40th Max-Born-Symposium, Wroclaw, 09-12 Oct 2019

Matter Under Planetary Interior Conditions

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Picture by courtesy of DLR Berlin

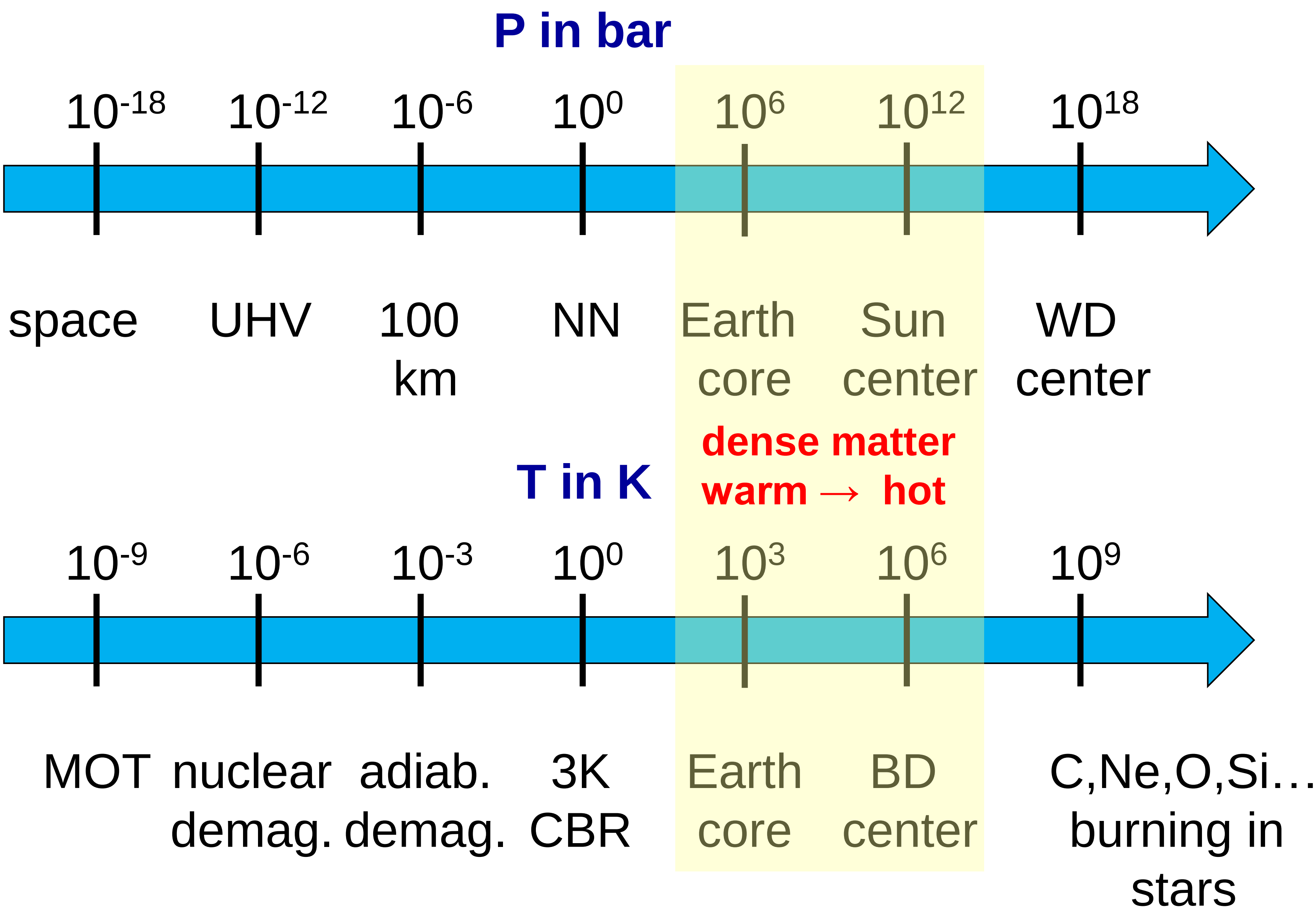
FOR 2440

Exoplanet Diversity DFG SPP-1992

SFB 652

DFG Deutsche Forschungsgemeinschaft

Extreme conditions



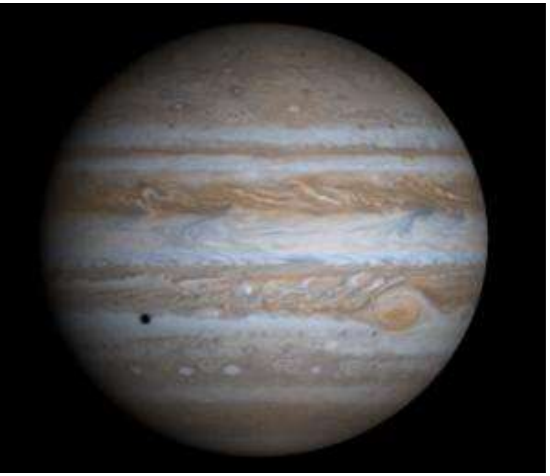
Astrophysical objects

Extreme states of matter (warm to hot, dense)

Planets $M<13M_J$

Brown Dwarfs $13M_J<M<75M_J$

Stars $M>75M_J$



Solar (8) and extrasolar planets

… in the Orion Nebula seen in the IR spectrum

Proxima Centauri M Dwarf

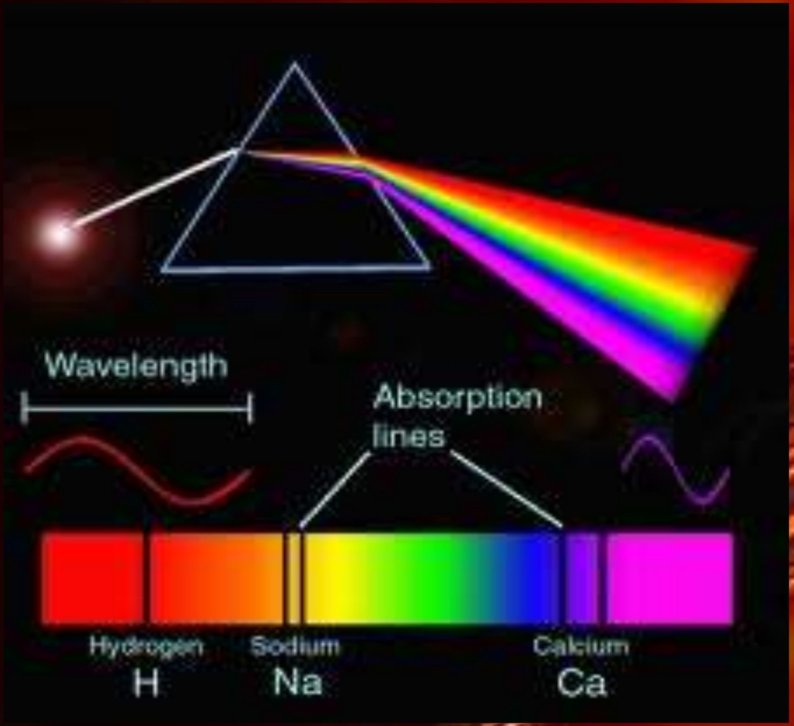
Interior (e.g. Jupiter):
$< 2x10^4$ K & 40 Mbar
warm dense matter

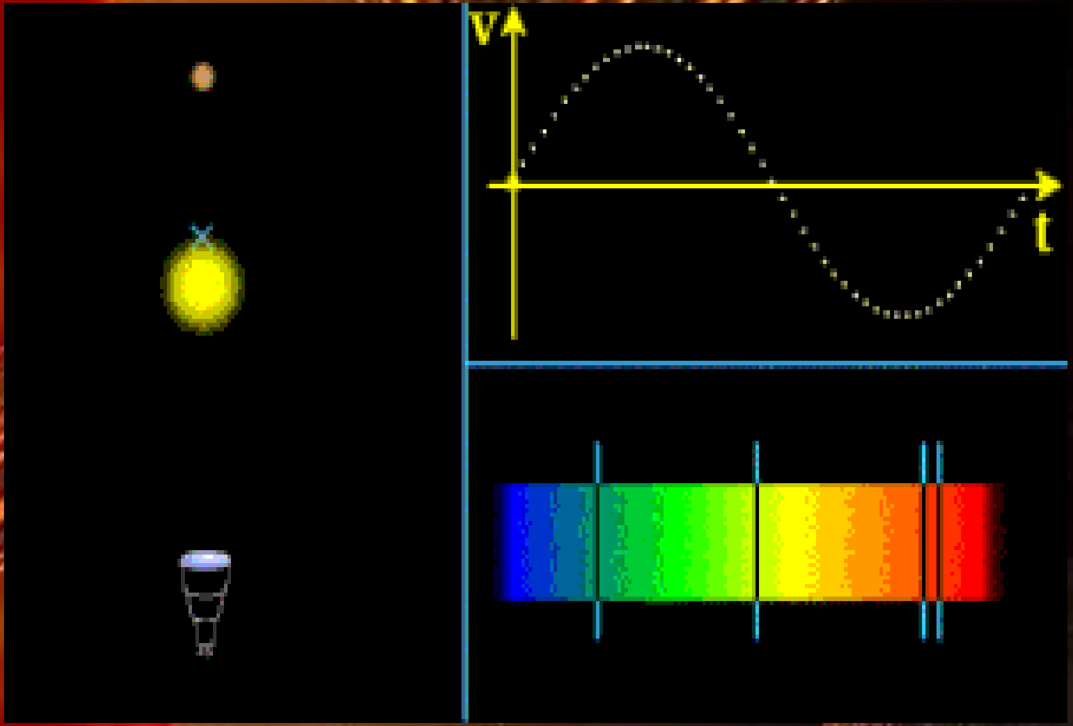
Interior (e.g. Gliese 229B):
$< 10^6$ K & 100 Gbar
degenerate dense matter

Interior of stars (e.g. Sun):
$< 15x10^6$ K & 250 Gbar
hot dense matter

Radial velocity measurement

Doppler effect





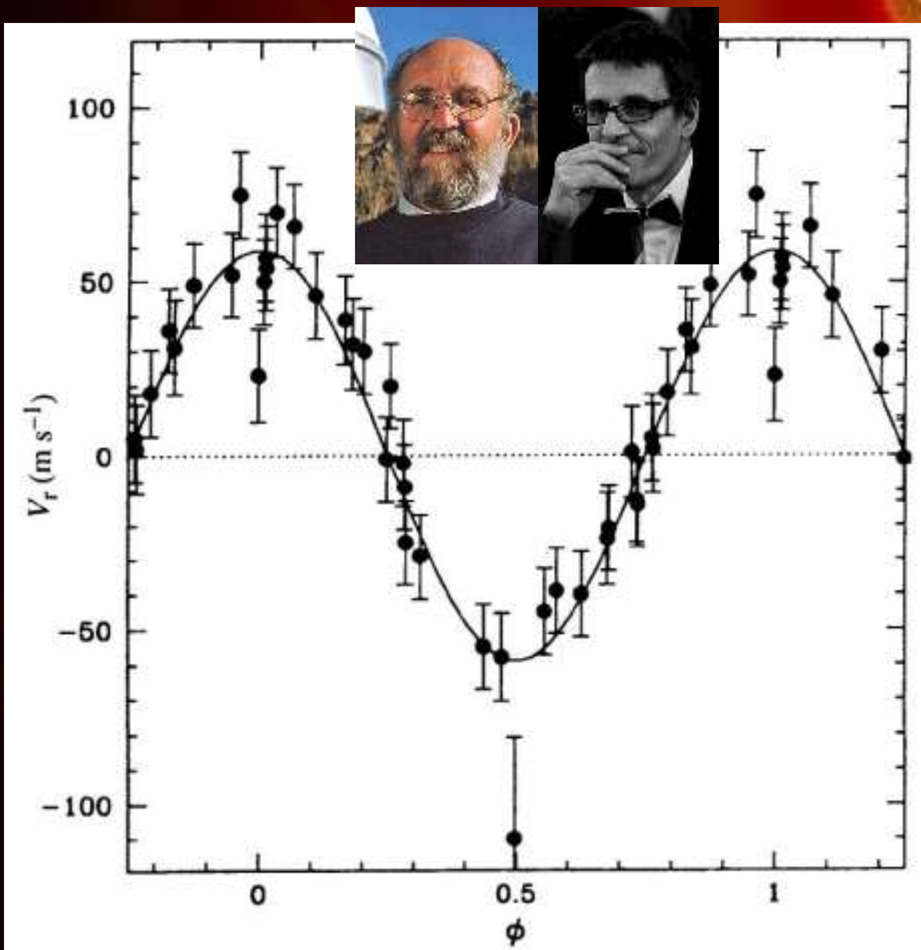
Effect in Solar System:

Jupiter	5.2 AU	12,7 m/s	11.856 a
Earth	1 AU	9 cm/s	1a

1st exoplanet: 51 Pegasi b (1995)

M. Mayor & D. Queloz, Nature **378**, 355 (1995)

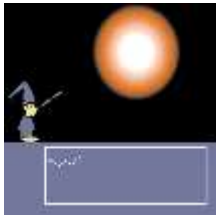
G5V star: 50 Ly away (Pegasus), 1.06 M_{sun}, 5565 K



- K = 55 m/s
- P = 4.23 days
- e = 0.00
- M = 0.45 M_{Jup}/sin(i)
- sine R-V curve

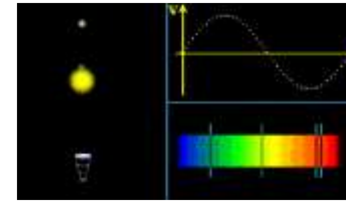
⇨ circular orbit

Nobel Prize 2019

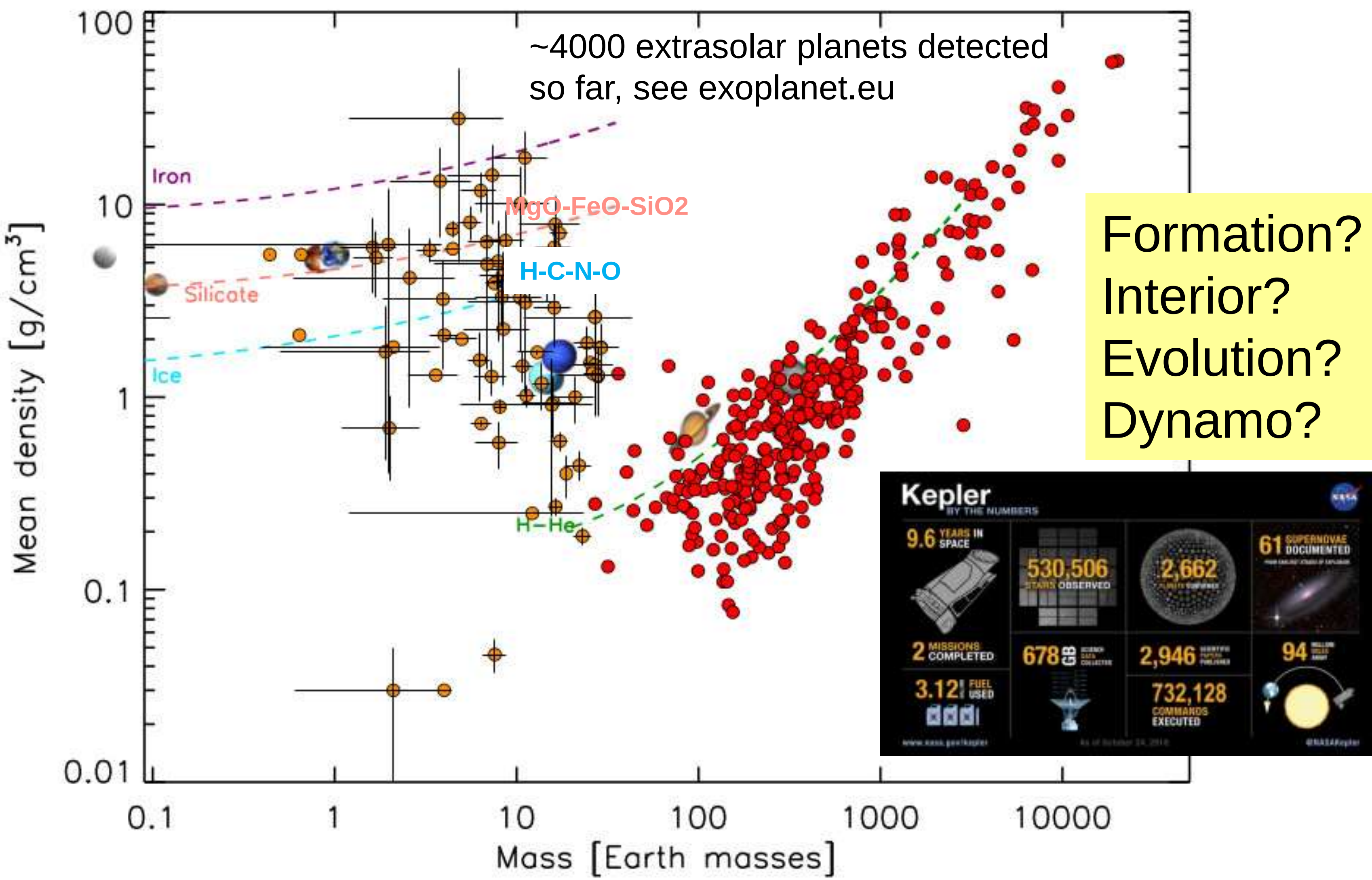


Extrasolar transiting planets

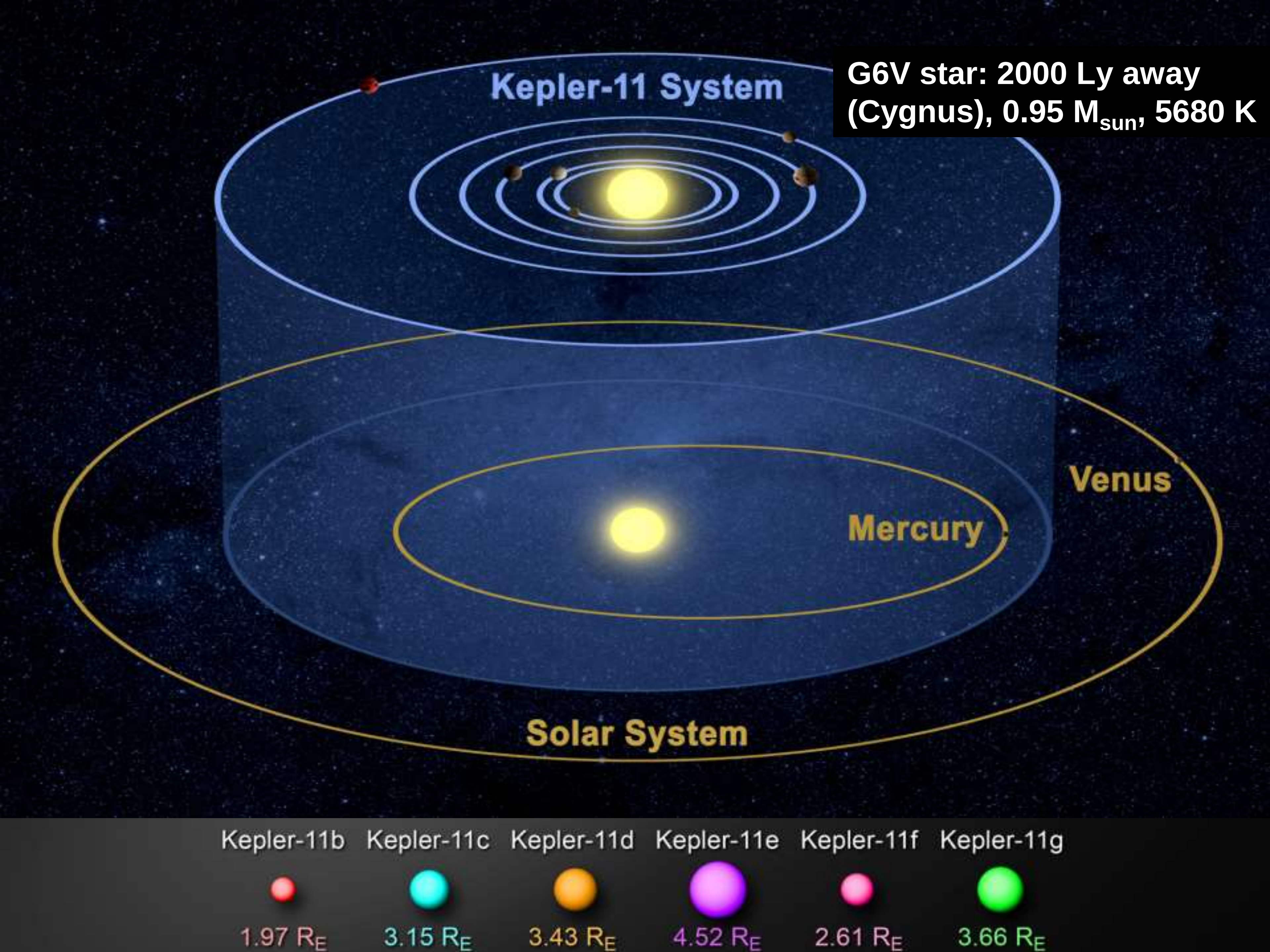
Mean density vs. mass



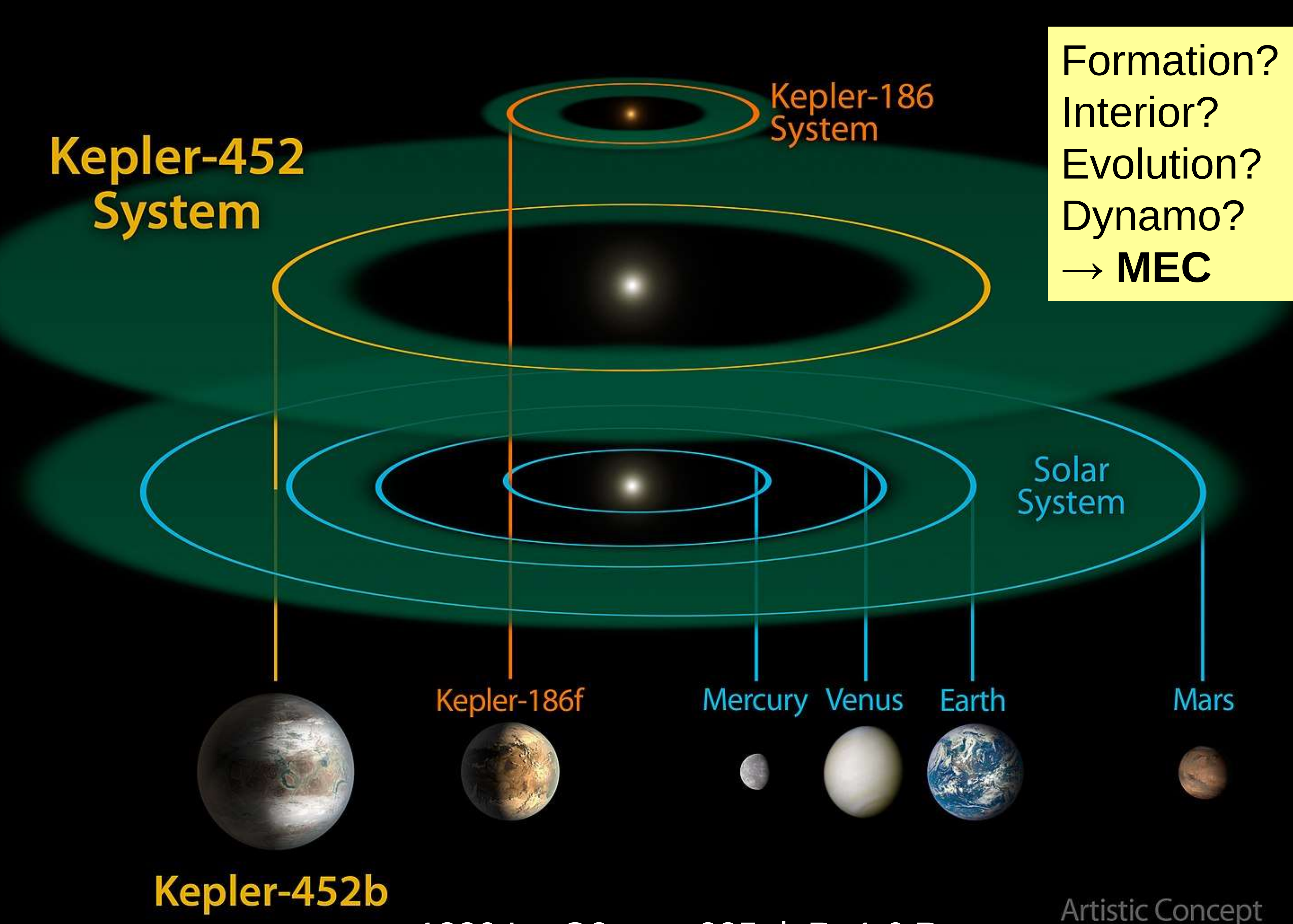
H. Rauer et al., Exp. Astron. **38**, 249 (2014)



Formation?
Interior?
Evolution?
Dynamo?


G6V star: 2000 Ly away
(Cygnus), 0.95 M_{sun}, 5680 K
Kepler-11 System
Venus
Mercury
Solar System
Kepler-11b
Kepler-11c
Kepler-11d
Kepler-11e
Kepler-11f
Kepler-11g
1.97 R_E
3.15 R_E
3.43 R_E
4.52 R_E
2.61 R_E
3.66 R_E

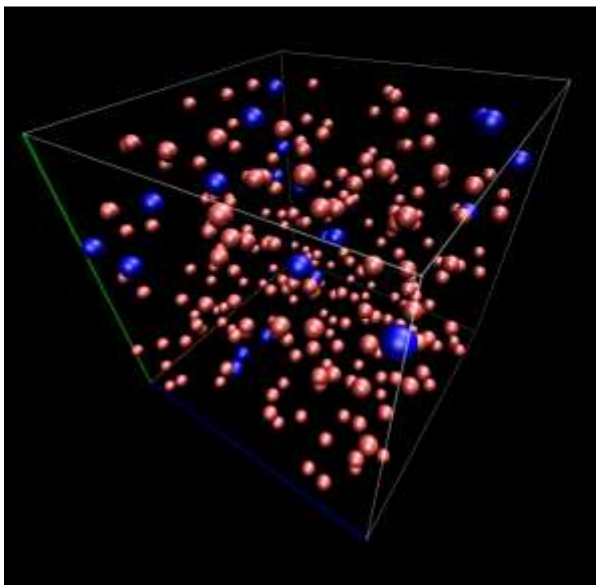
Formation?
Interior?
Evolution?
Dynamo?
→ **MEC**



1830 Ly, G2 star: 385 d, R=1.6 R_E

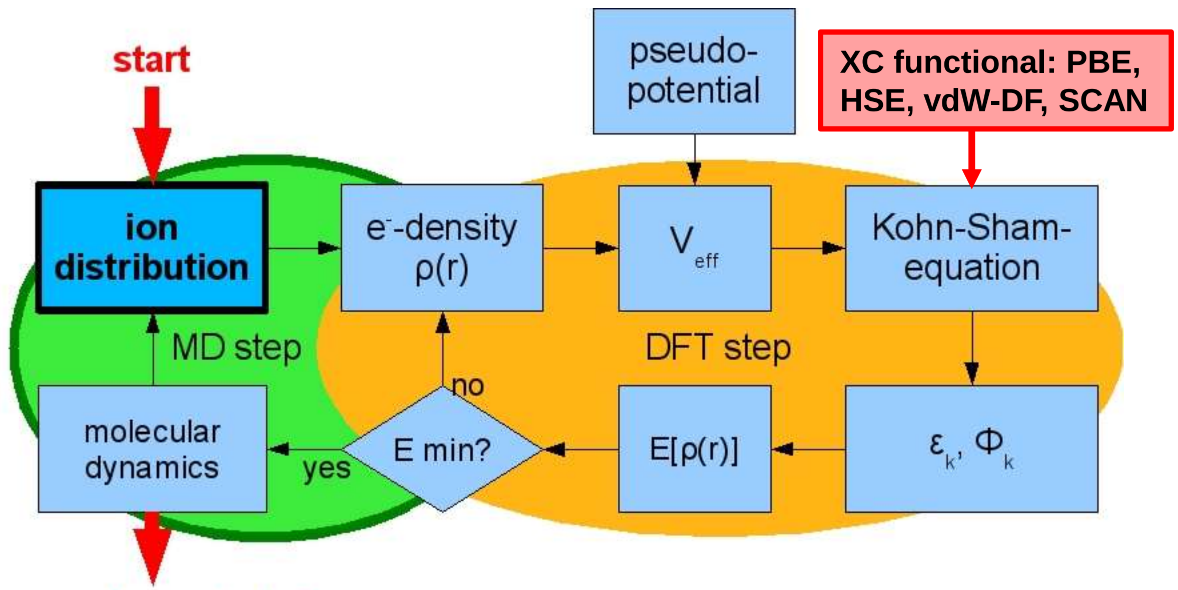
MEC: DFT-MD simulations

No effective pair potentials or assuming bound states – nuclei and electrons!
Born-Oppenheimer approximation: combination of (quantum) DFT (e) and (classical) MD (nuclei).
Warm Dense Matter: finite-temperature DFT-MD simulations based on
N.D. Mermin, Phys. Rev. **137,** A1441 (1965)
DFT codes: Vienna Ab-initio Simulation Package (VASP), Abinit, Quantum Espresso …
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)

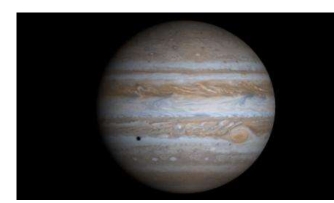


H-He (8.6%) @ 1 Mbar, 4000 K

box length ~ 10^{-9} m



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



GP size ~ 10^8 m

First Jupiter papers with David Blaschke

ISSN 1063-7796, Physics of Particles and Nuclei, 2008, Vol. 39, No. 7, pp. 1122–1127. © Pleiades Publishing, Ltd., 2008.

Warm Dense Matter in Giant Planets and Exoplanets¶

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Abstract—Interior models of giant planets are strongly connected with properties of hydrogen under extreme conditions. We present a detailed description of the modeling procedure and discuss results for Jupiter and Saturn.

PACS numbers: 96.15.De

DOI: 10.1134/S1063779608070277

The Astrophysical Journal, 683:1217–1228, 2008 August 20

AB INITIO EQUATION OF STATE DATA FOR HYDROGEN, HELIUM, AND WATER AND THE INTERNAL STRUCTURE OF JUPITER

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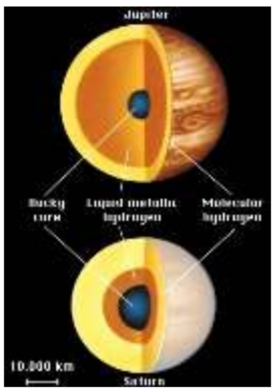
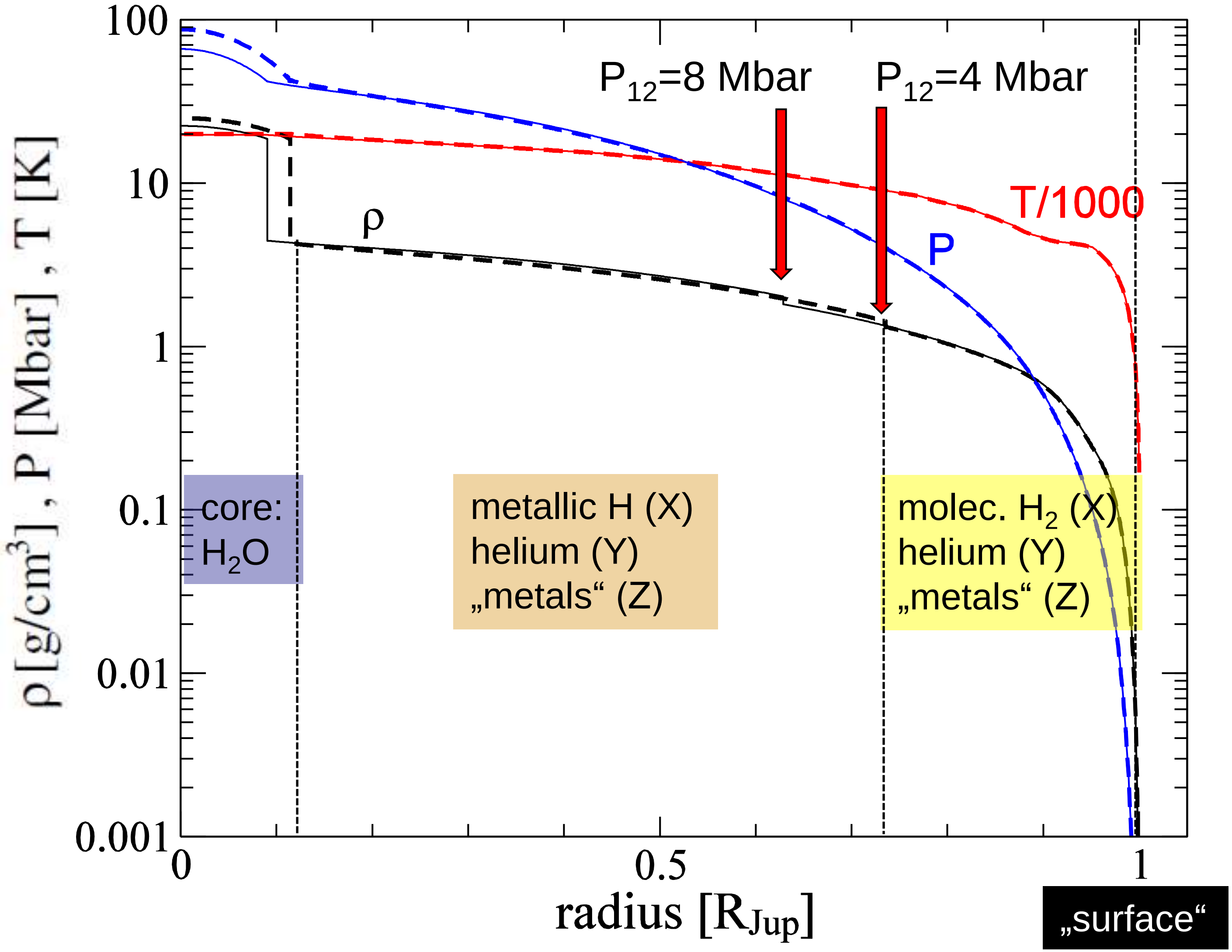
ABSTRACT

The equation of state of hydrogen, helium, and water affects interior structure models of giant planets significantly. We present a new equation of state data table, LM-REOS, generated by large-scale quantum molecular dynamics simulations for hydrogen, helium, and water in the warm dense matter regime, i.e., for megabar pressures and temperatures of several thousand kelvins, and by advanced chemical methods in the complementary regions. The influence of LM-REOS on the structure of Jupiter is investigated and compared with state-of-the-art results within a standard three-layer model consistent with astrophysical observations of Jupiter. Our new Jupiter models predict an important impact of mixing effects of helium in hydrogen with respect to an altered compressibility and immiscibility.

Jupiter`s interior with LM-REOS (H-He-H_2O)

Assuming a three-layer structure

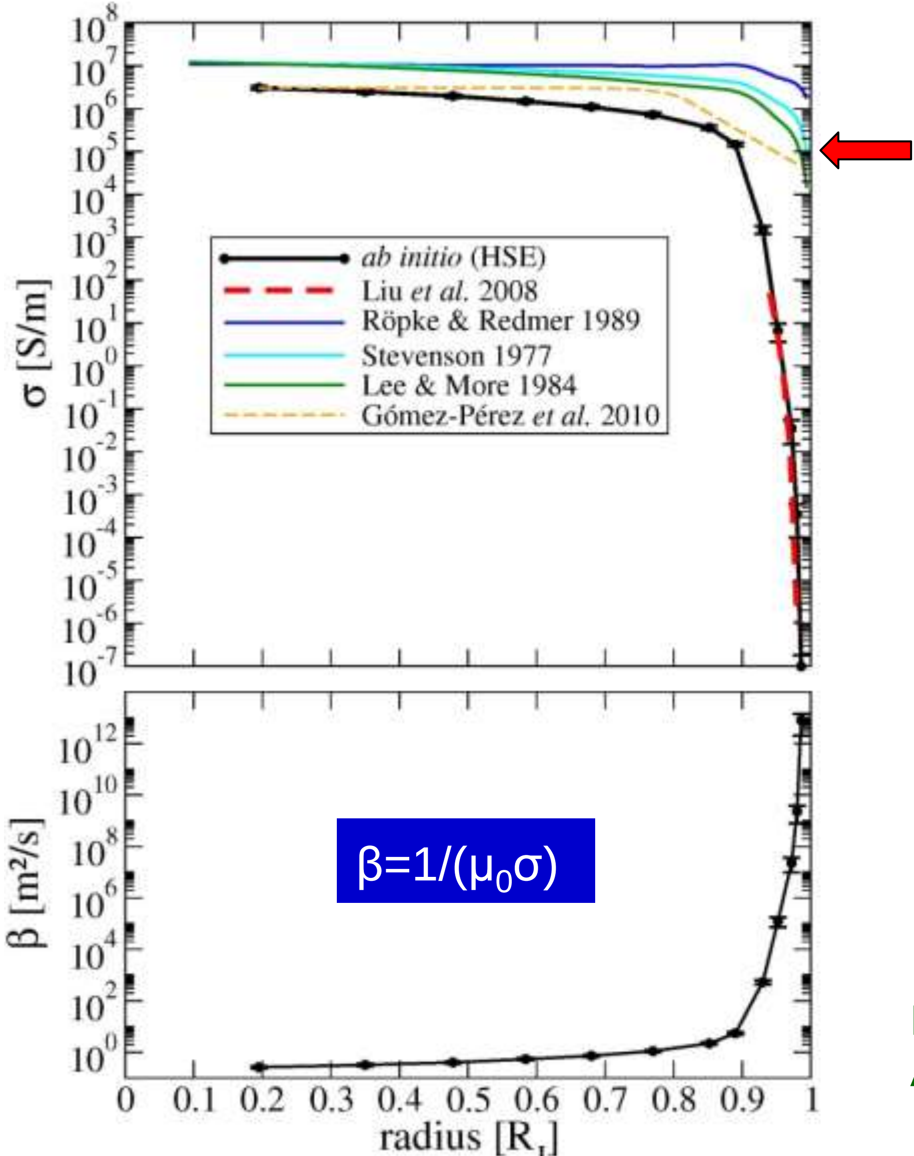




N. Nettelmann et al., ApJ **750**, 52 (2012), M. French et al., ApJS **202**, 5 (2012)

Electrical conductivity in Jupiter

M. French et al., ApJS **202**, 5 (2012): self-consistent EOS and material data from DFT-MD



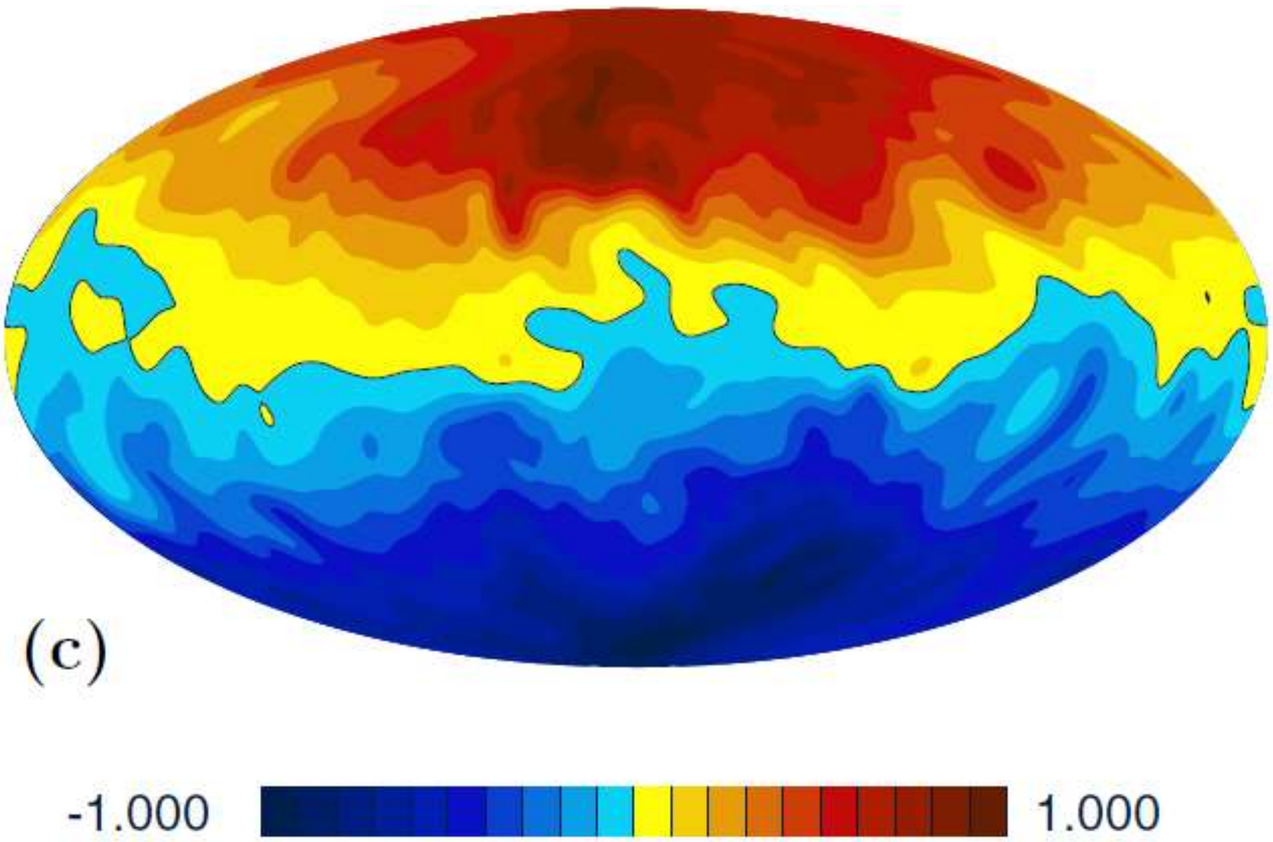
Continuous nonmetal-to-metal transition (Mott criterion)

Calculated as well:
specific heats
sound velocity
dynamic and kinematic viscosity
diffusion constants
thermal conductivity

For Brown Dwarf conditions:
A. Becker et al., Astron. J. **156**, 149 (2018)

Jupiter`s Magnetic Field

Dynamo simulations based on self-consistent EOS and material data from DFT-MD:
M. French et al., ApJS **202**, 5 (2012)



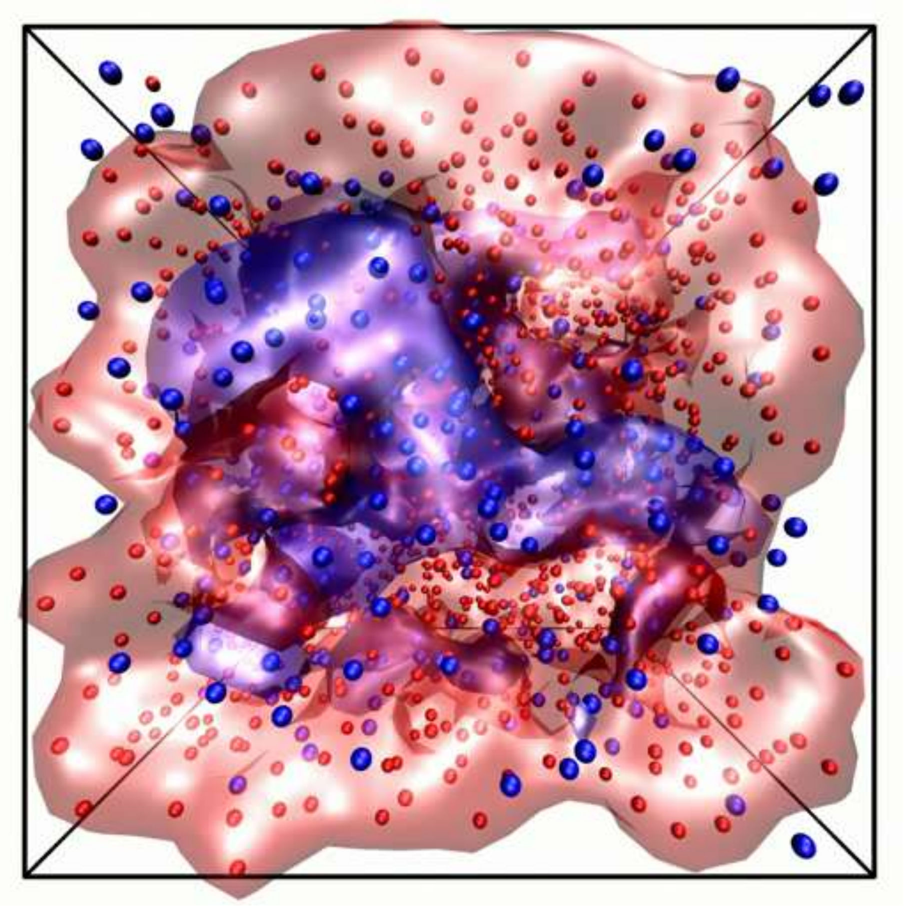
Snapshot of the radial component of the dipolar magnetic field of Jupiter from magneto-hydrodynamic simulations (dynamo).

C. Jones, Icarus **241**, 148 (2014)

Metalization in H drives H-He demixing

DFT-MD (PBE)

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

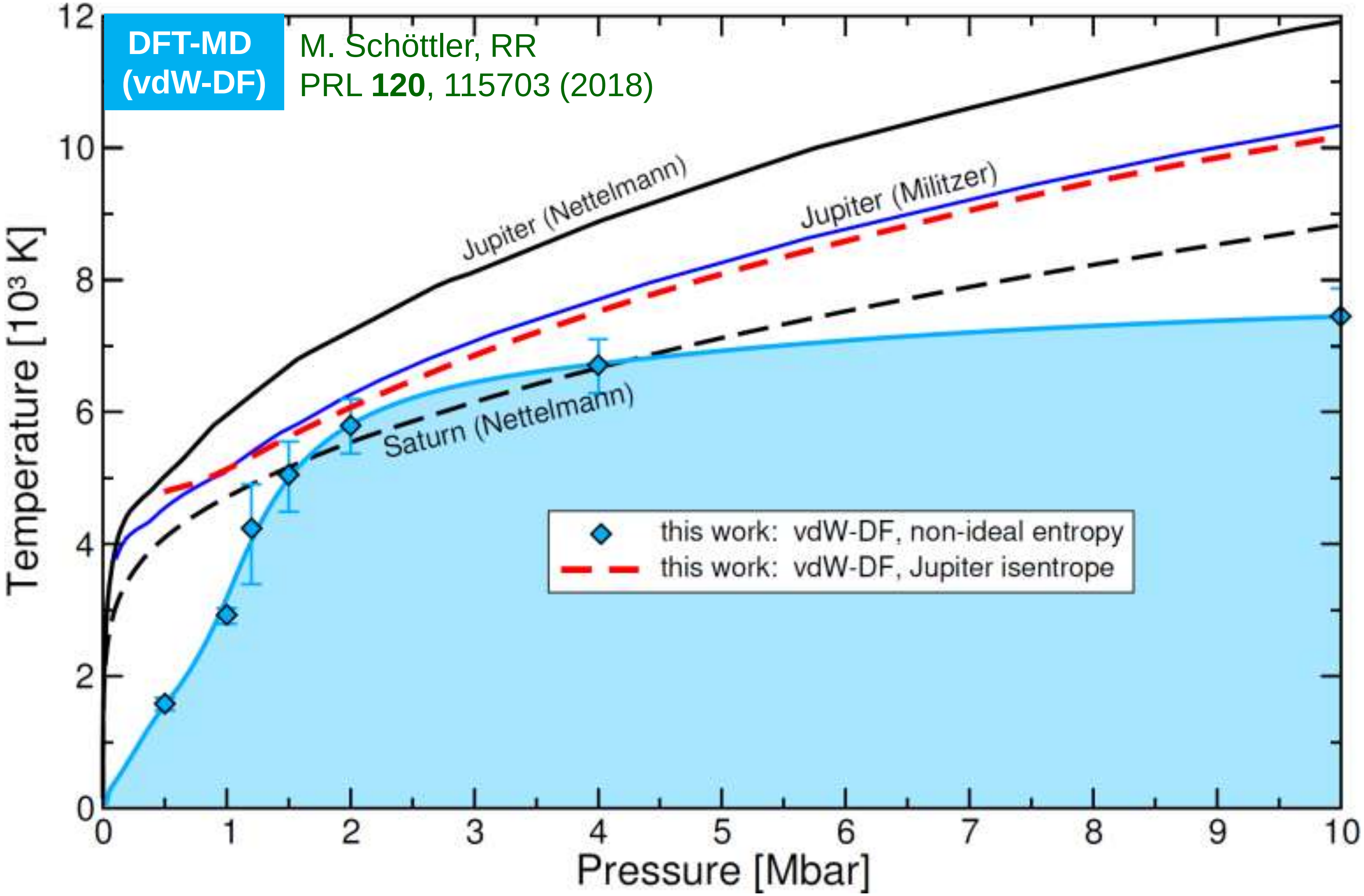


Simulation box with 1024 H atoms and 512 He atoms at ρ=4 g/cm^3, T=6000 K, P~20 Mbar. Shown are the ions (dots) and isosurfaces of the particle density: **He - blue**, **H - red**.

H-He demixing in Gas Giants

Isentropes for Jupiter and Saturn: He rain?

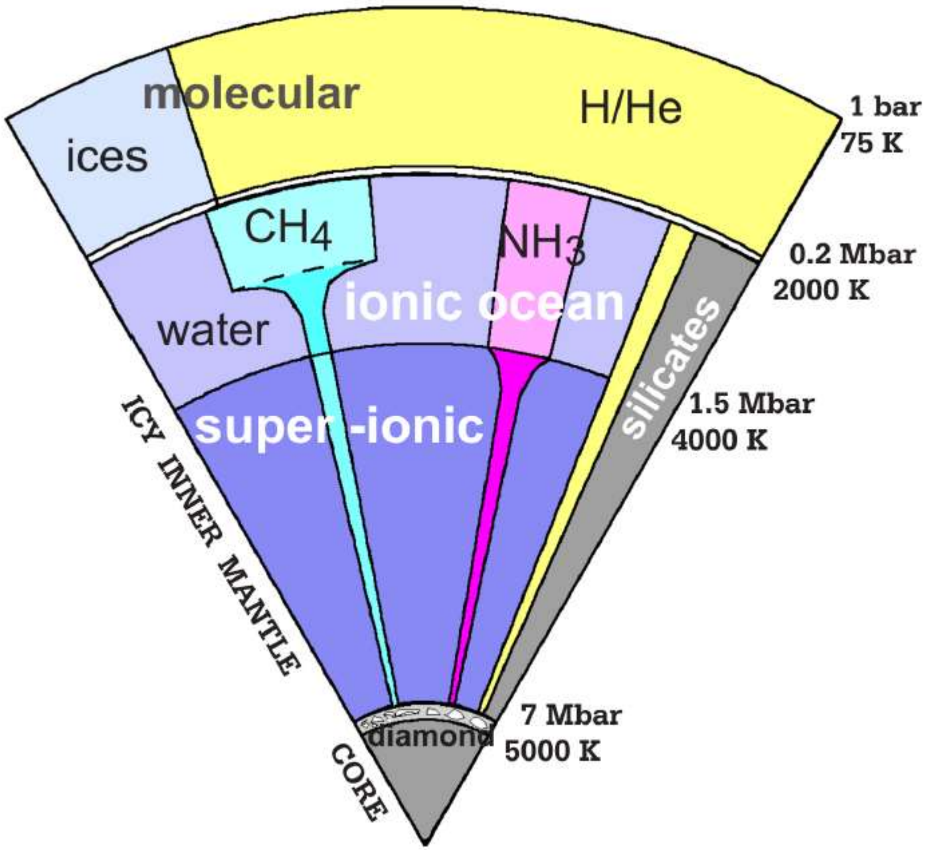
For Saturn, see R. Püstow et al., Icarus **267**, 323 (2016)



Jupiter: N. Nettelmann et al., ApJ **683**, 1217 (2008)
Jupiter: B. Militzer and W.B. Hubbard, ApJ **774**, 148 (2013)
Saturn: N. Nettelmann et al., Icarus **225**, 548 (2013)

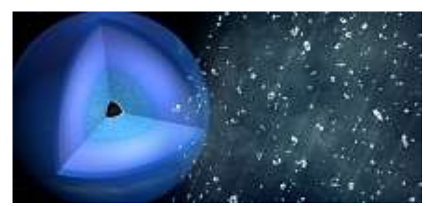
Interior of ice giants: H-C-N-O mixtures

Complex system!



U & N
Neptune-like exos
mini-Neptunes

Physical origin and location of layer boundaries:
→ ice phase diagram
→ superionic phase?
→ carbon rain?
→ solubility of rock material?
→ inhomogeneous zone from formation: thermal boundary layer?



D. Kraus et al., Nat. Astron. **1**, 606 **(**2017)

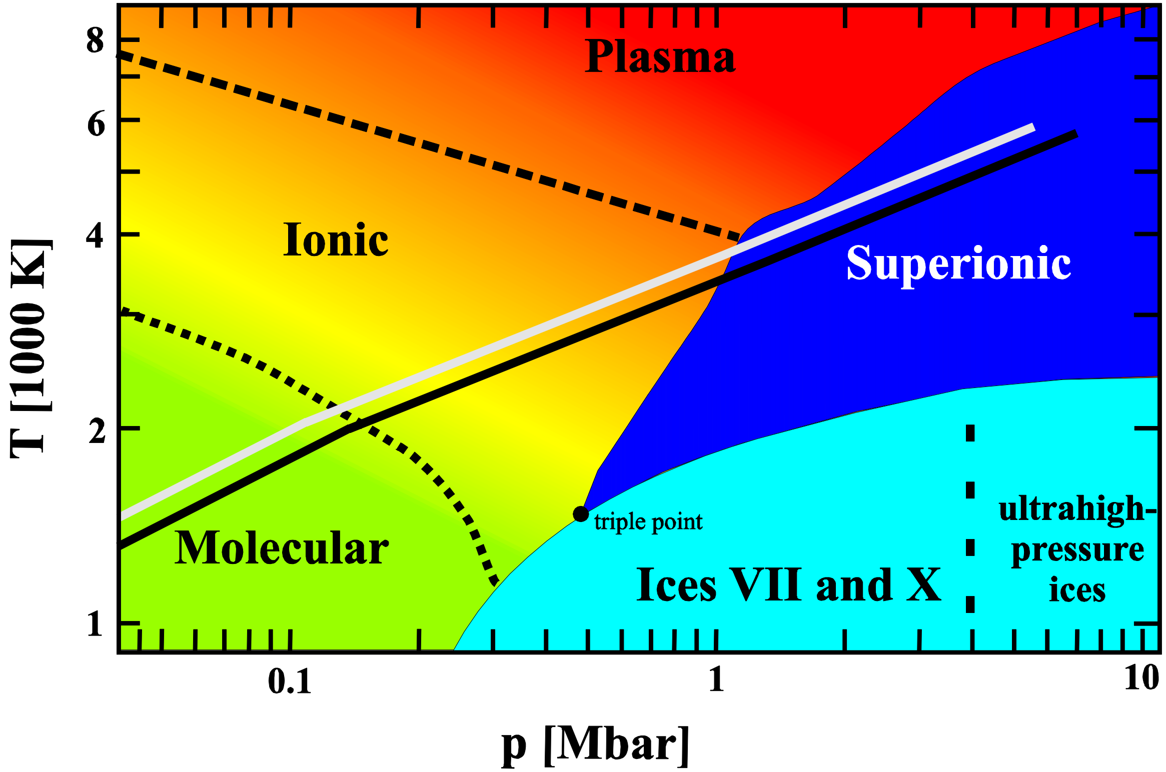
Interior structure models of this type are not uniquely defined.
Accurate EOS data for warm dense H-He-C-N-O mixtures are needed and information on the high-P phase diagram.

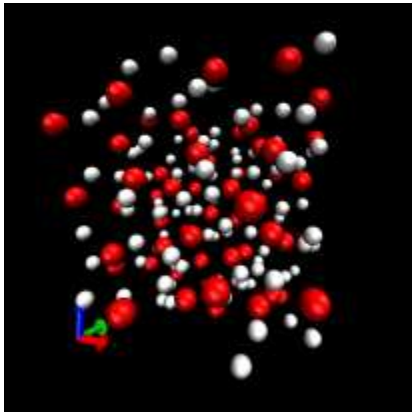
See e.g. Hubbard et al. (1980, 89, 95), Helled et al. (2009, 10, 11), Nettelmann et al. (2013, 2019)

High-pressure phase diagram of H_2O

H_2O: see RR et al., Icarus **211**, 798 (2011)
NH_3: M. Bethkenhagen, M. French, RR, JCP **138**, 234504 (2013)
NH_3-H_2O: M. Bethkenhagen et al. JPCA **119**, 10582 (2015)
H-C-N-O: M. Bethkenhagen et al. ApJ **848**, 67 (2017)

Uranus (white), Neptune (black), ice giants, mini-Neptunes

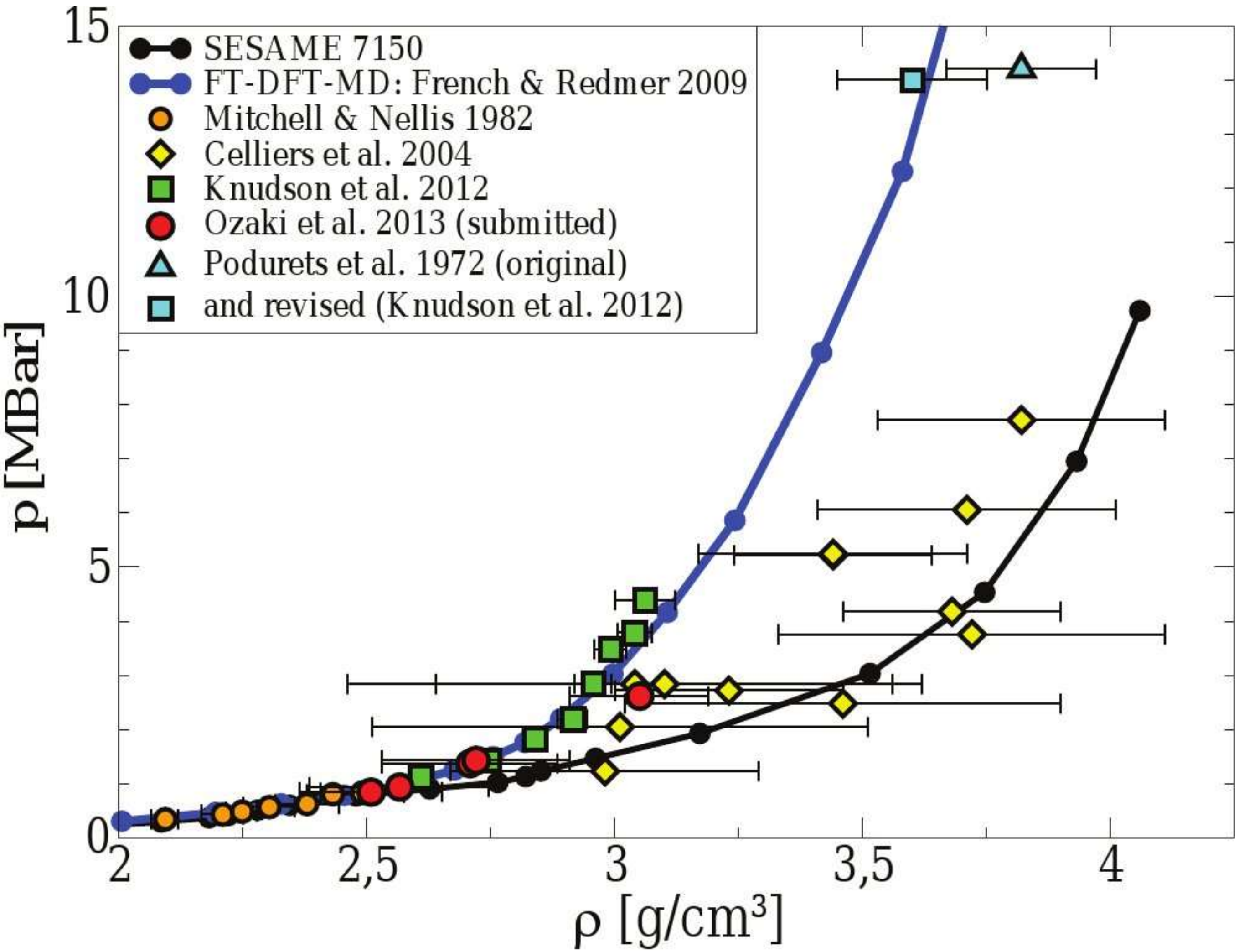


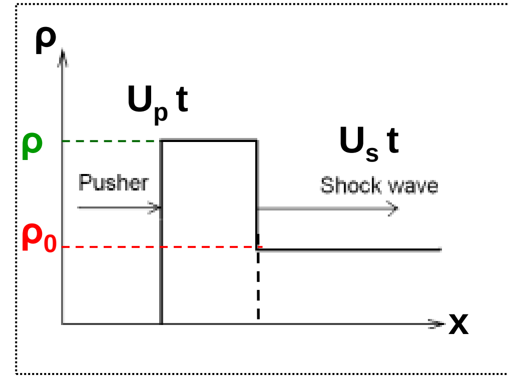


C. Cavazzoni et al., Science **283**, 44 (1999)
T.R. Mattsson, M.P. Desjarlais, PRL **97**, 017801 (2006)
E. Schwegler et al., PNAS **105**, 14779 (2008)
H.F. Wilson et al., PRL **110**, 151102 (2013)
Experiment: M. Millot et al. Nature **569**, 251 (2019)

EOS and phase diagram:
M. French et al., PRB **79**, 054107 (2009), PRE **93**, 022140 (2016)
Transport properties (diffusion, conductivity):
M. French et al., PRB **82**, 174108 (2010), PoP **24**, 092306 (2017)

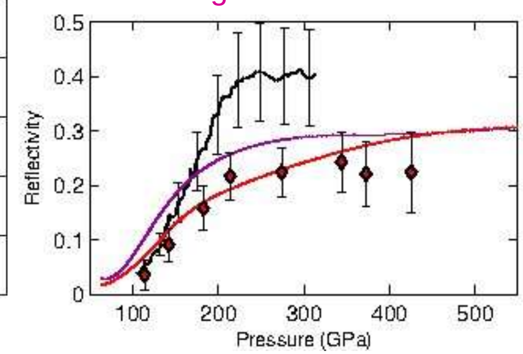
Benchmark: Hugoniot curve for H_2O





Data:
Red ◊ □ : Sandia Z
Open □ : Laser shocks

Theory: FT-DFT-MD
Red: HSE
Magenta: PBE

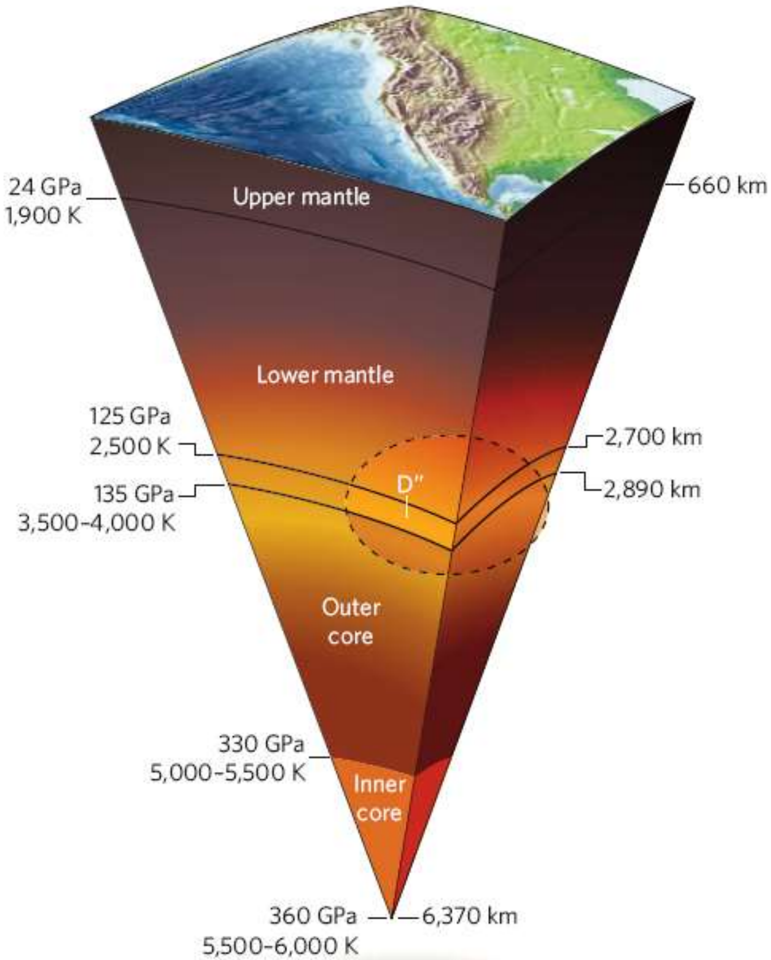


M.D. Knudson et al., PRL 1**08**, 091102 (2012) – Sandia Z machine
Drivers: High-power lasers, e.g., NIF, Omega, LULI, Vulcan, Phelix …

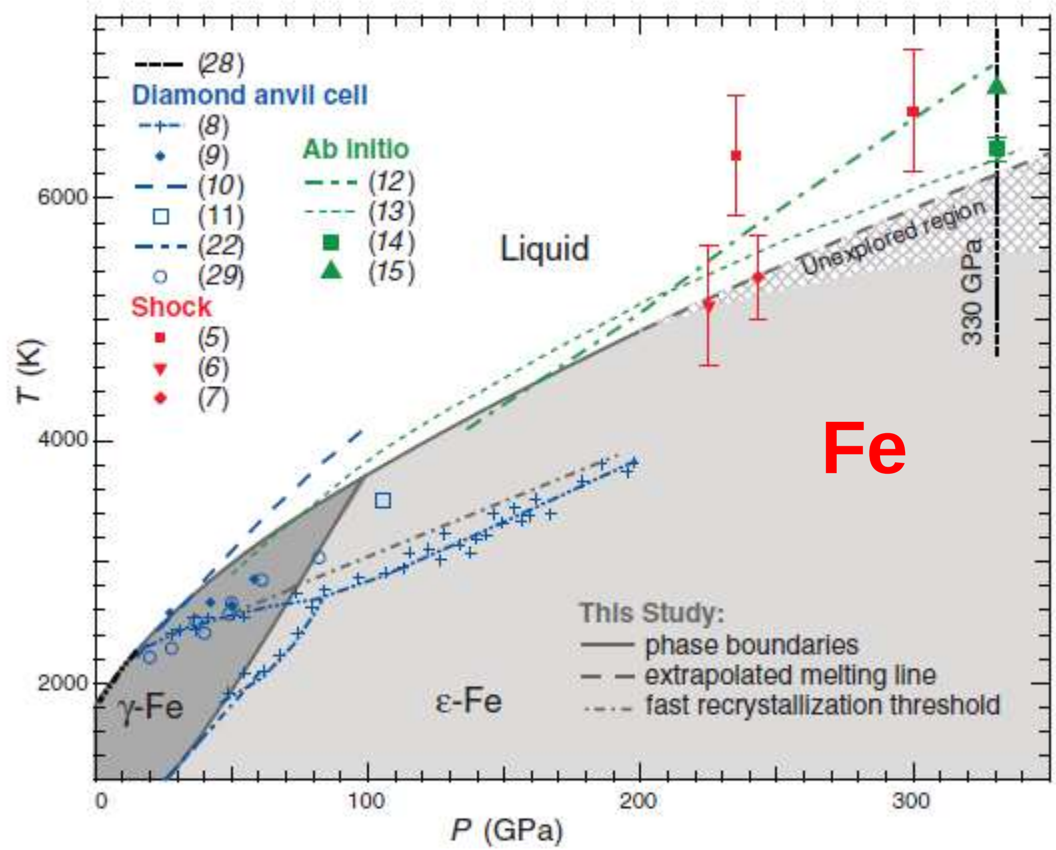
Earth - mineralogy at the extreme

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

Super Earths 1-10 M_E
Kepler, CoRoT, PLATO 2.0
Completely different?

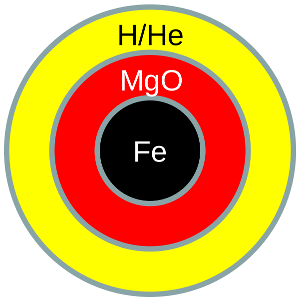


T.S. Duffy, Nature **451**, 269 **(**2008)



S. Anzellini et al., Science **340**, 464 **(**2013)

M-R relation and interior models for super-Earth Kepler 10b



G star 560 Ly away

Kepler 10b:

$R \sim 1.475\ R_E$

$M \sim 4.6\ M_E$

a=0.01864 AU

T=0.8375 d

Kepler 10c:

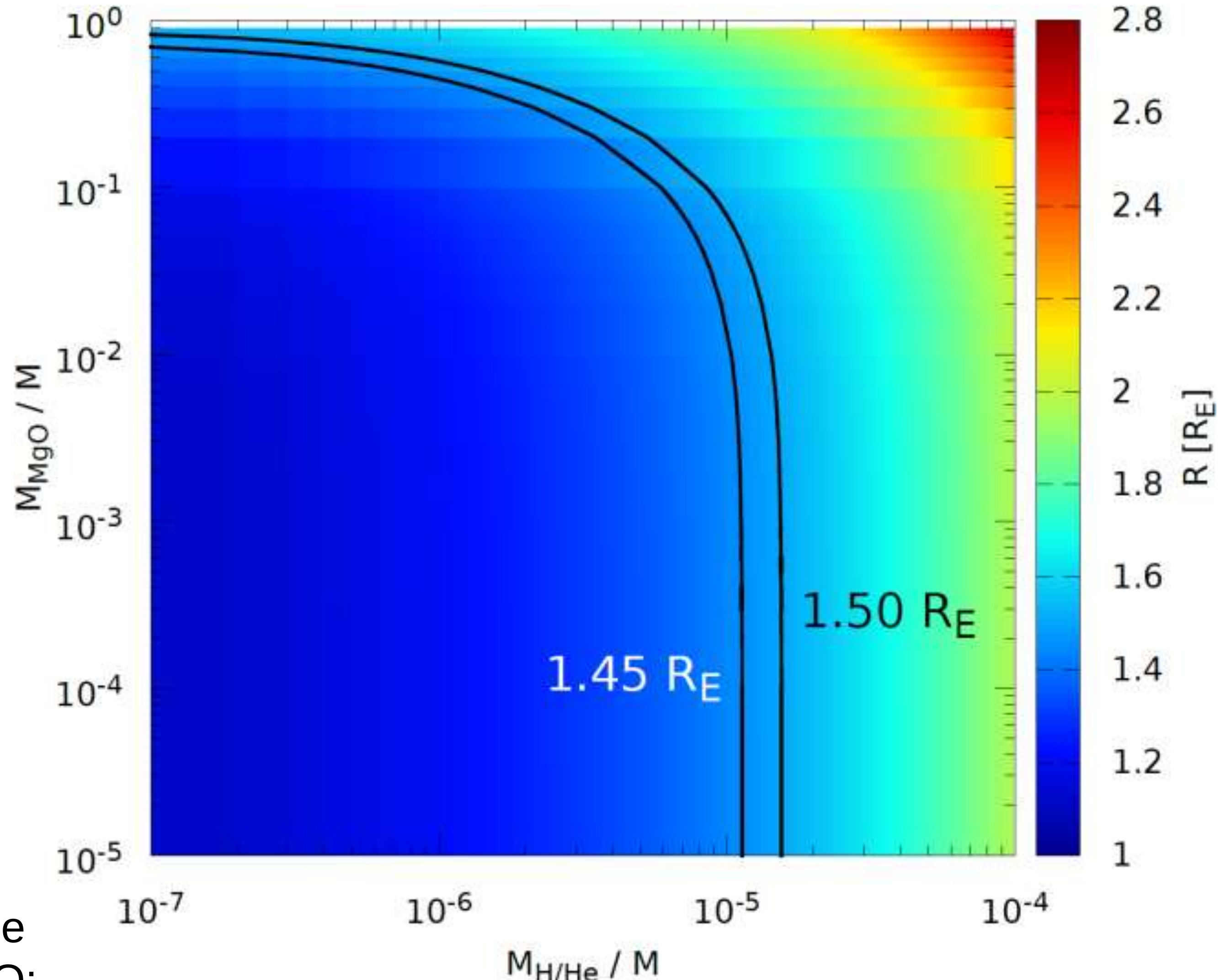
$R \sim 2.35\ R_E$

$M \sim 17.2\ M_E$

a=0.241 AU

T=45.3 d

Solutions depend on the structure assumed and the EOS used (H/He and MgO: DFT-MD)



C. Kellermann, RR, A&A **615**, A39 (2018)

Summary

- Modeling solar/extrasolar planets based on ab initio EOS and material data
  → develop advanced planetary models
  → structure, composition, evolution, magnetic fields
  → combine inerior and atmosphere models
  → gas giants – ice giants – mini-Neptunes – super-Earths
  → structure and evolution of planetary systems
- Large scale DFT-MD simulations performed for MEC
  → agreement with available shock wave experiments
  → predict high-pressure phase diagrams
  → nonmetal-to-metal transitions (H)
  → demixing phenomena at high pressures (H-He, H-C-N-O)
  → superionic water (NH_3 and mixtures)
  → minerals at high pressure (MgO-FeO-SiO_2, Fe)

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