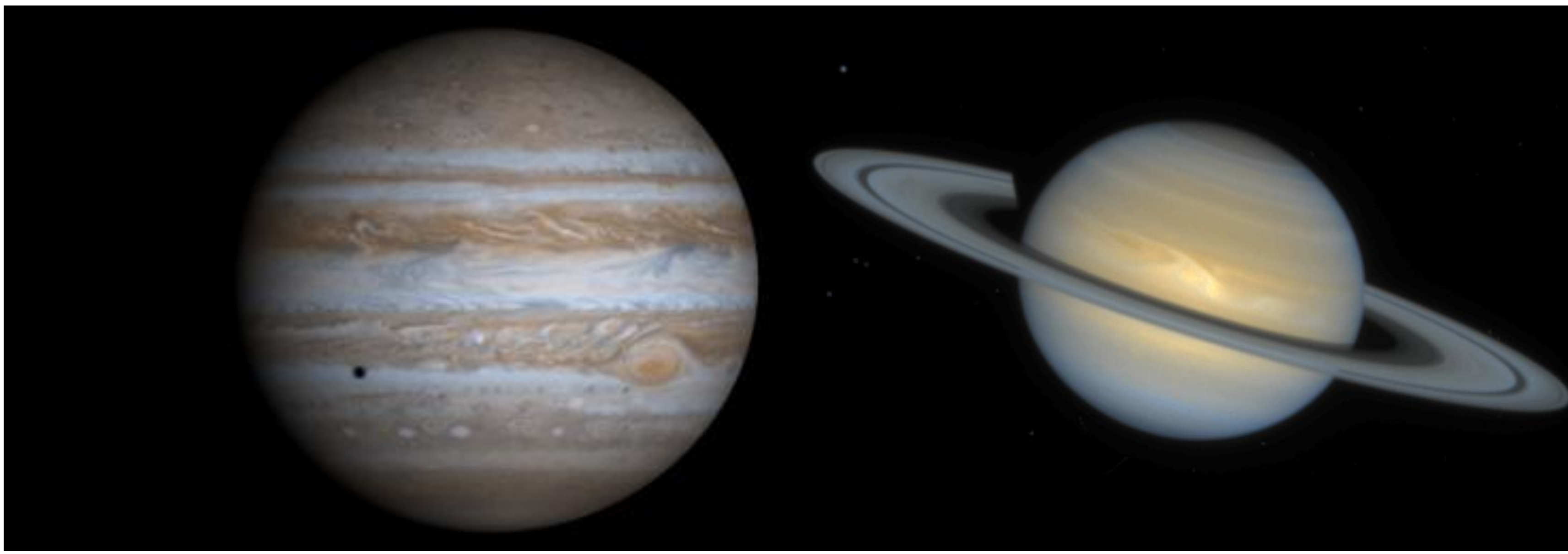
YETI Workshop in Jena, 15-17 November 2010

The Interior of Giant Planets



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AIMD simulations:

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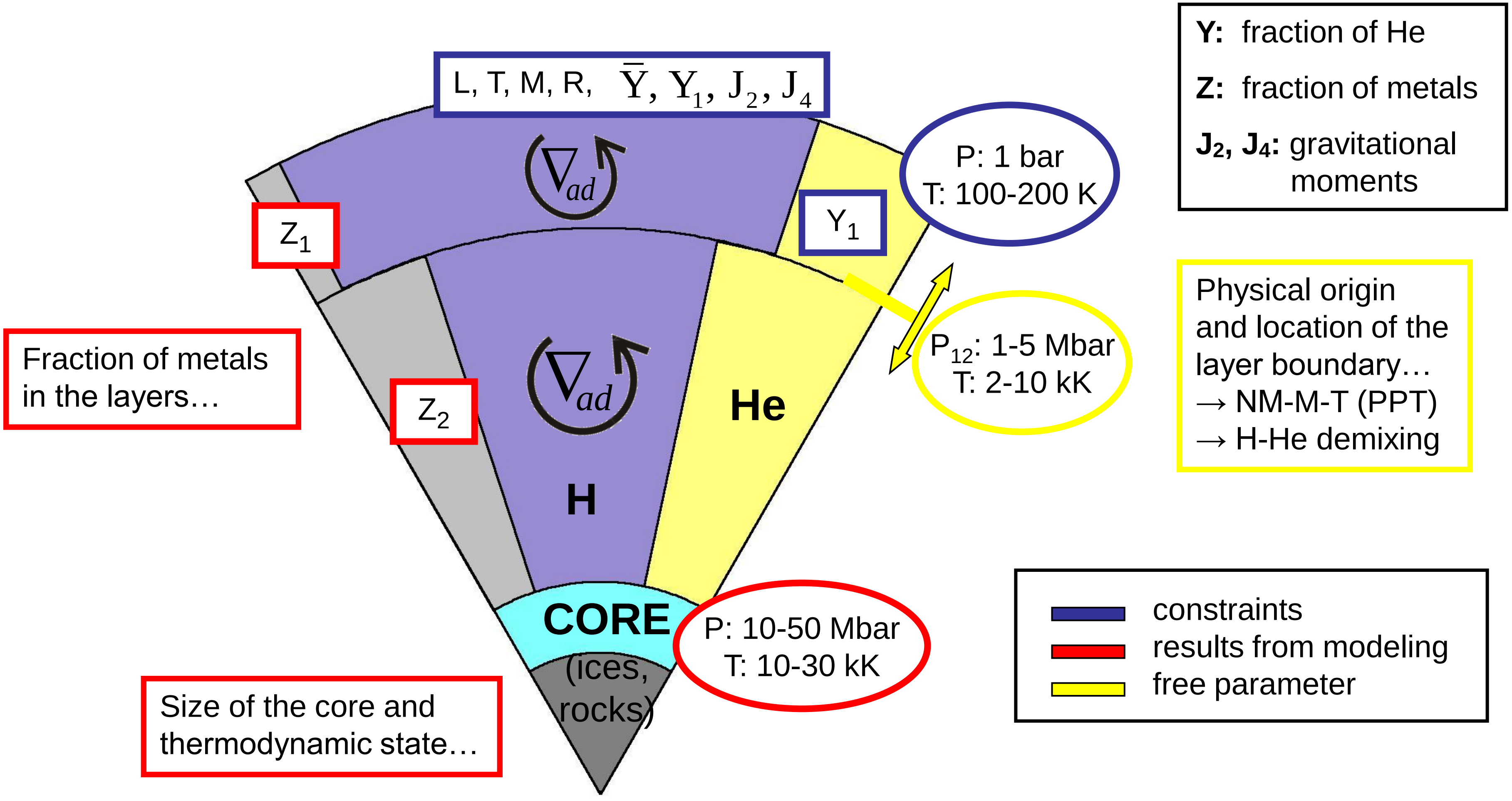
Computing Center of the University of Rostock

Contents

Interior of solar giant planets:

Matter under extreme conditions!



- **Three-layer interior models are uniquely defined by the observables, except P_{12}**
- **Input: EOS data for warm dense H and He, metals (C-N-O), and the isothermal rocky core**
- **Predictions of chemical models and new ab initio simulation data**

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:

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

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).
Planetary interior program: N. Nettelmann (2009).
Mass distribution along isentropes according to the EOS data used for the relevant materials (H, He, C-N-O, rocks).

EOS and phase diagram of light elements at high pressures ?

Poorly known above 1 Mbar but important for interior models: EOS data, isentropes, origin and location of layer boundaries, conductivity and magnetic field structure, opacity etc

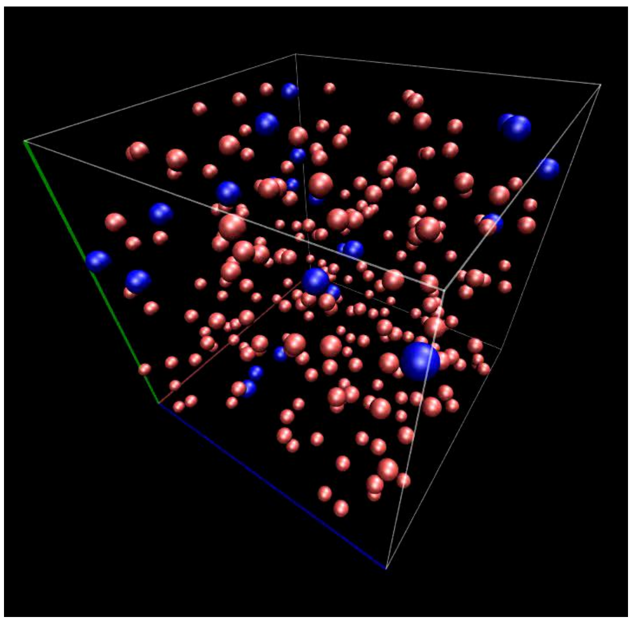
Apply ab initio methods and novel high-pressure experiments e.g. at NIF, Z for conditions deep in planetary interiors, i.e. for
→ 1-100 Mbar and 10^3-10^5 K
→ light elements, their hydrides and mixtures
(H, He, H-He, H2O, CH4, NH3 ...)

↓

1. Metallization in H: 1st-order phase transition (PPT)?
2. Is there a H-He demixing region as proposed earlier?
3. Superionic phases at high pressures (H2O)?

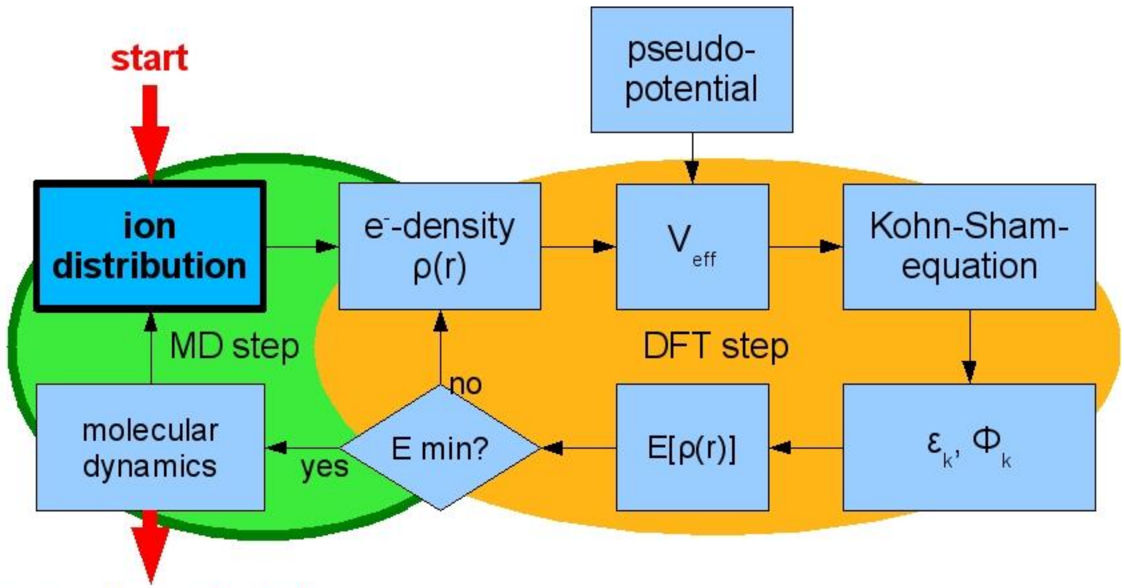
Ab initio MD (AIMD) simulations for WDM

Born-Oppenheimer approximation: combination of (quantum) DFT and (classical) MD
WDM: 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



thermodynamic data
pair correlation functions
electrical conductivity
diffusion coefficients
high-pressure phase diagram

GP size ~ 10^{8} m

Some details of the AIMD simulations

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

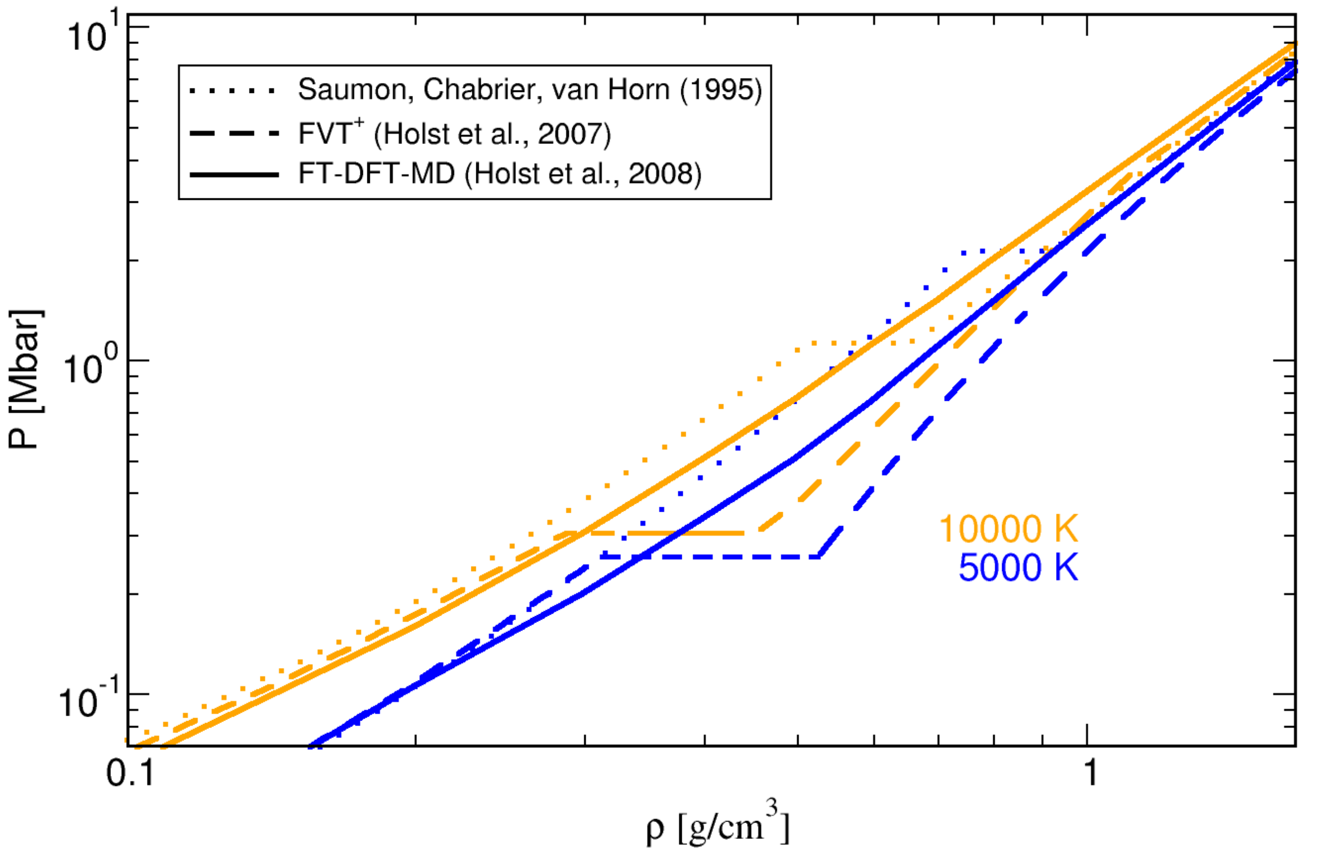
- Plane wave basis set: energy cut-off at about 1 keV
- **Exchange-correlation functional: GGA [1]**
- **PAW pseudopotentials [2]: 1 e/H, 2 e/He, 6(8) e/O**
- Ion temperature control by Nosé thermostat [3]
- Evaluation of electronic states in BZ at (few) special points (EOS)
- Higher k-point sets are needed for σ
- **N≤1024 electrons in a box of volume *V* at temperature *T***
- **Simulation time: up to 20 ps with several 1000 time steps**
- **Check convergence with respect to E_{cut}, k-points, N, Δt …**
- Parallel code runs on “Mercury” at Computing Center U Rostock
- CPU time at High Performance Computing Center North (HLRN)

[1] J.P. Perdew, K. Burke, M. Ernzerhof, PRL **77**, 3865 (1996)
[2] P.E. Blöchl, PRB **50**, 17953 (1994), G. Kresse, J. Joubert, PRB **59**, 1758 (1999)
[3] S. Nosé, J. Chem. Phys. **81**, 511 (1984)

Example: EOS of warm dense H2

AIMD compared with chemical models – no PPT above 5000 K

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

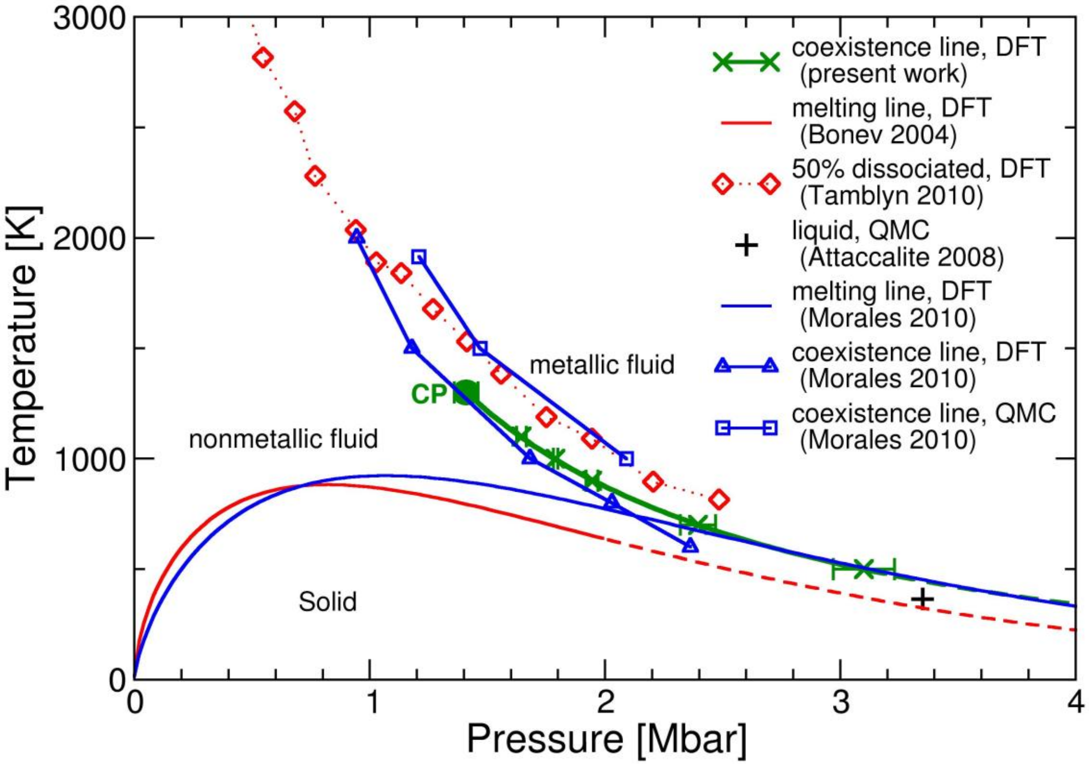


First exp. signature of a PPT ? See V.E. Fortov et al., PRL **99**, 185001 (2007)

AIMD EOS data on H2/D2: see also e.g. L. Collins et al., PRE **52**, 6202 (1995),
S.A. Bonev et al., PRB **69**, 014101 (2004), F. Gygi and G. Galli, PRB **65**, 220102(R) (2002).
QMC method: K.T. Delaney et al., PRL **97**, 235702 (2006).

New hydrogen phase diagram at high pressure:

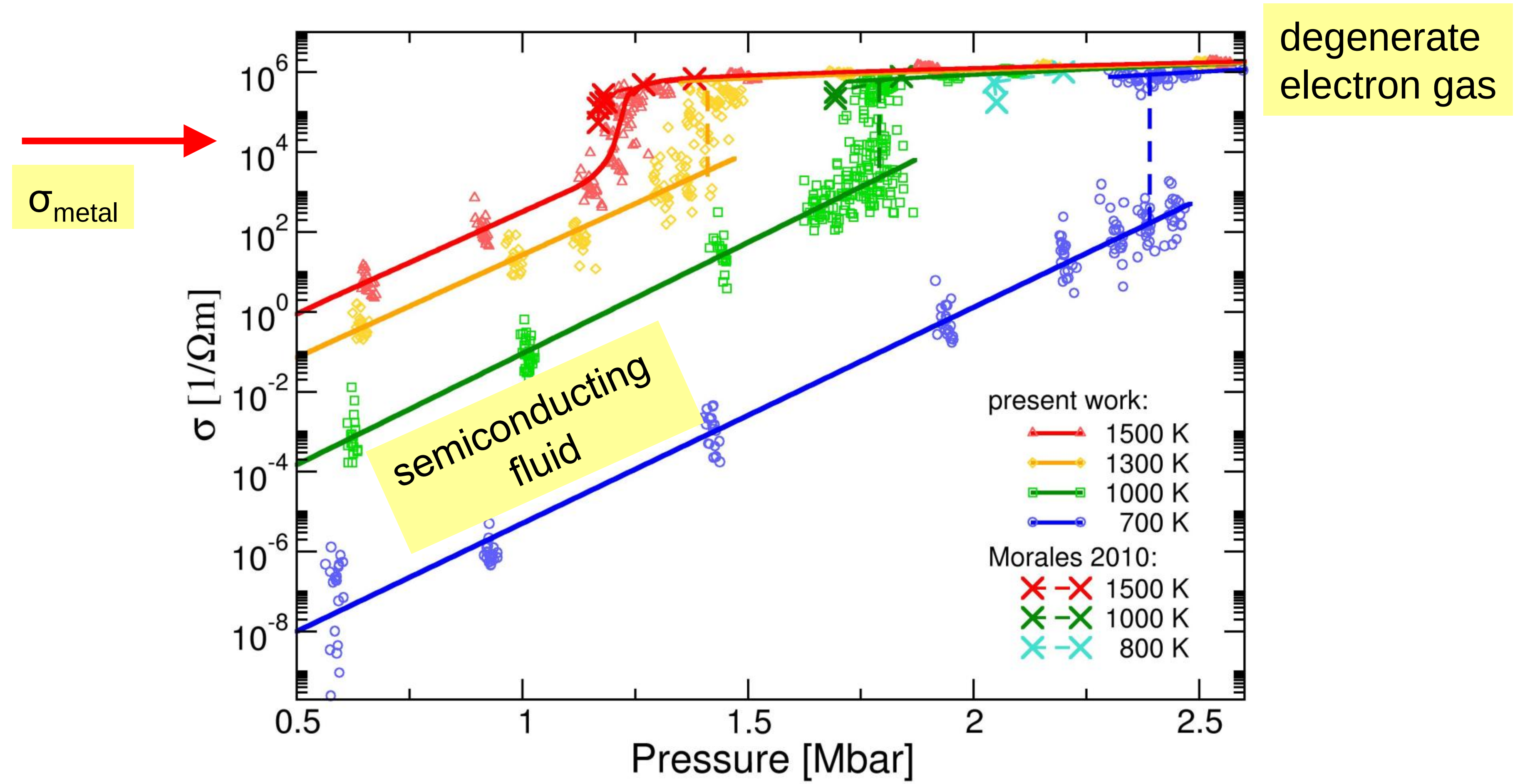
1st-order liquid-liquid phase transition (PPT)



1st-order liquid-liquid phase transition has been predicted below 2000 K:
M.A. Morales et al., PNAS **107**, 12799 (2010): AIMD and QMC;
see also I. Tamblyn, S.A. Bonev, PRL **104**, 065702 (2010)
We confirm these results with special emphasis to the NM-M-T:
critical point located below 1500 K at 0.82 g/ccm, 1.4 Mbar
W. Lorenzen, B. Holst, R. Redmer PRB **82**, 195107 (2010)

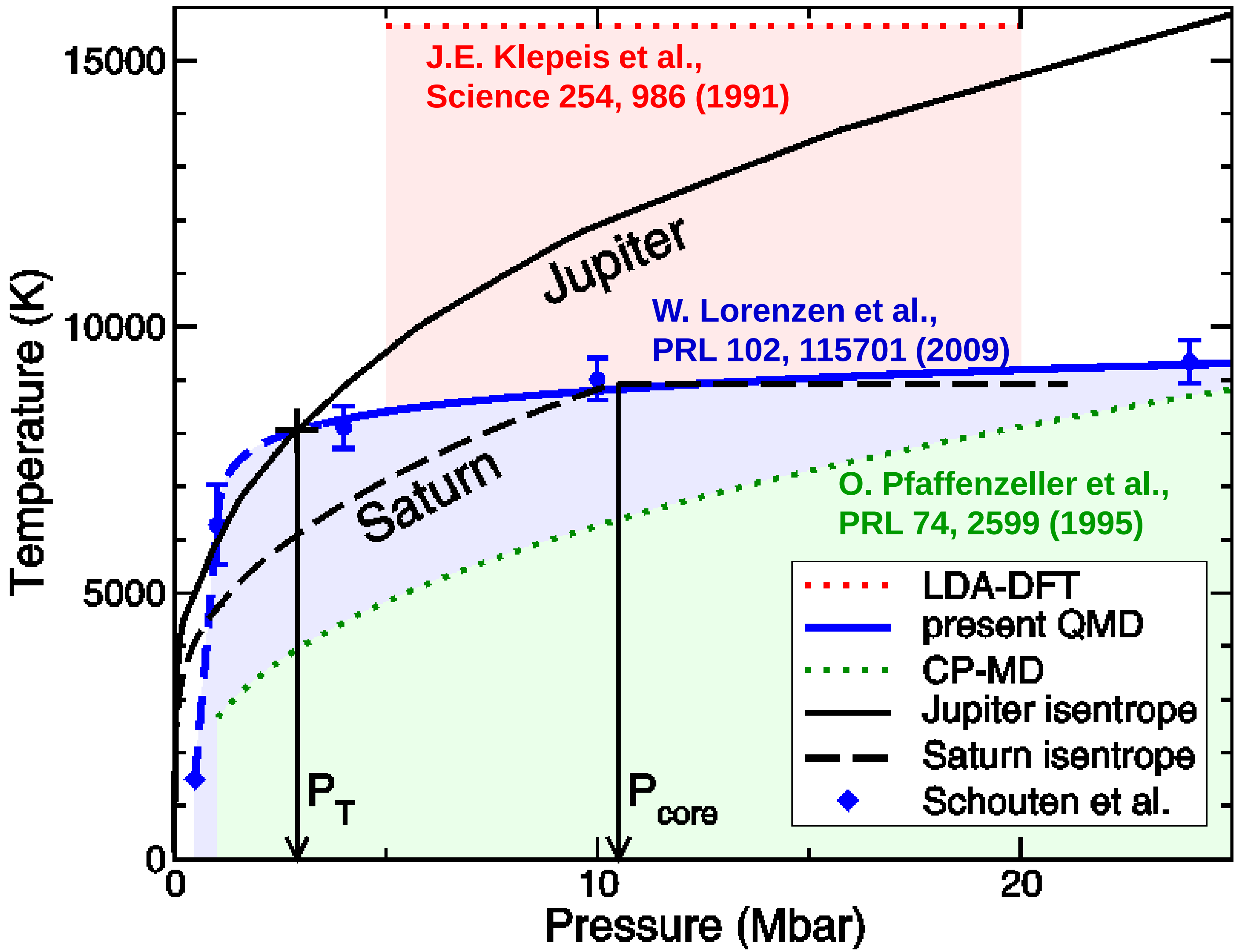
Electrical conductivity in liquid hydrogen

NM-M-T drives the 1st-order phase transition
Continuous above critical point - along the Jupiter isentrope



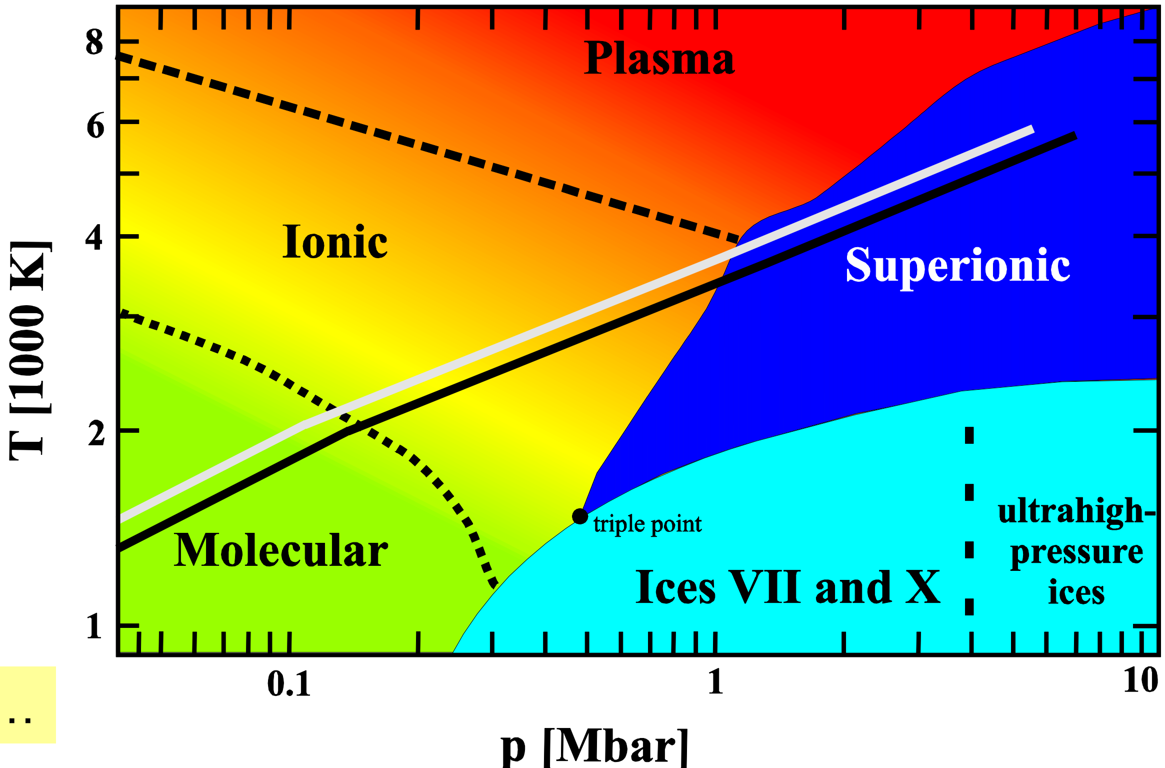
W. Lorenzen, B. Holst, R. Redmer, PRB **82**, 195107 (2010)

Consequences of the NM-M-T for GPs:
Demixing of H-He - relevant for Jupiter (?) and Saturn (!)



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

Water phase diagram at ultra-high pressures



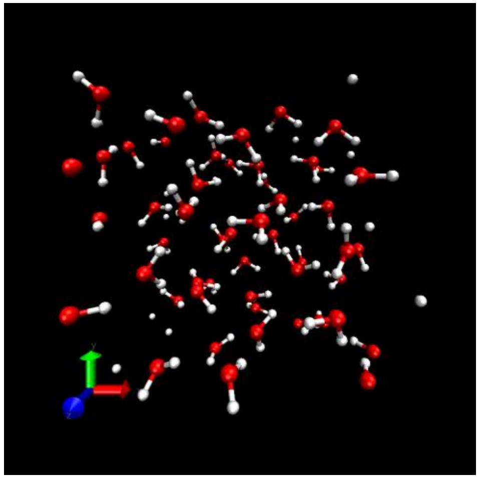
Relevant for the interiors of Neptune (black) and Uranus (white)

Representative of metals in J & S (Z)

Core material?

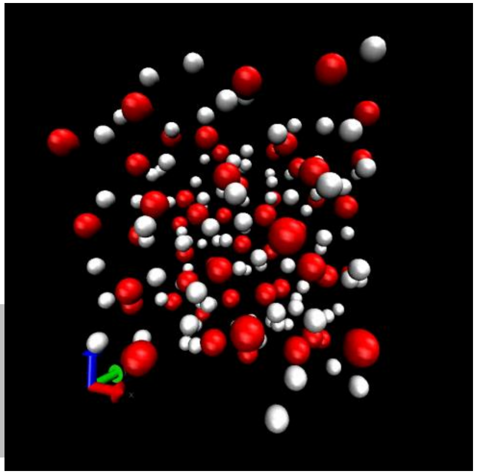
Normal ice…

… 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)

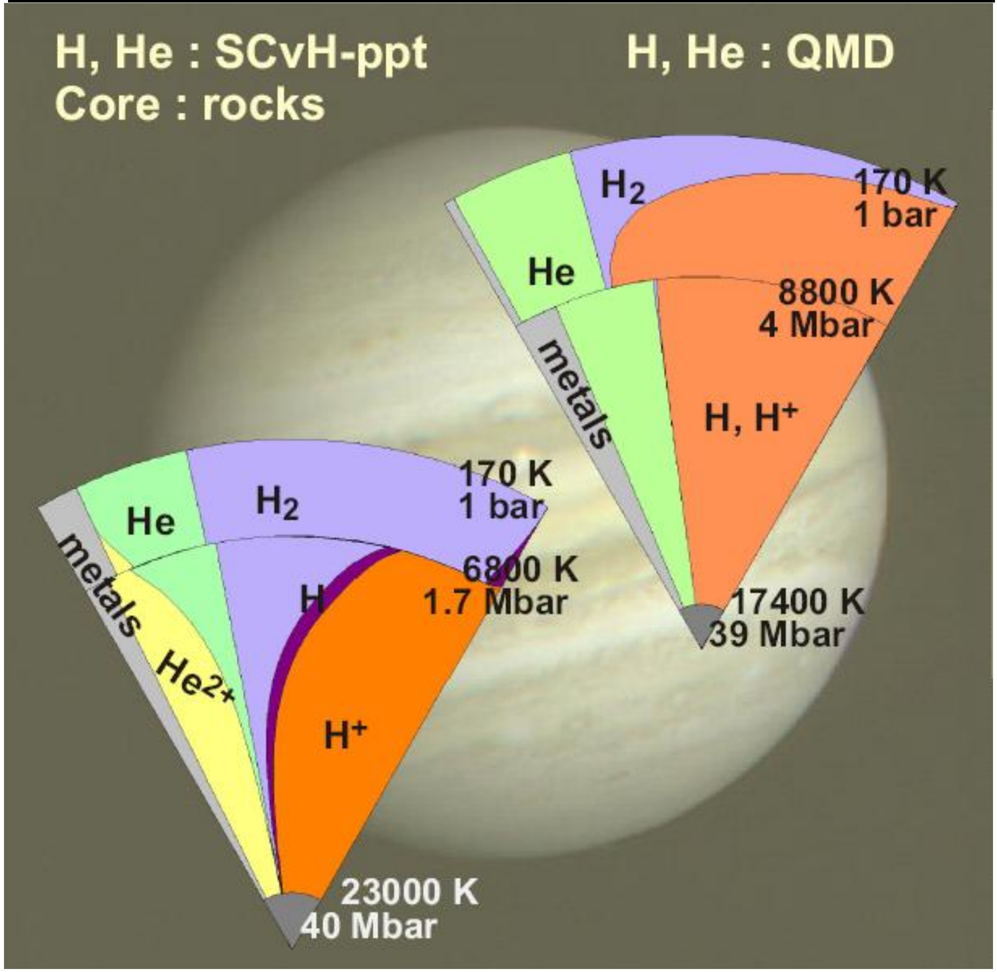


Interior of Jupiter with LM-REOS

N. Nettelmann et al., ApJ **683,** 1217 (2008)

Alternative two-layer Jupiter model by B. Militzer et al., ApJ 688, L45 (2008)

Abundances of chemical species for 2 models using different EOS



Standard SCvH-EOS within an advanced chemical model:

- **well separated *'molecular'* and *'metallic'* layer**
- **P_{12} around 1.7 Mbar**
- **metals almost uniformly distributed**
- **reason for the layer boundary:**

plasma phase transition in H?

Ab initio LM-REOS based on a strict physical picture covers 97% of Jupiter mass:

- **strong discontinuity in metals**
- **earlier onset of 'ionization'**
- **also small core with $M_c = (1\text{-}6)\ M_E$**
- **P_{12} around 4 Mbar**
- **reason for the layer boundary:**

H-He phase separation?

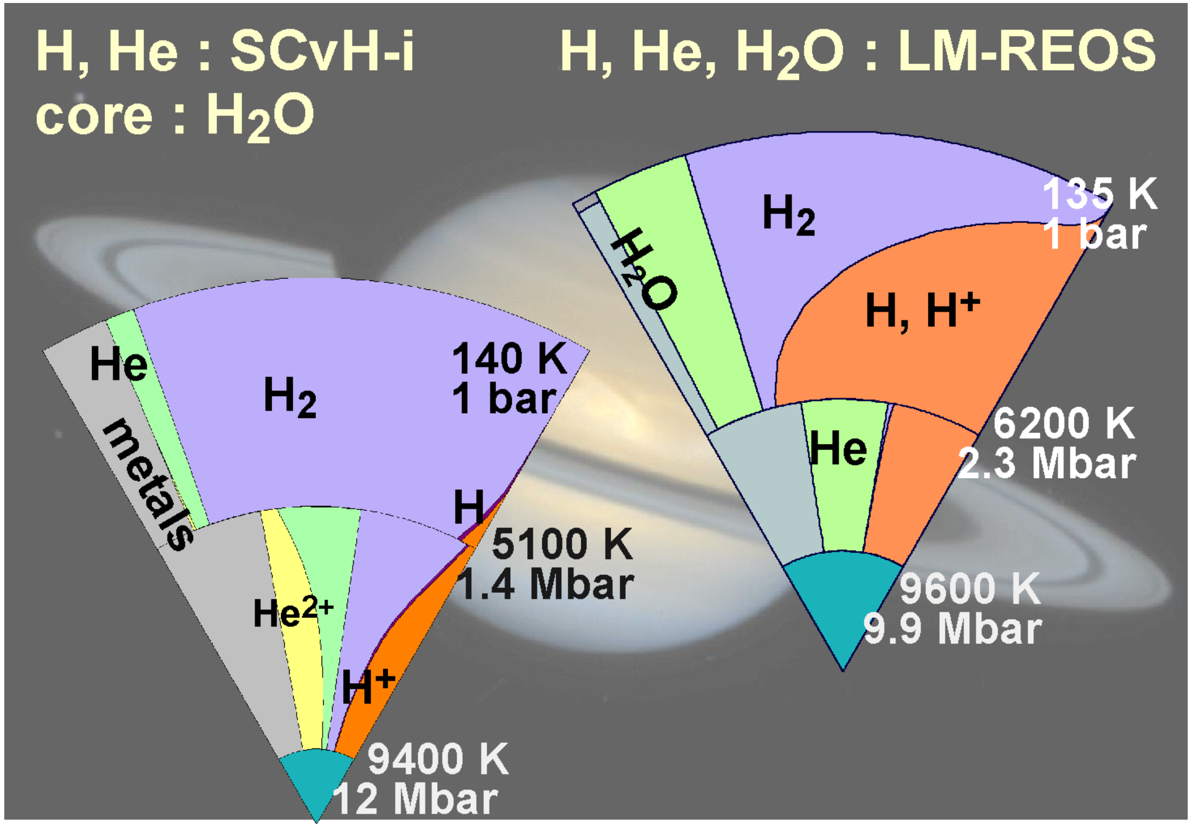
as proposed earlier by Stevenson, Salpeter, Fortney, Hubbard …

H-He EOS of D. Saumon, G. Chabrier, H.M. Van Horn, ApJS **99**, 713 (1995)

H_2O EOS from Sesame tables (1972)

Interior of Saturn with LM-REOS

J.J. Fortney, N. Nettelmann, Space Sci. Rev. **152**, 423 (2009)

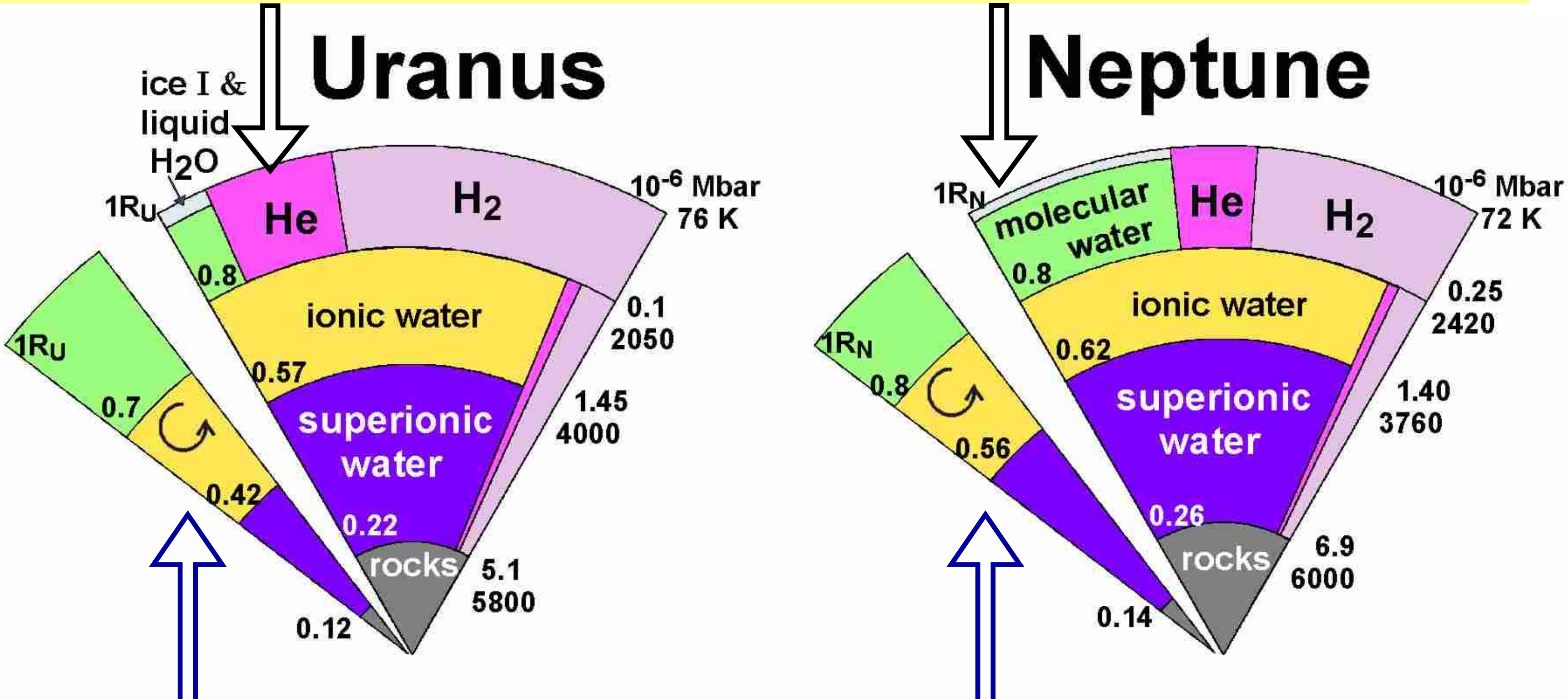


Saturn`s interor in comparison with that of Jupiter:

- **lower temperatures → larger molecular outer envelope**
- **strong candidate for H-He demixing → higher luminosity and age?**
- **higher fraction of metals (up to 40%)**
- **greater core → superionic water in the core?**

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 (LM-REOS):
J.J. Fortney, N. Nettelmann, Space Sci. Rev. **152**, 423 (2009),
R. Redmer et al., Icarus (in print)



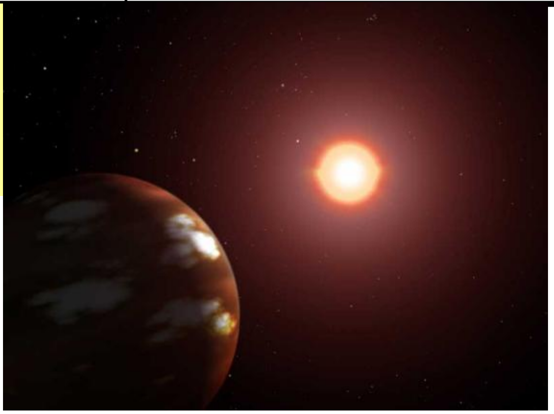
Independent **dynamo models** reproduce the non-dipolar and non-axisymmetric magnetic fields of N and U by assuming a rather thin conducting shell (yellow) and a central region (magenta) that is stable against convection but of similar conductivity (here: superionic!):
S. Stanley and J. Bloxham, Nature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

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 μm)
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)

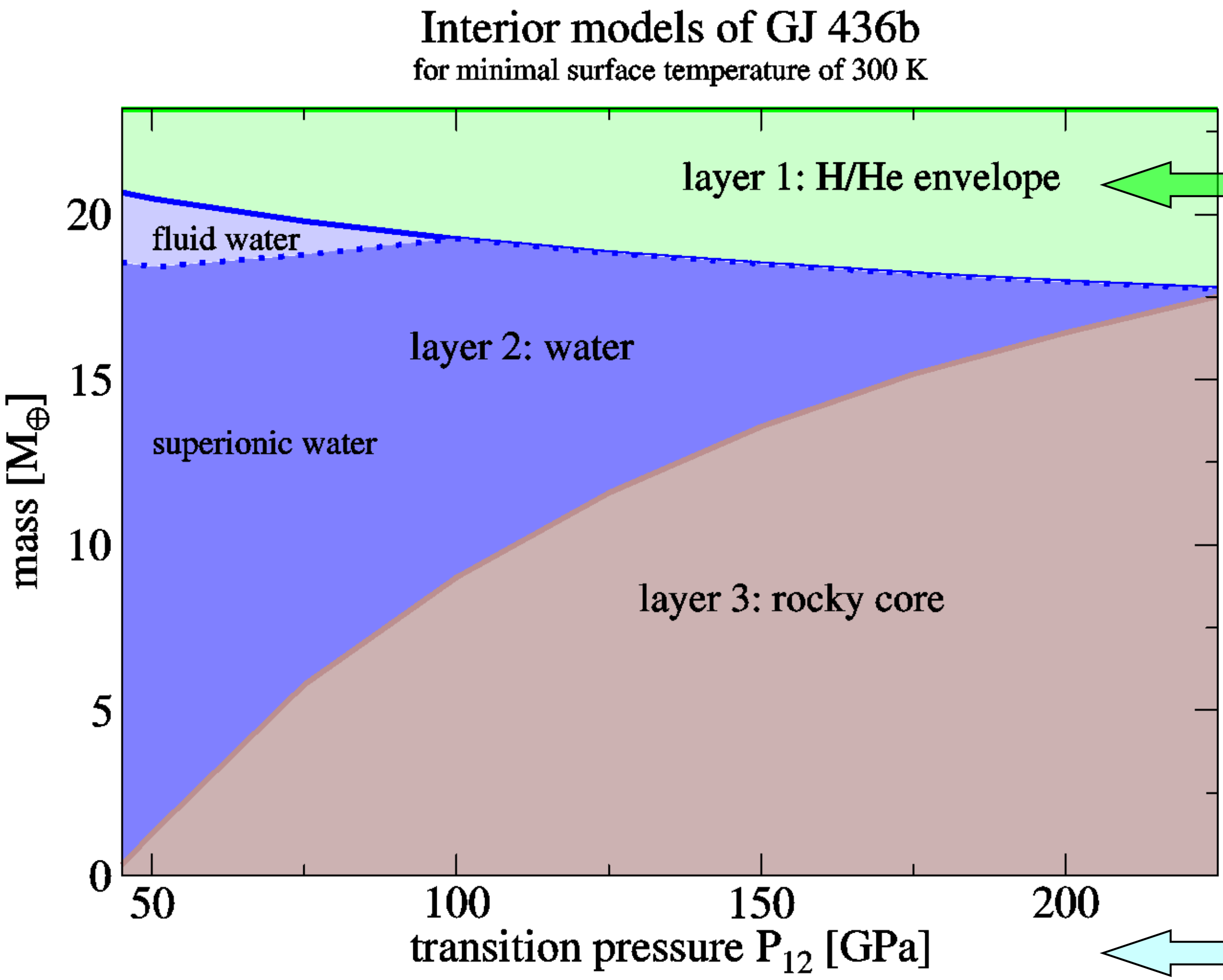


Observational parameters:
M. Gillon et al., A&A **471**, L51 (2007),
B.-O. Demory et al., A&A **475**, 1125 (2007)

GJ 436b: Water or rocky planet?

What information can we derive from a known M(R) relation within a three-layer model?

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



Isothermal H_2-He mixture (27.5%):
T(1 bar)=300 K
Z_1=2%
high metallicity

Results of modelling **strongly** depend on surface temperature! Coupling of planetary atmosphere to stellar radiation important!

Limiting cases by varying P_{12} yield **water or rocky planet.** Is the water **superionic ?**

Summary

- Paramount importance for modeling GPs:
  → accurate high-pressure EOS data: LM-REOS
  → identify the phase diagram and coexistence lines
  → compare with shock compression experiments

- Develop and evaluate interior models:
  → solar GPs
  → determine material data (σ, η, c_s …) along the isentropes
  → additional constraint: *U. Kramm, Love number k2*
  → extrasolar GPs: *N. Nettelmann, GJ 1214b*

- Young transiting planets: *R. Neuhäuser et al., YETI*
- Planetary atmospheres: *P. Hauschildt et al., J.J. Fortney*
- Planetary magnetism: *DFG-SPP 1488*