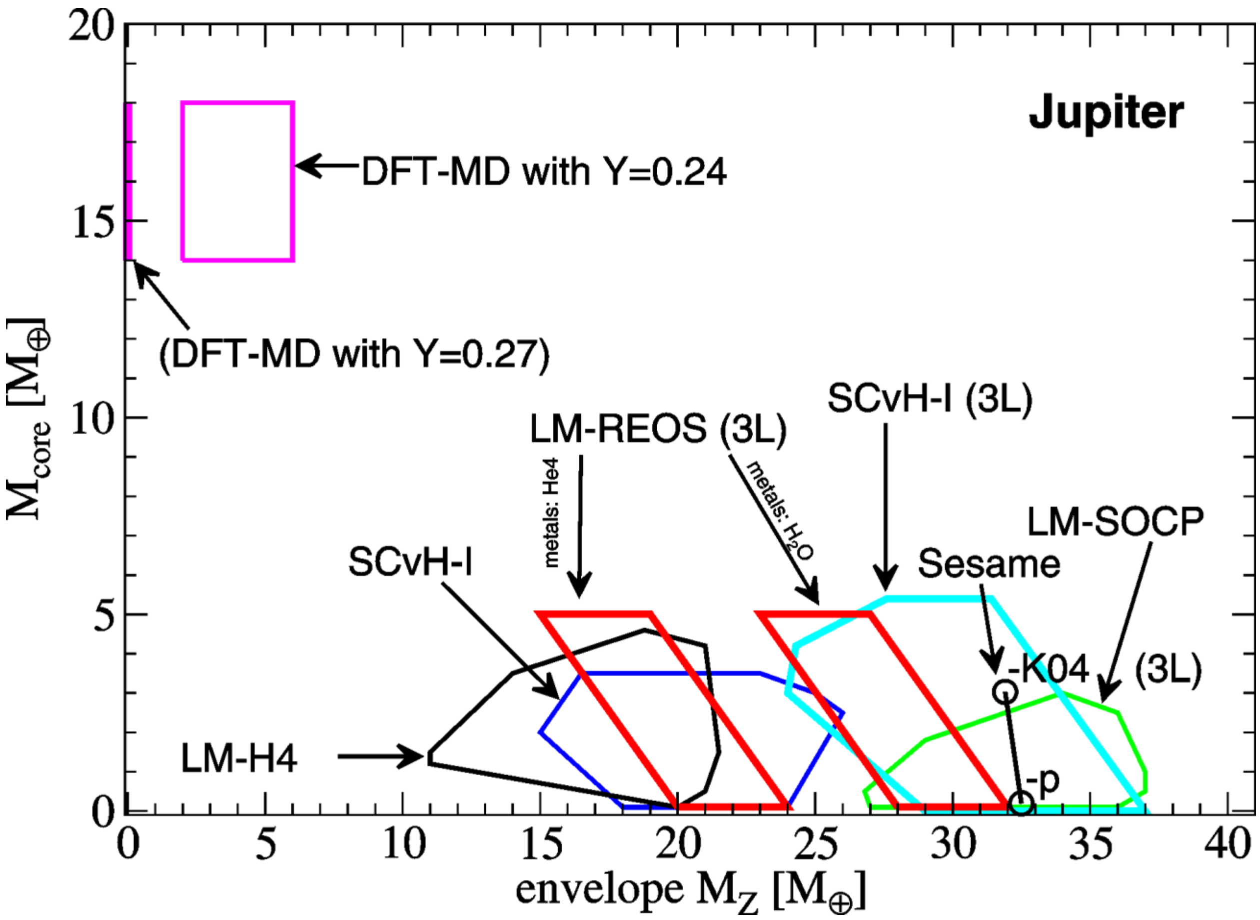


Density, pressure and temperature along Jupiter`s isentrope.

Jupiter – EOS predictions

(N. Nettelmann)

Core mass and mass of metals in the envelope for different EOS as labeled



CONCLUSION:

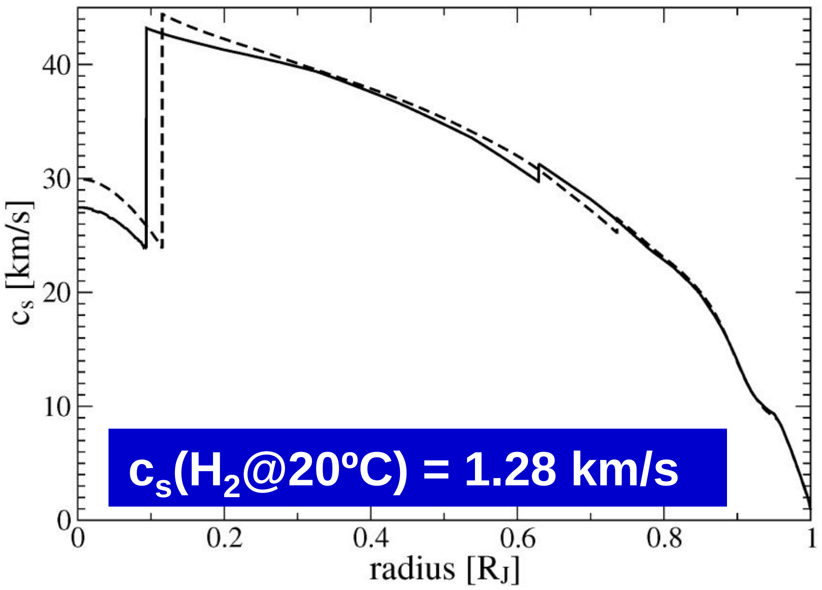
The average metallicity is 2-8 x solar.

Reproduced with H-REOS.2 Nettelmann et al., ApJ 750, 52 (2012)

- **Guillot, Planet. Space Sci. 47, 1183 (1999)**
- **Saumon & Guillot, ApJ 609, 1170 (2004)**
- **Militzer et al., ApJ 688, L45 (2008)**
- **Fortney & Nettelmann, Space Sci. Rev. 152, 423 (2010)**

Material properties along Jupiter`s isentrope

M. French et al. (2012): self-consistent set of *ab initio* EOS and material data that can now be used for planetary modeling (interior, dynamo, evolution)

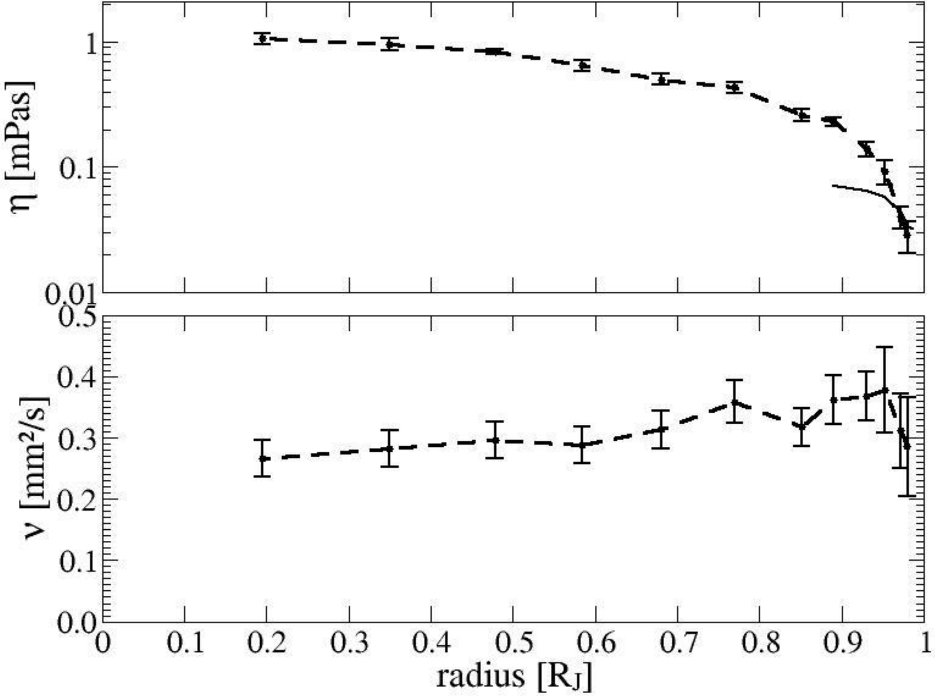


$c_s(H_2@20ºC) = 1.28$ km/s

Sound velocity c_s along Jupiter`s Isentrope (processes EOS data).

$$c_s = \sqrt{\left(\frac{\partial P}{\partial \rho}\right)_S}$$

$\eta(H_2O@20ºC) = 1$ mPas

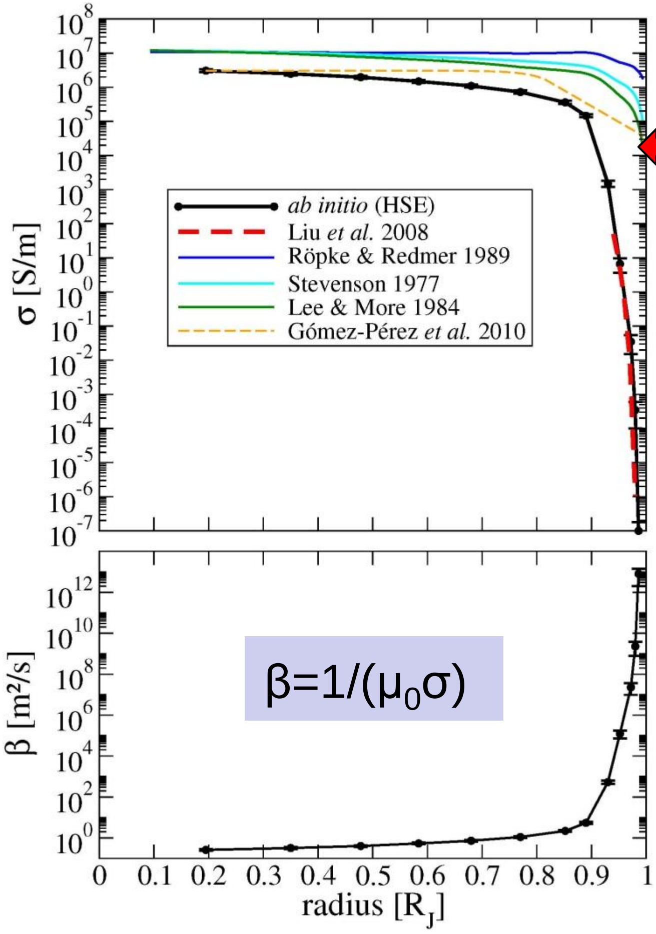


Dynamic (η) and kinematic (ν=η/ρ) viscosity along Jupiter`s isentrope.

$$\eta = \frac{\Omega}{3k_B T}\int_0^\infty dt \sum_{ij=\{xy,yz,zx\}} \left\langle p_{ij}(0)\, p_{ij}(t)\right\rangle$$

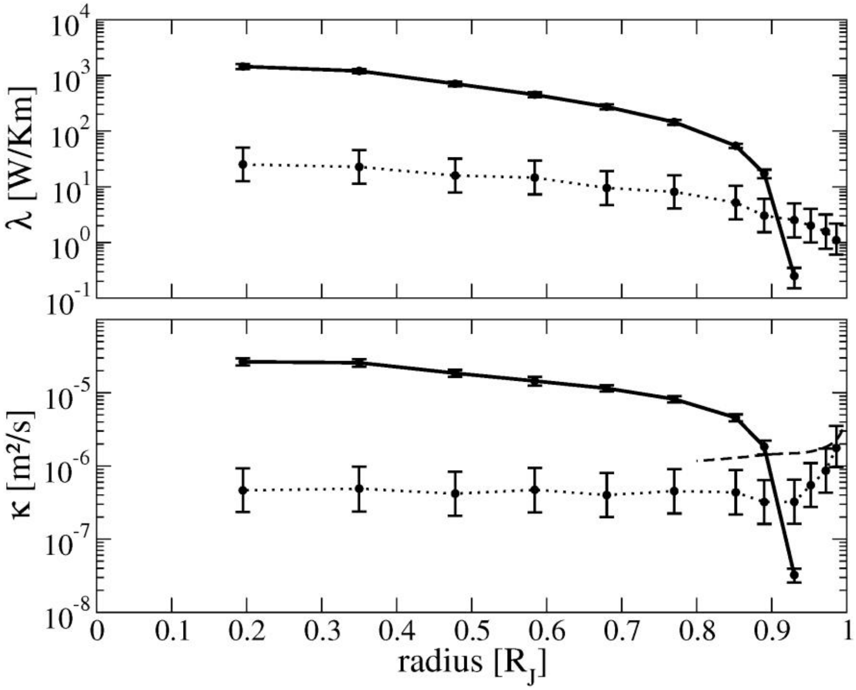
Material properties along Jupiter`s isentrope

M. French et al. (2012): self-consistent set of *ab initio* EOS and material data that can now be used for planetary modeling (interior, dynamo, evolution)



$\beta = 1/(\mu_0 \sigma)$

MIT



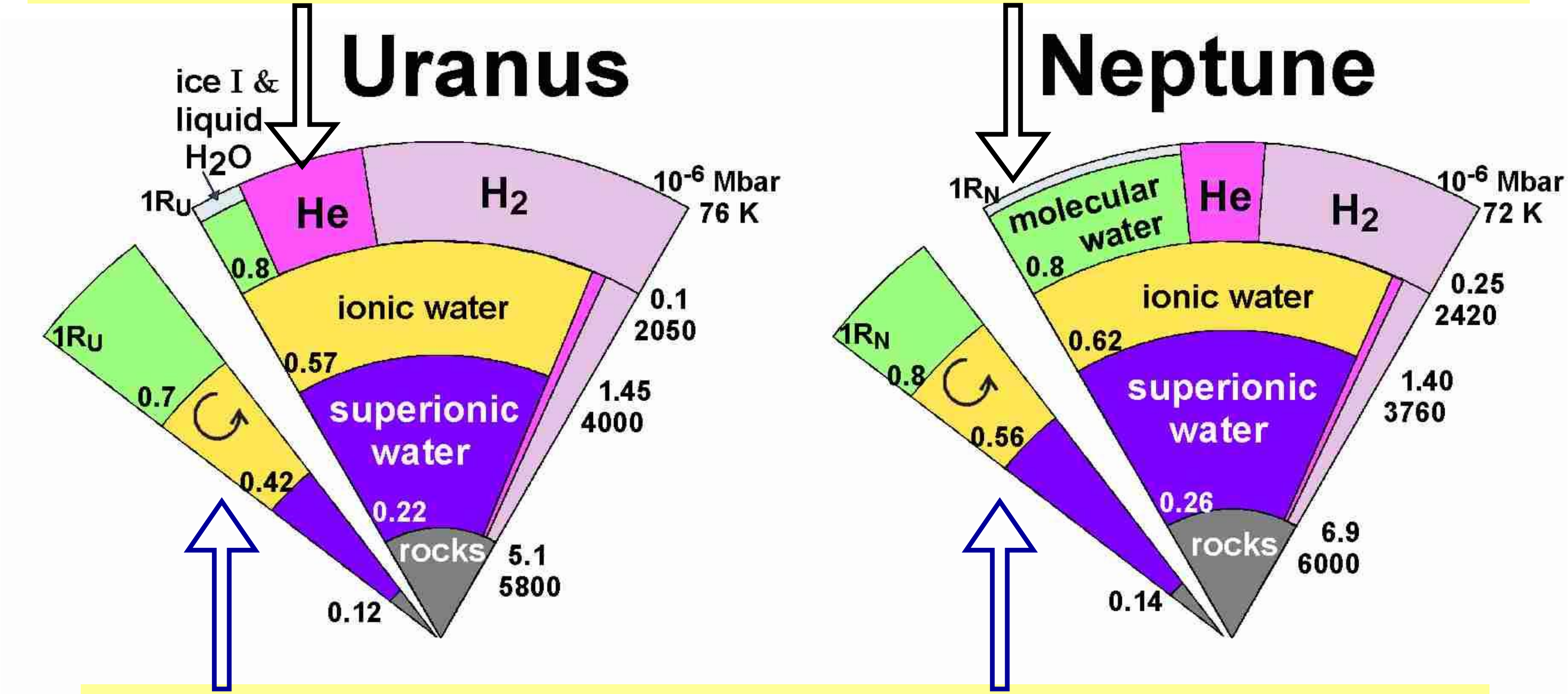
Thermal conductivity λ and thermal diffusivity κ along Jupiter`s isentrope. Solid: electronic, dotted: ionic.

Electrical conductivity σ and magnetic diffusivity along Jupiter`s isentrope.

$\kappa = \lambda/(\rho c_p)$

Interior of Neptune and Uranus

Our **interior models** reproduce the gravity data based on the EOS and the phase diagram of H_2O and H, He:
J.J. Fortney, N. Nettelmann, Space Sci. Rev. **152**, 423 (2009),
R. Redmer et al., Icarus **211**, 798 (2011)



Independent **dynamo models** reproduce the non-dipolar and non-axisymmetric magnetic fields of N and U by assuming a rather thin conducting shell (yellow) and a central region (magenta) that is stable against convection but of similar conductivity (here: superionic!):
S. Stanley and J. Bloxham, Nature **428**, 151 (2004).

Constraints for modeling GPs (observables)

(N. Nettelmann)

Observable	Solar Giant Planets	Extrasolar Giant Planets
Mass M_p	14.5 – 318 M_{Earth}	✓ (RV & Transit)
Radius R_p	equatorial radius R_{eq}	mean R (Transit)
Pressure $P\,(R_p)$	1 bar	1 mbar
$T\,(R_p)$	70 - 170 K	500 - 2000 K
mean helium mass fraction Y	0.27 (solar)	0.25 - 0.28
atmospheric He mass fraction Y_1	$\leq$ 0.27	$Y_1 = Y$
atmospheric metallicity Z_1	$\geq$ 2 x solar	spectroscopy
period of rotation ω	9 – 17 h	$\omega \approx$ orbital period (days)
gravitational moments J_{2n}	J_2, J_4, J_6	-
Love number k_2	-	k_2 (e, TTV)
age	4.56 Gyr	0.3 – 10 Gyr
T_{eff}	60 - 120 K	model atm. grid / imaging

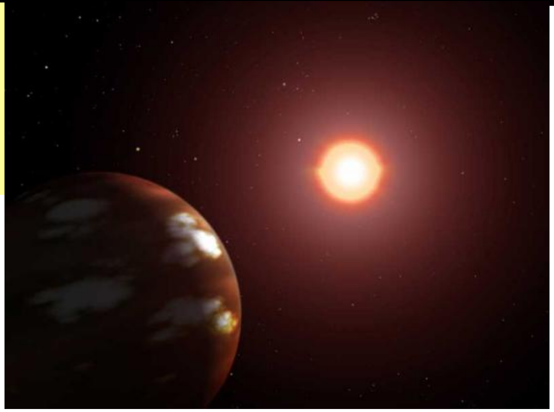
Hot Neptune GJ 436b

Mass-radius relation for transiting planets known (plus radial velocity method)

	Neptune	**GJ 436b**
mass [$M_{\oplus}$]	17.13	22.6 ± 9%
radius [$R_{\oplus}$]	3.86	3.95 ± 9%
surface temperatur [K]	70 (at 1 bar)	520 (T_e) – 720 (8 ❍m)
semi major axis [AU]	30	0.03
period	165 years	2.64 days

Host star is M Dwarf with T_{eff}=3350 K and M=0.44 M_{Sun}, 33 Ly away (Leo)
H.L. Maness et al., PASP **119**, 90 (2007)

Observational parameters:
M. Gillon et al., A&A **471**, L51 (2007),
B.-O. Demory et al., A&A **475**, 1125 (2007)

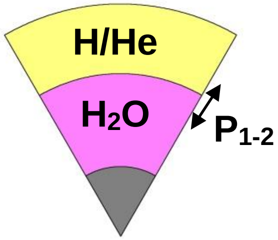


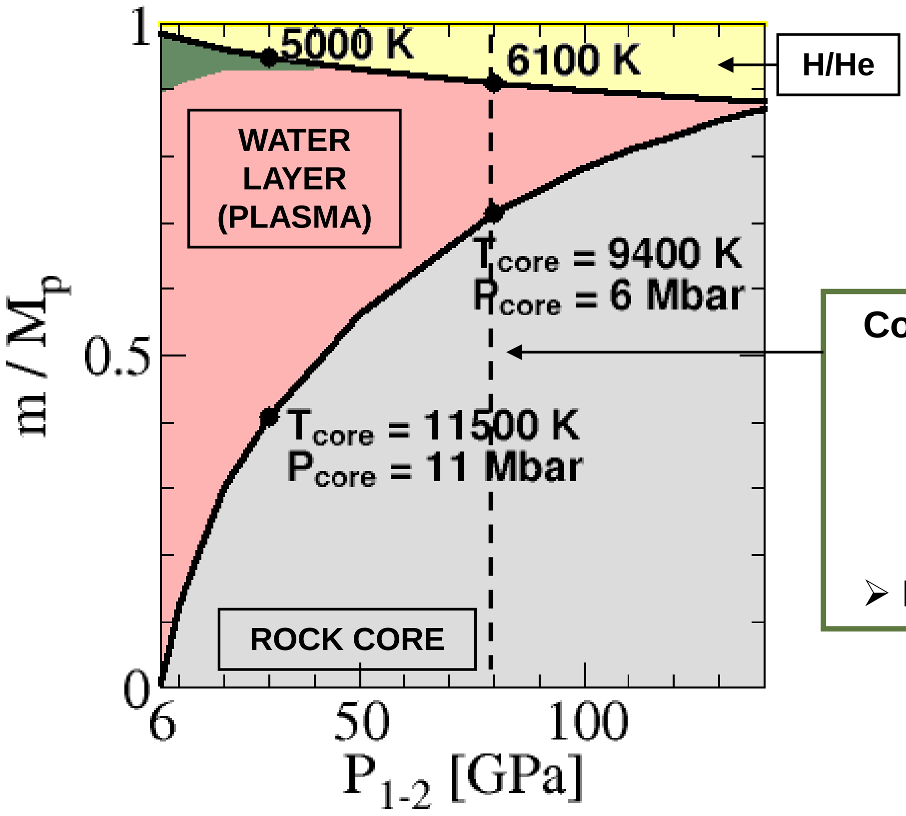
GJ 436b: Water or rocky planet?

N. Nettelmann et al., A&A **523**, A26 (2010)

Structure calculations limit the H/He mass fraction down to 1 - 12% M_p.

Illustration





Constraints from formation:

H/H=10-20%

ice=17-40%

rock=45-70%

- **Figueira et al., A&A (2009)**

CONCLUSION: Models with M_{core} ~ 0.7 M_p are consistent with all constraints.

Summary

- Large scale AIMD simulations are performed for WDM
  → agreement with available shock wave experiments
  → predict high-pressure phase diagram of matter (H,He,H_2O)
  → nonmetal-to-metal and 1st-order phase transition (H)
  → demixing phenomena at high pressures (H-He, H-H_2O …)
  → superionic water (NH_3?)
  → experimental verification

- Modeling planets based on AIMD EOS and material data
  → develop new and advanced planetary models
  → structure, composition, evolution of solar/extrasolar planets
  → gas giants – ice giants – Super Earths
  → diversity of magnetic fields
  → structure and evolution of planetary systems

Outlook warm dense matter

- Laboratory experiments are increasingly capable of driving matter to extreme conditions: NIF (lasers), Z, FELs …

- Simulations based on first-principles techniques are in very good agreement with high-pressure data (predictive)

- Some key issues:
  → finite-temperature DFT functionals
  → orbital-free DFT for high temperatures **F. Lambert, J. Kress**
  → electron dynamics via TD-DFT (optics and transport)
  → treatment of non-equilibrium states
  → quantum Monte Carlo methods
  → develop new (and renew existing) computational methods