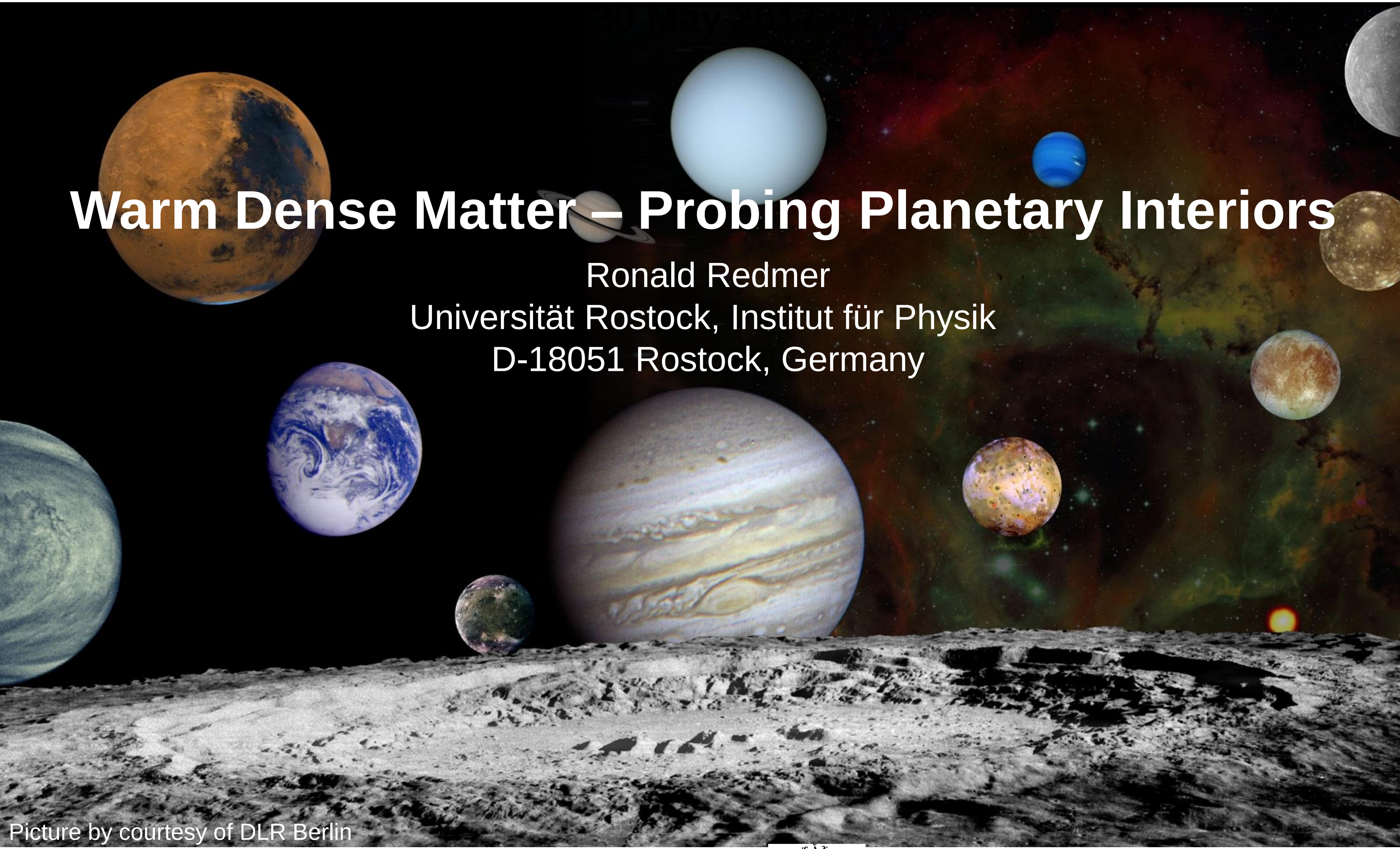
Seminar at the High Energy Density Science Center
Lawrence Livermore National Laboratory, USA, Nov 9, 2017



Warm Dense Matter – Probing Planetary Interiors

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Picture by courtesy of DLR Berlin

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LCLS

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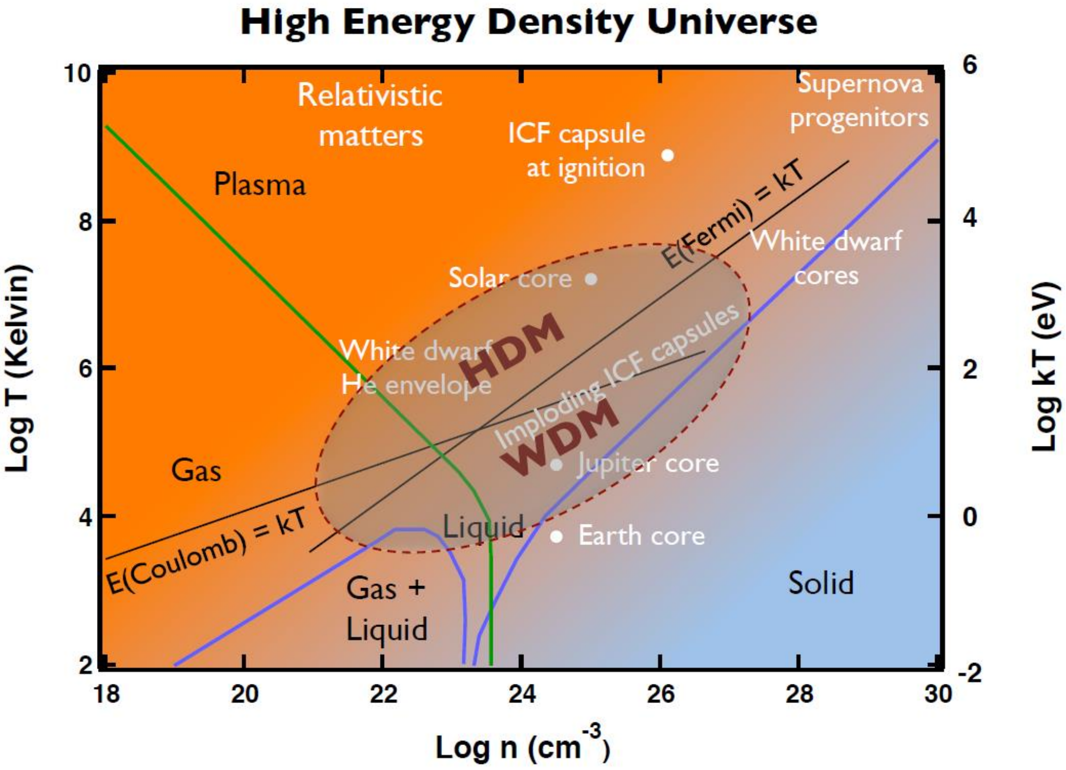
Contents

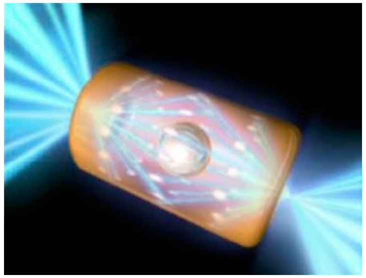
Warm Dense Matter (WDM)

See: Basic Research Needs for High Energy Density Laboratory Physics (DOE Office of Science and NNSA, 2010)



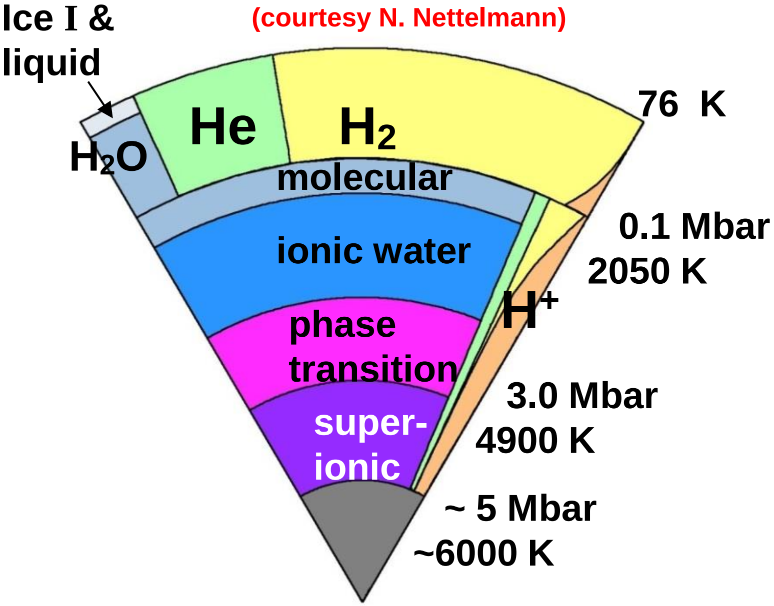
DENSITY ~ solid density (0,1 – 10)
TEMPERATURE ~ few eV
PRESSURES ~ Mbar-Gbar

Inertial Confinement Fusion
(courtesy NIF)



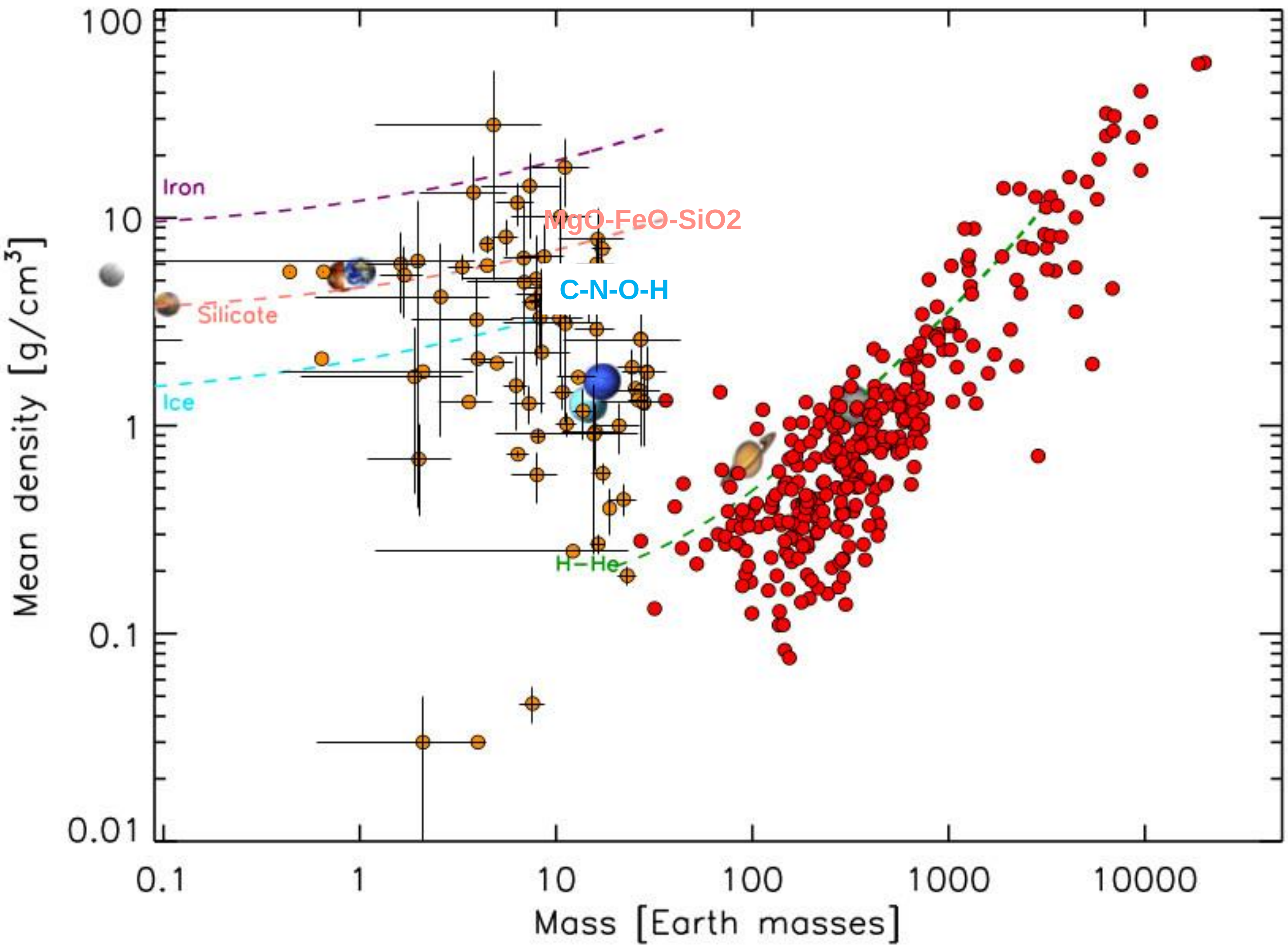
T > 10^8 K
P > 100 Gbar

Planetary Physics: e.g. Uranus
(courtesy N. Nettelmann)

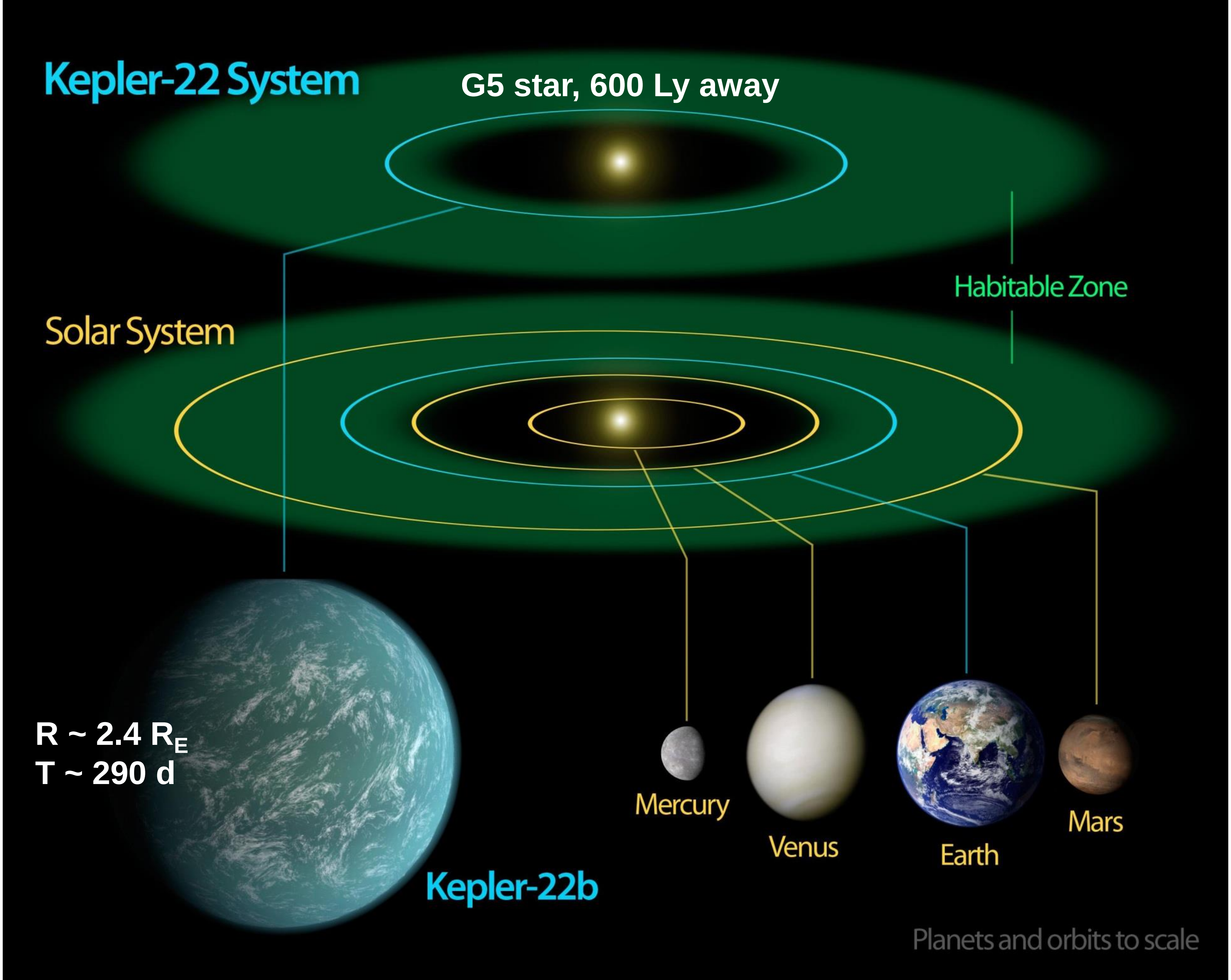


Mean Density vs. Mass

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

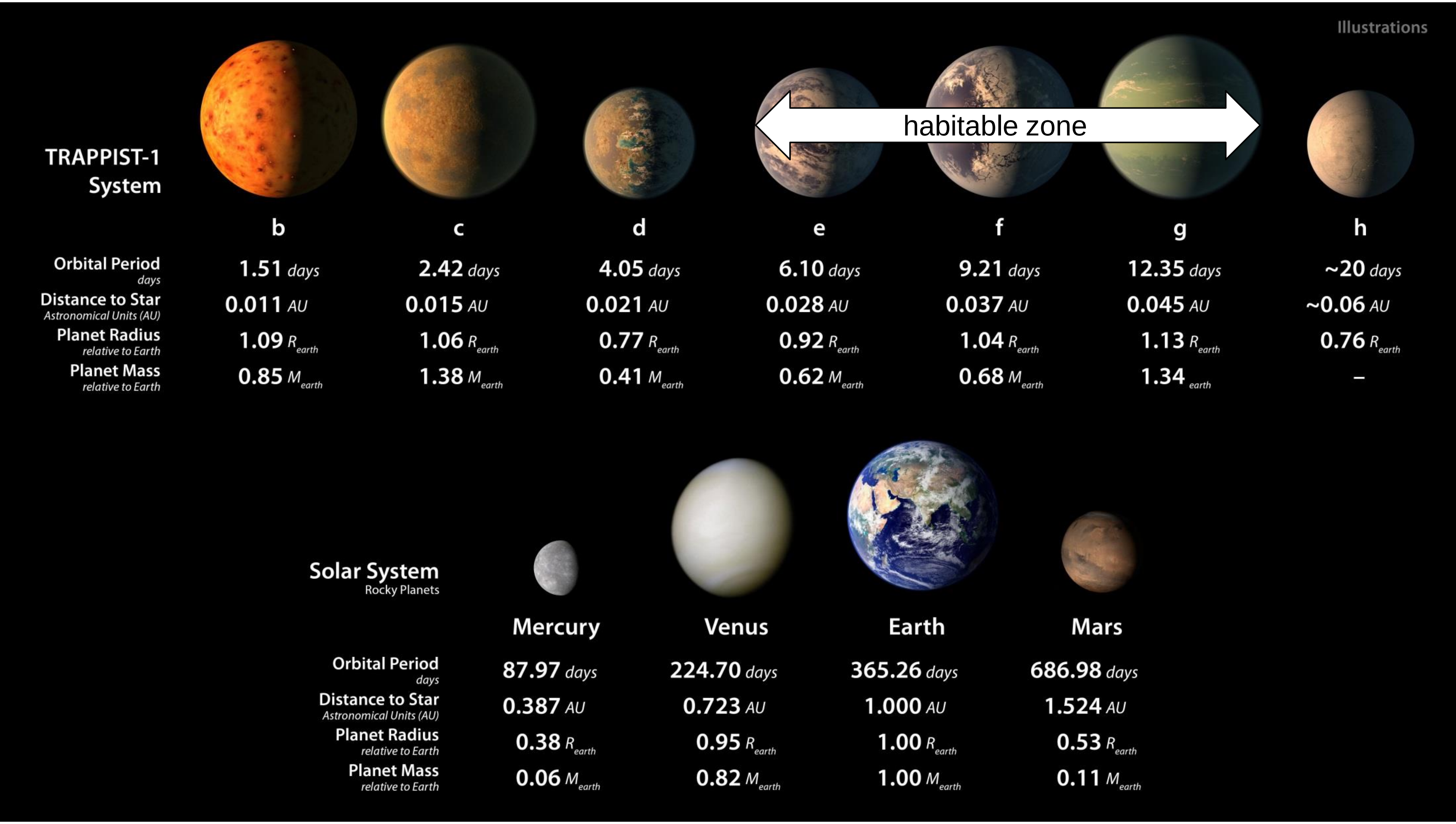


G5 star, 600 Ly away



$R \sim 2.4\ R_E$
$T \sim 290$ d

M8 star: 40 Ly away, 0.082 M_{Sun}



TRAPPIST-1 System

	b	c	d	e	f	g	h
Orbital Period *days*	1.51 *days*	2.42 *days*	4.05 *days*	6.10 *days*	9.21 *days*	12.35 *days*	~20 *days*
Distance to Star *Astronomical Units (AU)*	0.011 *AU*	0.015 *AU*	0.021 *AU*	0.028 *AU*	0.037 *AU*	0.045 *AU*	~0.06 *AU*
Planet Radius *relative to Earth*	1.09 R_{earth}	1.06 R_{earth}	0.77 R_{earth}	0.92 R_{earth}	1.04 R_{earth}	1.13 R_{earth}	0.76 R_{earth}
Planet Mass *relative to Earth*	0.85 M_{earth}	1.38 M_{earth}	0.41 M_{earth}	0.62 M_{earth}	0.68 M_{earth}	1.34 $_{earth}$	–

Solar System Rocky Planets

	Mercury	Venus	Earth	Mars
Orbital Period *days*	87.97 *days*	224.70 *days*	365.26 *days*	686.98 *days*
Distance to Star *Astronomical Units (AU)*	0.387 *AU*	0.723 *AU*	1.000 *AU*	1.524 *AU*
Planet Radius *relative to Earth*	0.38 R_{earth}	0.95 R_{earth}	1.00 R_{earth}	0.53 R_{earth}
Planet Mass *relative to Earth*	0.06 M_{earth}	0.82 M_{earth}	1.00 M_{earth}	0.11 M_{earth}

Transiting Planets and Planetesimals Small Telescope (TRAPPIST), La Silla Observatory, Chile: M. Gillon et al., Nature **542**, 456 (2017)

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:

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

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:

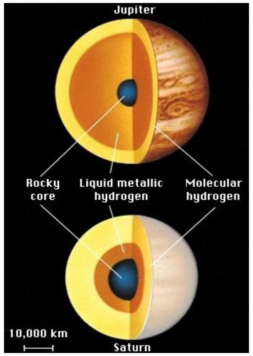
$$J_{2i} = -\frac{1}{MR_{eq}^{2i}} \int d^3 r' \boxed{\rho(r'(\theta'))}\, r'^{2i} P_{2i}(\cos\theta')$$

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/isotherms according to EOS data for WDM – most important input!

Interior of Gas Giants: H-He

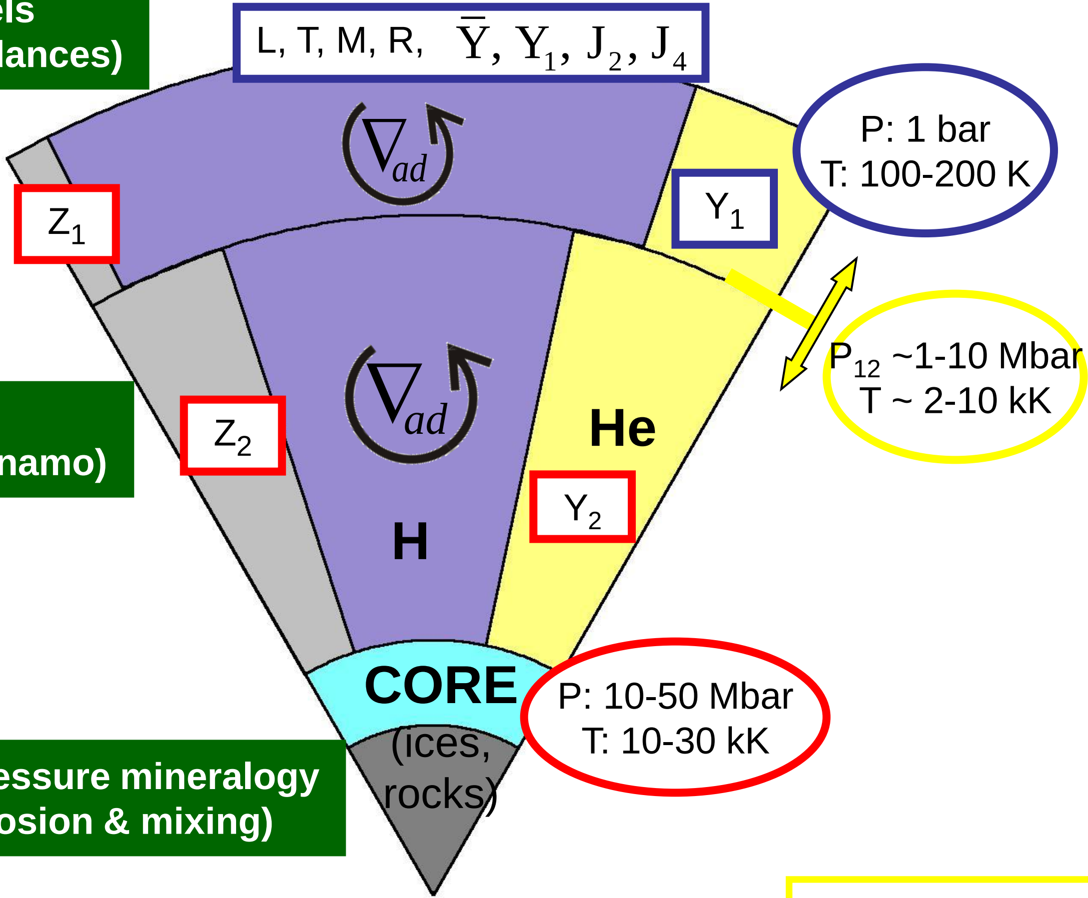
Three-layer model, input and constraints



Atmosphere models (luminosity, abundances)

Magnetic field generation (dynamo)

High-pressure mineralogy (core erosion & mixing)



L, T, M, R, $\bar{Y}, Y_1, J_2, J_4$

P: 1 bar
T: 100-200 K

P_{12} ~1-10 Mbar
T ~ 2-10 kK

P: 10-50 Mbar
T: 10-30 kK

🟦 constraints
🟥 results from modeling
🟨 free parameter

Physical origin and location of the layer boundary:
→ MIT (PPT)
→ H-He demixing

Matter under extreme conditions (WDM):
- **High-pressure H-He phase diagram**
- **EOS of complex mixtures**
- **Electrical & thermal conductivity**
- **Diffusion & viscosity**

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

Interior of Jupiter: Juno Mission

High-precision measurement of gravitational moments J_{2i}

Juno's Instruments

Gravity Science and Magnetometers
Study Jupiter's deep structure by mapping the planet's gravity field and magnetic field

Microwave Radiometer
Probe Jupiter's deep atmosphere and measure how much water (and hence oxygen) is there

JEDI, JADE and Waves
Sample electric fields, plasma waves and particles around Jupiter to determine how the magnetic field is connected to the atmosphere, and especially the auroras (northern and southern lights)

UVS and JIRAM
Using ultraviolet and infrared cameras, take images of the atmosphere and auroras, including chemical fingerprints of the gases present

JunoCam
Take spectacular close-up, color images

SPACECRAFT DIMENSIONS

Diameter: 66 feet (20 meters)
Height: 15 feet (4.5 meters)

For more information:
missionjuno.swri.edu & www.nasa.gov/juno

National Aeronautics and Space Administration

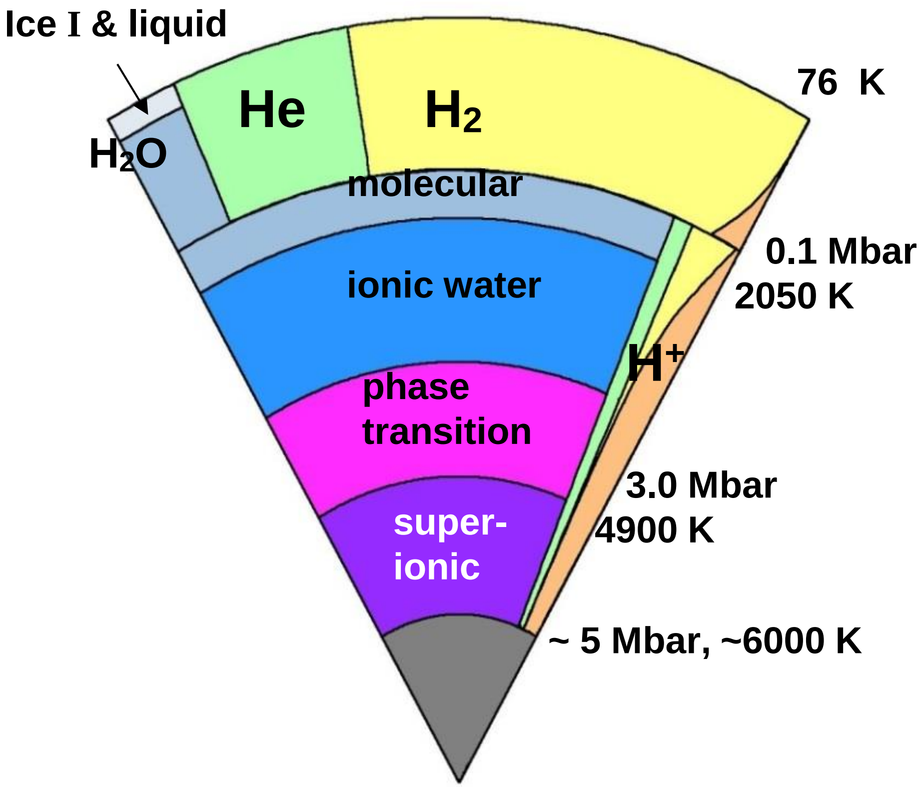
Jet Propulsion Laboratory
California Institute of Technology
Pasadena, California

www.nasa.gov

See e.g.
W.B. Hubbard and B. Militzer, ApJ **820**, 80 (2016)
S. Wahl et al., J. Geophys. Res. **44**, 4649 (2017)
N. Nettelmann, A&A **606**, A139 (2017)

Interior of Ice Giants: C-N-O-H Mixture

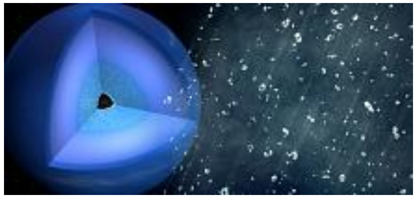
Multi-layer models



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)

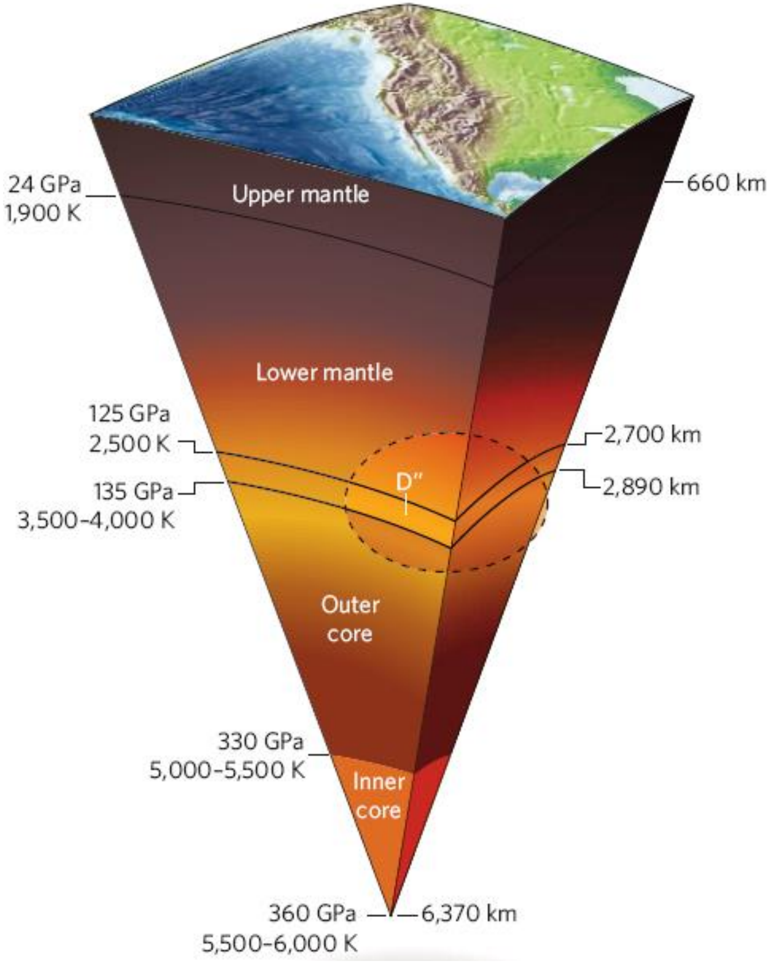
Interior structure models of this type are not uniquely defined.
Accurate EOS data for warm dense C-N-O-H-He mixtures are needed and information on the high-P phase diagram.

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

From Earth to Super-Earths – Mineralogy at the Extreme

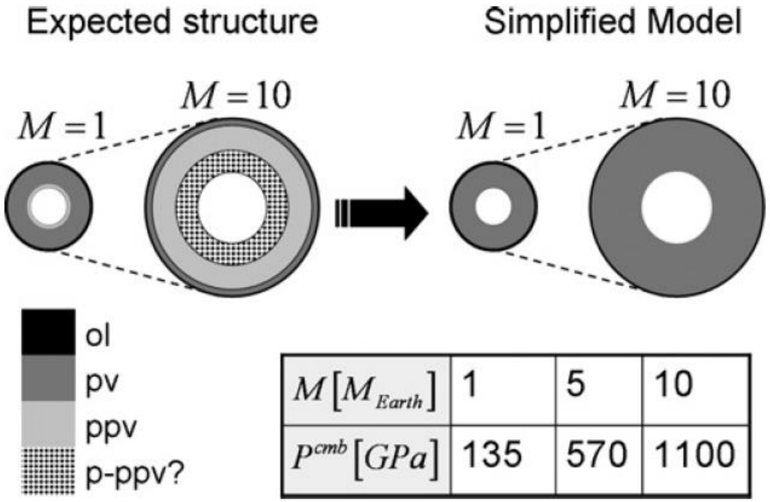
Upper mantle: olivine $(Mg,Mn,Fe)_2[SiO_4]$
Lower mantle: perovskite $MgSiO_3$, PPv
Core: (Fe,Ni)[Si,O,S,C…] – melting line, dynamo

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



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

V. Stamenkovic et al., Icarus **216**, 572 **(**2011)



$M[M_{Earth}]$	1	5	10
$P^{cmb}[GPa]$	135	570	1100

High-P crystal structures?
High-P EOS data and phase diagram?
Slope of melting line?
Electrical and thermal conductivity?
Viscosity?

Diamond Anvil Cells (DACs)

Conventional DAC technique is limited to static pressures of few Mbar and low T using resistive or pulsed laser heating.

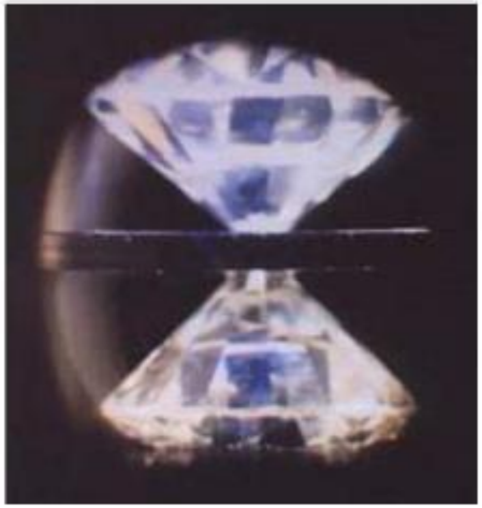
Dynamic dDAC (for molecular solids) > 2 Mbar
Evans et al. 2007
Double-stage dsDAC – potential to reach 10 Mbar
Dubrovinsky et al. 2012: Re >6 Mbar
Dubrovinsky et al. 2015: Os ~8 Mbar
X-ray diagnostics at 3rd generation synchrotrons:

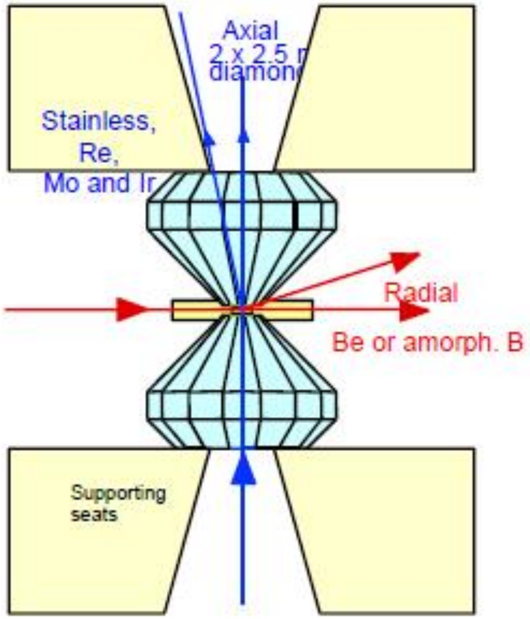
- ESRF, ECB@PETRA III, APS, Diamond …
- Structure, phase transitions, EOS, reflectivity …

Laser-driven shocks: NIF, Omega, Nike … Orion, Vulcan, LMJ, LULI, PeTAL, Phelix …

Combination of pre-compressed samples (DACs) and shock waves (lasers)
Jeanloz et al. 2007, Eggert et al. 2008,
Loubeyre et al. 2012, Torchio et al. 2016

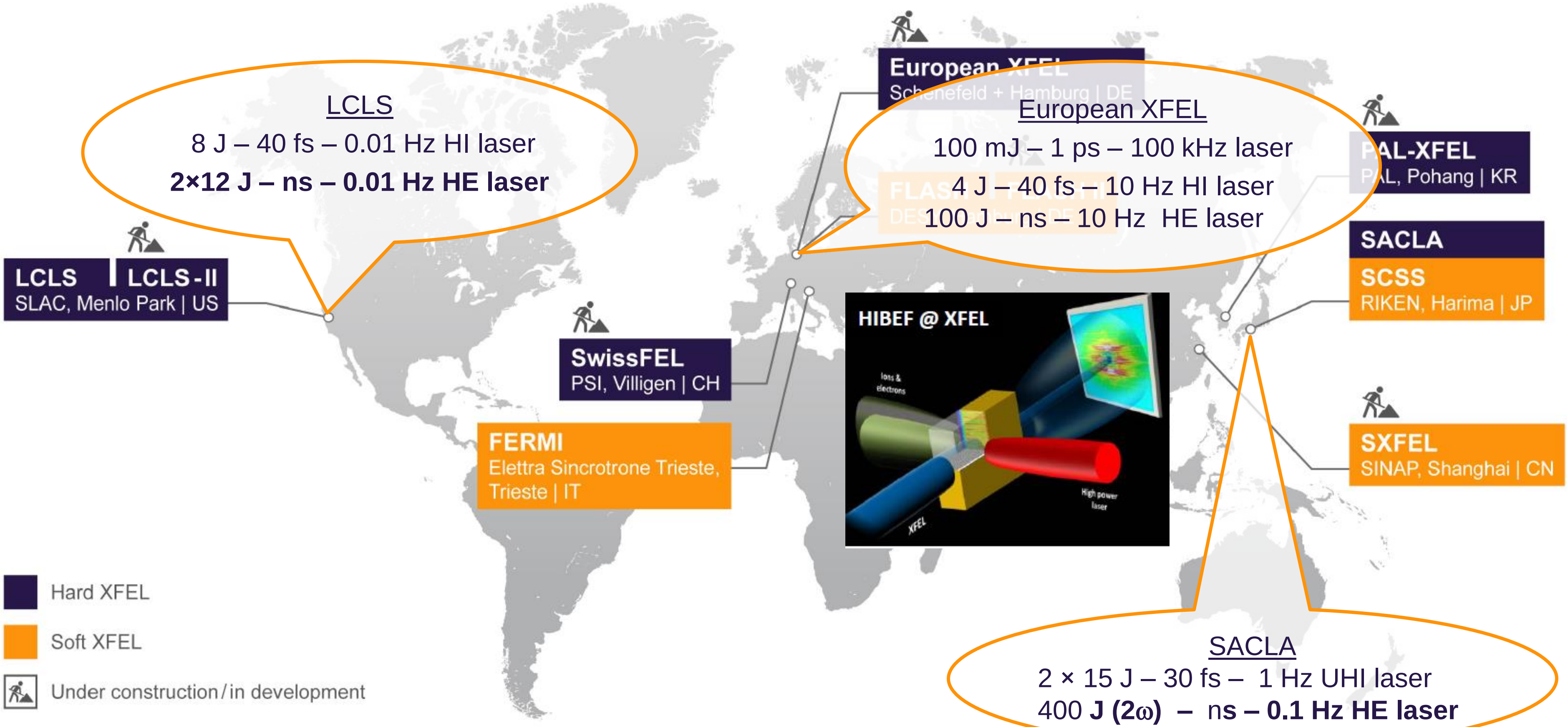
By courtesy of H.-P. Liermann (DESY)





X-ray free-electron lasers worldwide with big OLs

The European XFEL will put Europe in the lead among industrialized nations in a highly competitive scientific and technical environment.



LCLS
8 J – 40 fs – 0.01 Hz HI laser
2×12 J – ns – 0.01 Hz HE laser

European XFEL
100 mJ – 1 ps – 100 kHz laser
4 J – 40 fs – 10 Hz HI laser
100 J – ns – 10 Hz HE laser

SACLA
2 × 15 J – 30 fs – 1 Hz UHI laser
400 **J (2ω)** – ns **– 0.1 Hz HE laser**

- ■ Hard XFEL
- ■ Soft XFEL
- Under construction / in development

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    - Planetary Interiors
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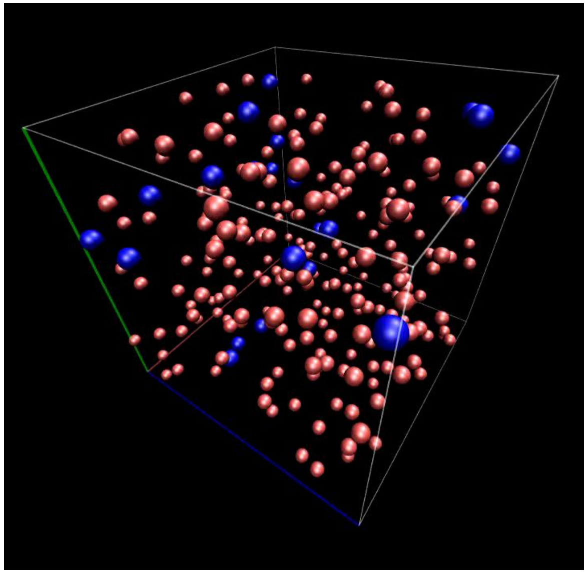
    - C-N-O-H: Uranus and Neptune
    - MgO-FeO-SiO_2: Rocky Planets
4. Outlook

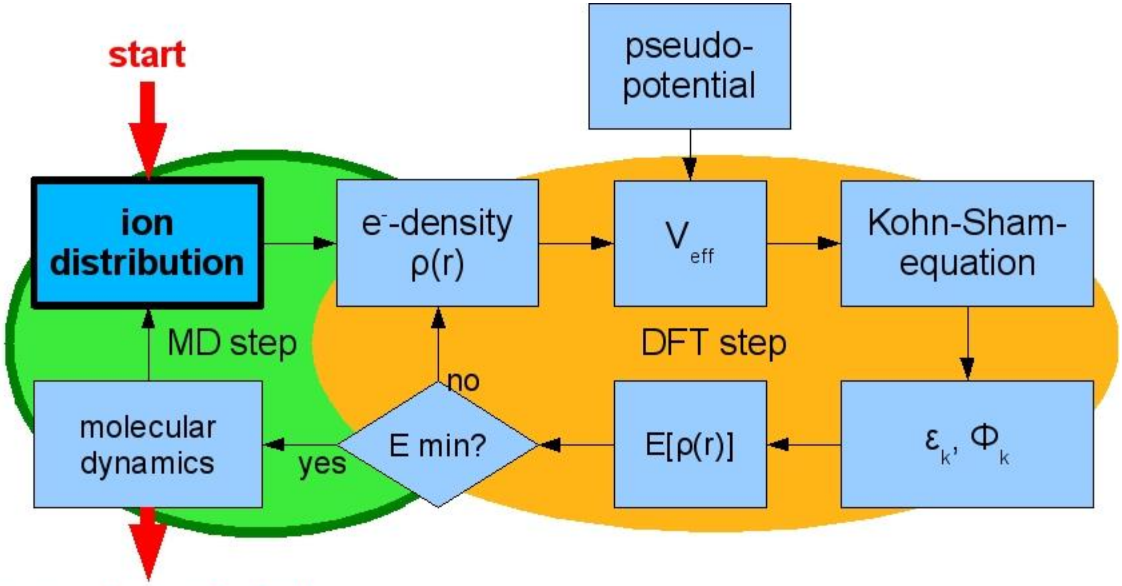
DFT-MD Simulations for WDM

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)
Codes: **Vienna Ab-initio Simulation Package** (VASP) or 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)

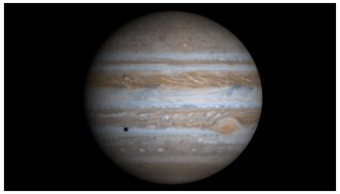


H-He (8.6%) @ 1 Mbar, 4000 K

box length ~ 10^{-9} m

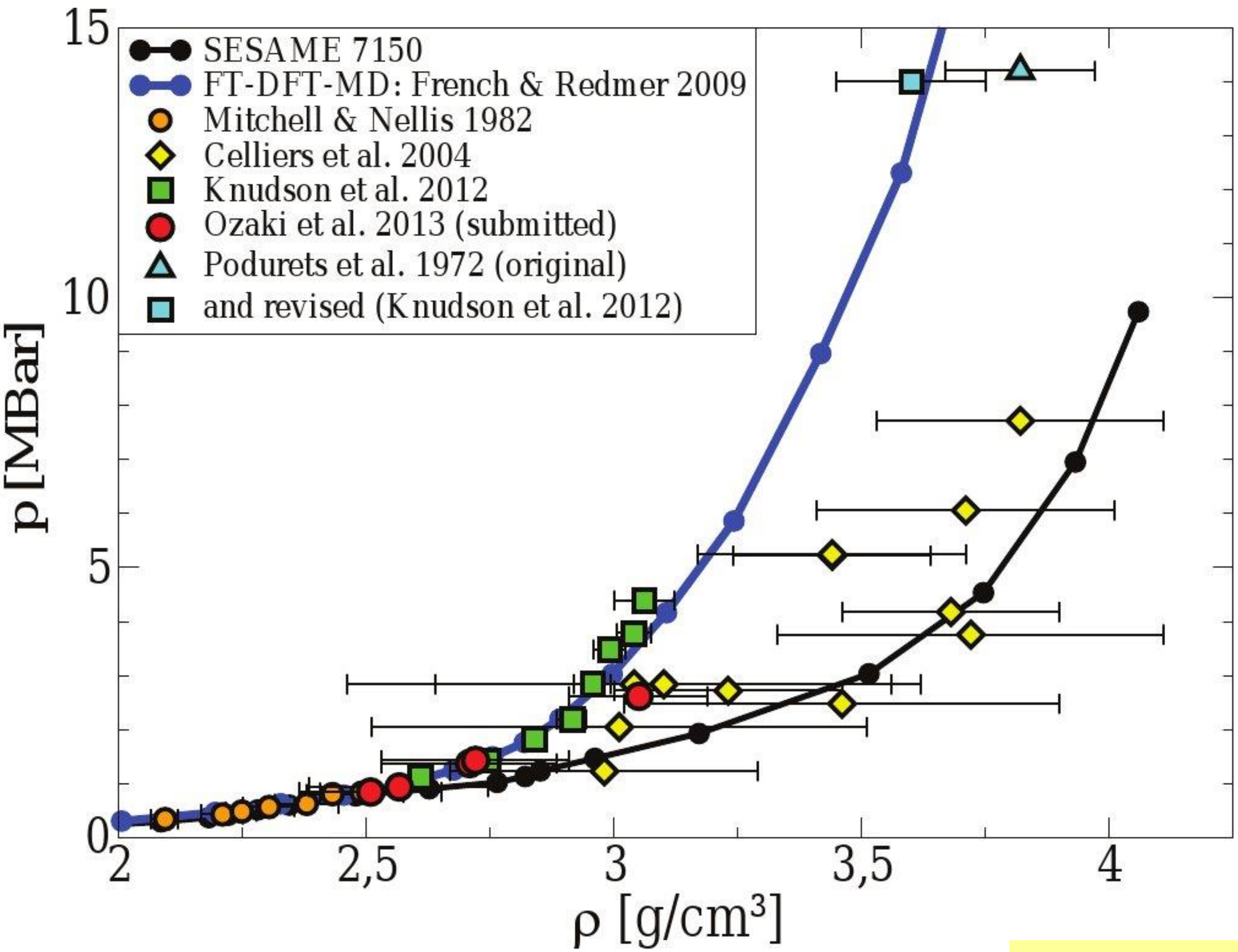


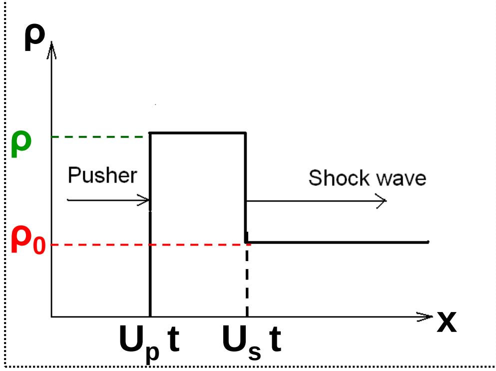
thermodynamic data
high-pressure phase diagram
pair correlation functions
electrical & thermal conductivity
diffusion coefficient
viscosity, opacity



GP size ~ 10^{8} m

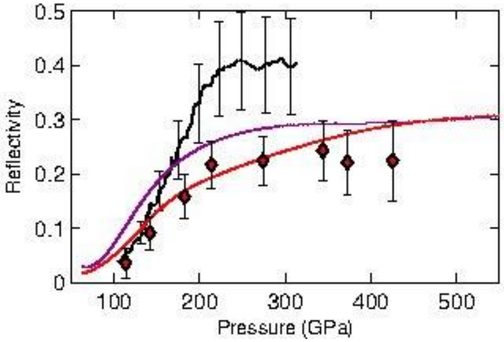
Benchmark:
Hugoniot Curve for H_2O





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

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



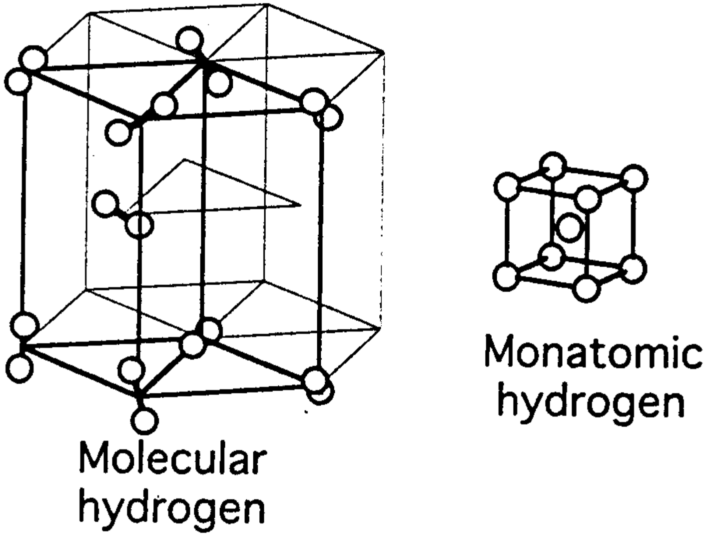
M.D. Knudson et al., PRL 1**08**, 091102 (2012)
Experiments at Sandia`s Z machine

GOOD NEWS:
Very good agreement for EOS and reflectivity (PBE, HSE)

Contents

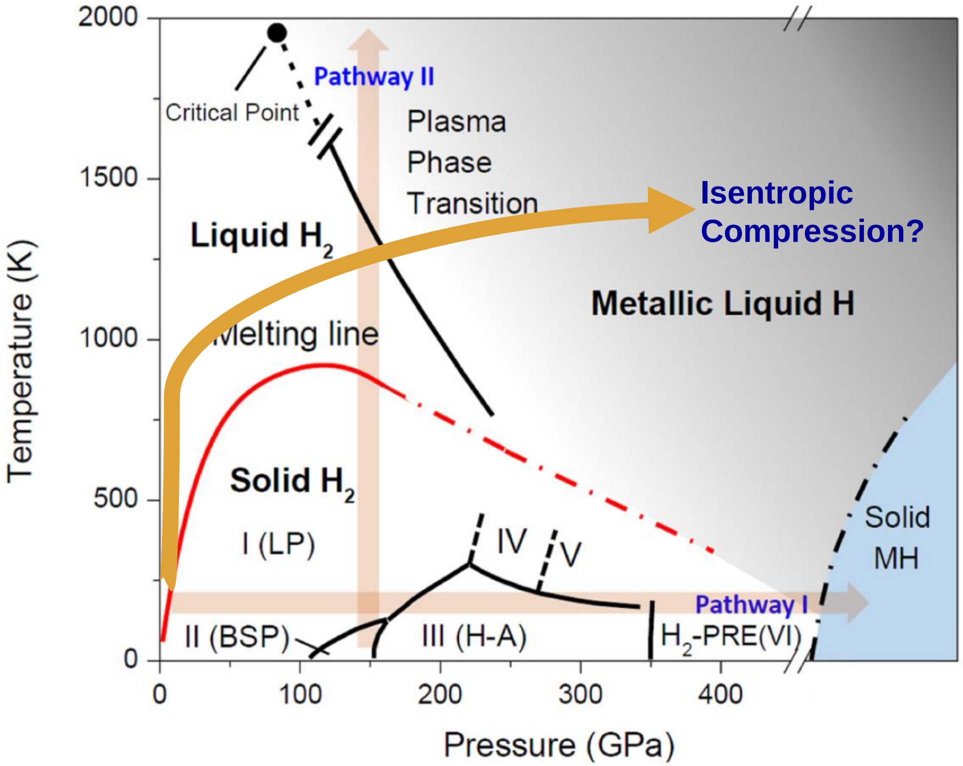
Solid Metallic Hydrogen at T=0 K?

Proposed by Wigner and Huntington already in 1935 (at 25 GPa).
Verified in recent **DAC** experiments at 5 Mbar?
Rich phase diagram obtained in solid H: phases I, II, III, IV, V.



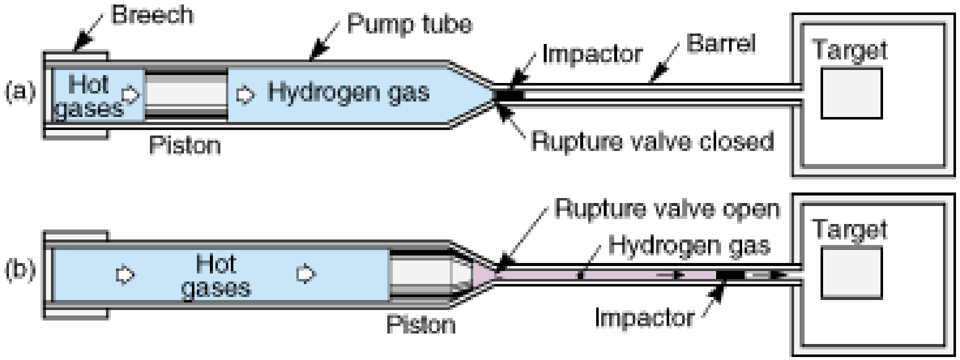
H.K. Mao & R.J. Hemley, RMP **66**, 671 (1994)

Metallization by band-gap closure:
From 15 eV in the hcp molecular insulator to zero in the bcc metal

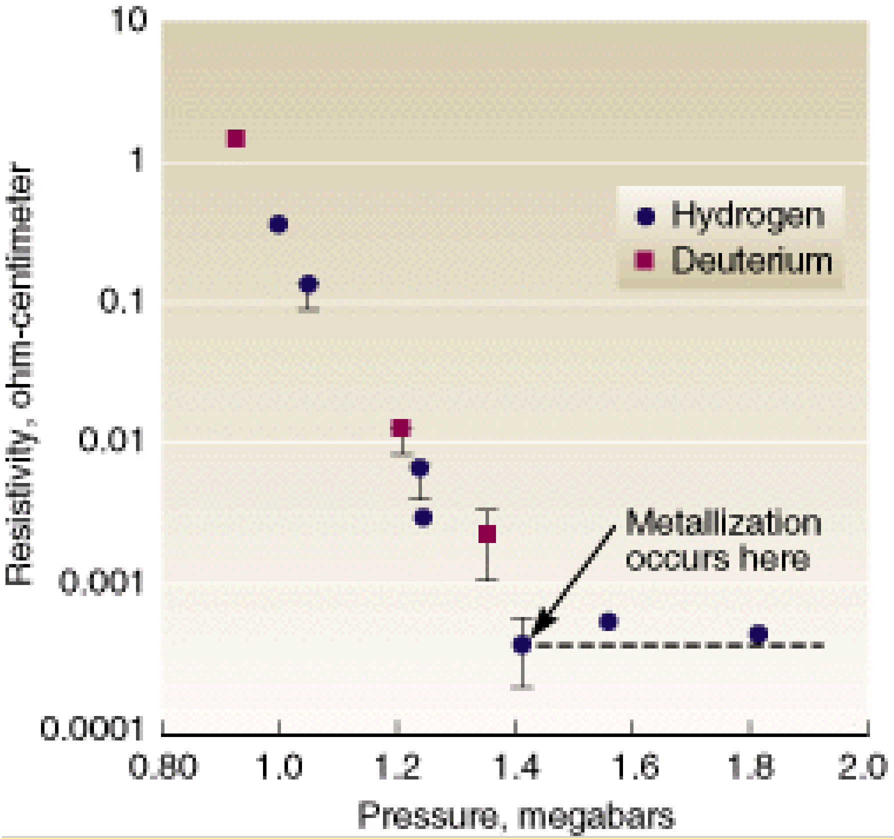


R.P. Dias, I.F. Silvera, Science **355**, 715 (2017)
For recent DAC studies, see also:
P. Dalladay-Simpson et al., Nature (2016)
R.S. McWilliams et al., PRL (2016)

Gas Guns: Fluid Metallic Hydrogen



(a) In the first stage of the gas gun (blue shading), hot-burning gases from gunpowder drive a piston, which in turn compresses hydrogen gas. (b) In the second stage (pink shading), the high-pressure gas eventually ruptures a second-stage valve, accelerating the impactor down the barrel toward its target.



Reverberating shock waves in sandwich target

$\longrightarrow$ quasi-isentropic process

$\longrightarrow$ „low“ temperatures

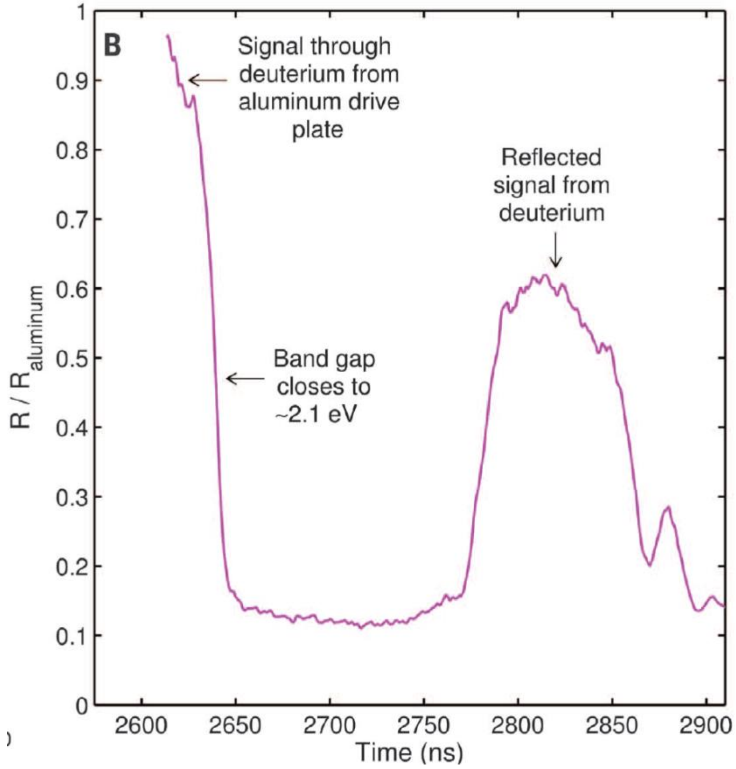
Metallic conductivity observed at ~3000 K and 1.4 Mbar

But no indication of a first-order phase transition!

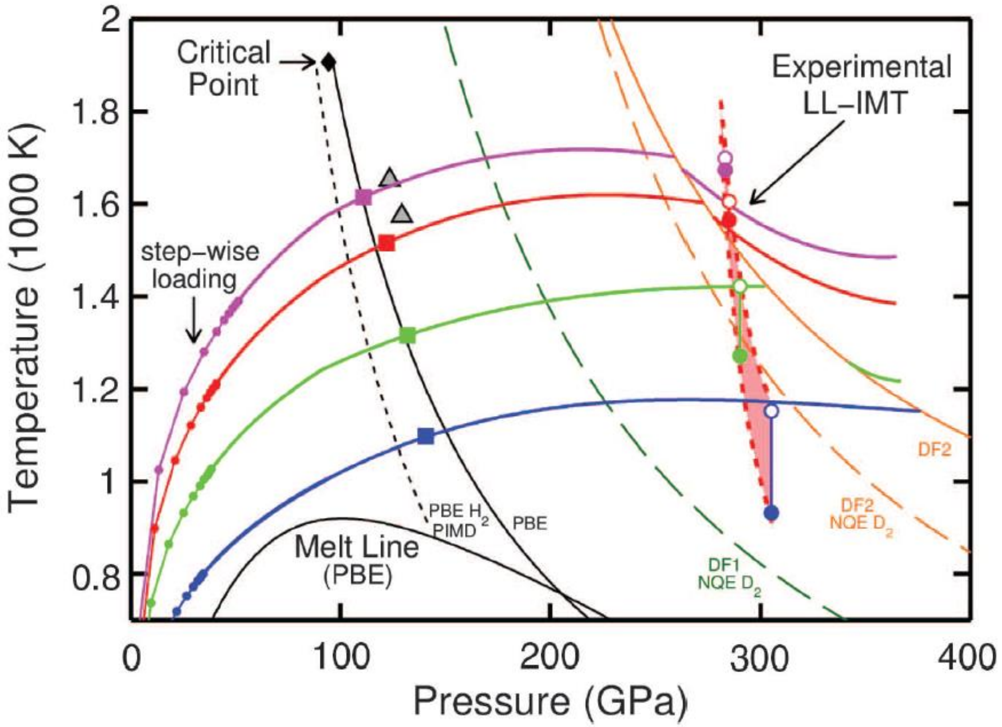
W.J. Nellis et al., PRL **68**, 2937 (1992)
S.T. Weir et al., PRL **76**, 1860 (1996)

Abrupt Insulator-to-Metal Transition - Typical of a first-order LL-PT

M.D. Knudson, M.P. Desjarlais, A. Becker, R.W. Lemke, K.A. Cochrane, M.E. Savage, D.E. Bliss, T.R. Mattsson, RR, Science **348**, 1455 (2015)



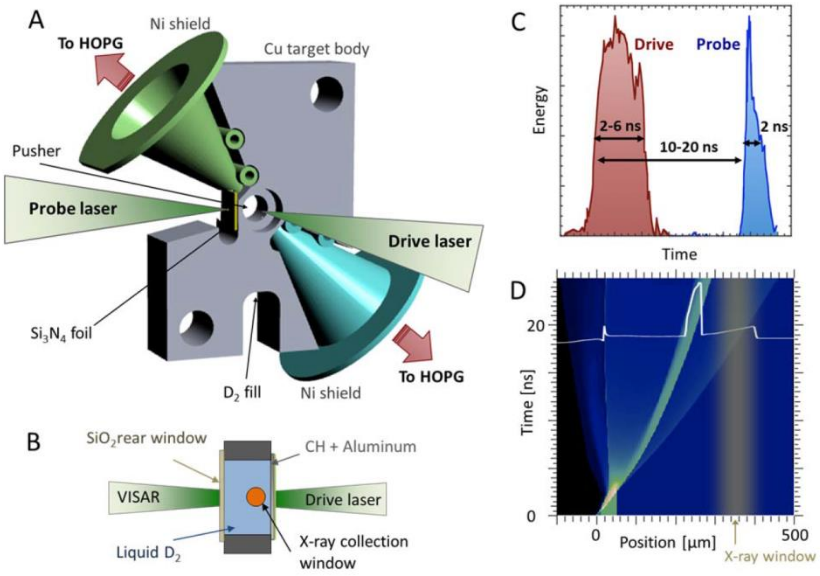
Measure the shock compression path and reflectivity, check with DFT-MD (Z Fundamental Science Program).

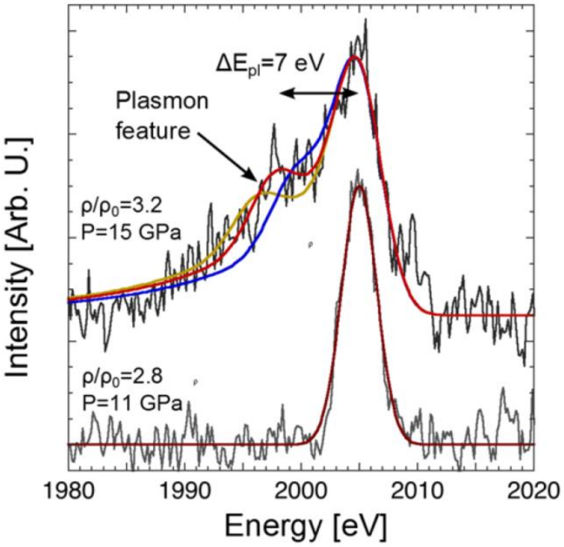


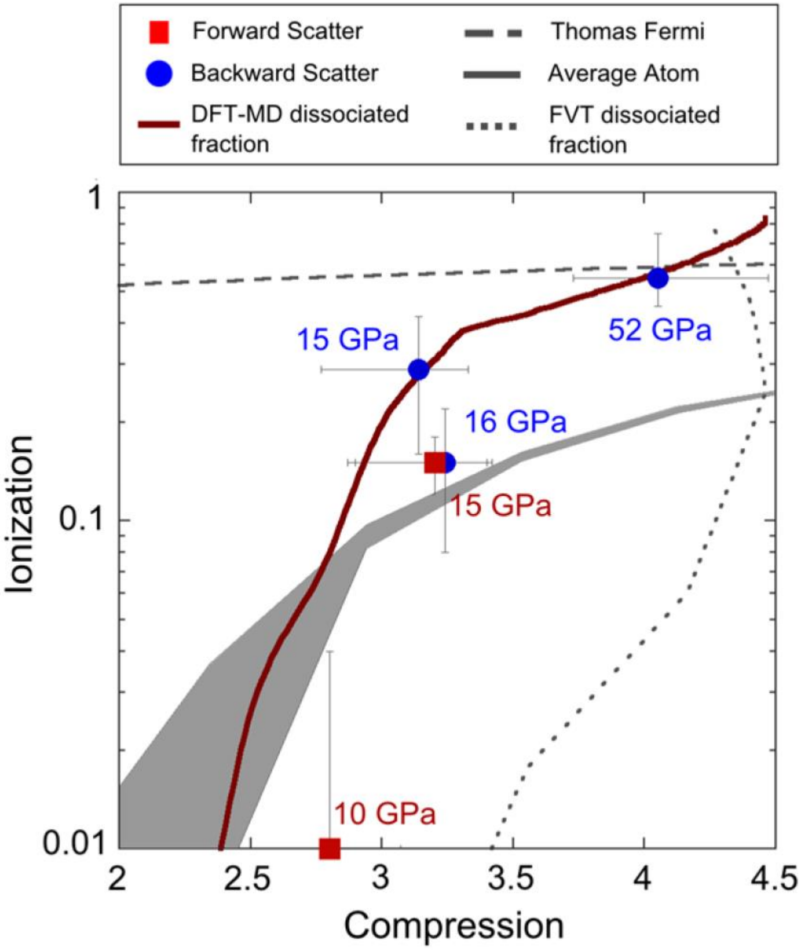
LL-IMT at ~3 Mbar below 2000 K: Indication of a first-order LL-PT.

X-ray Thomson Scattering Probes Onset of Dissociation in Jupiter

P. Davis et al., Nature Commun. **7**, 11189 (2016)
Experiment: Janus Laser Facility (LLNL)
DFT-MD: A. Becker (U Rostock)





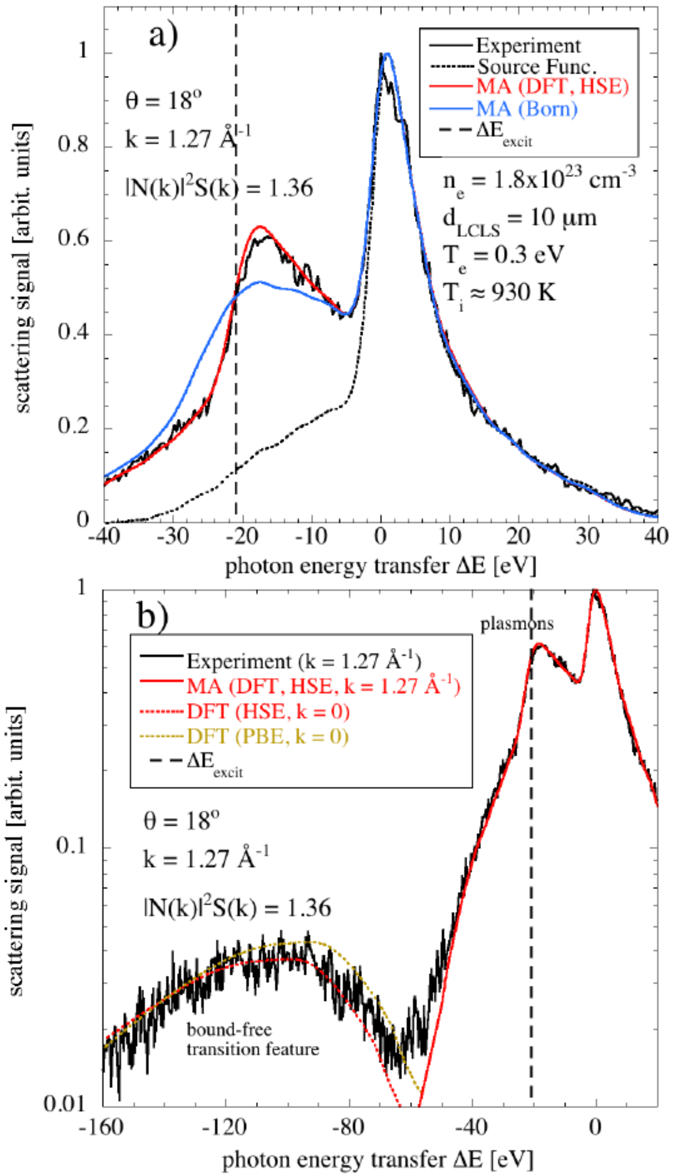


XRTS Experiments at FELs: LCLS

P. Sperling et al., PRL **115**, 115001 (2015)
B. Witte et al., PRL **118**, 225001 (2017)

BMA

DFT-MD



Al

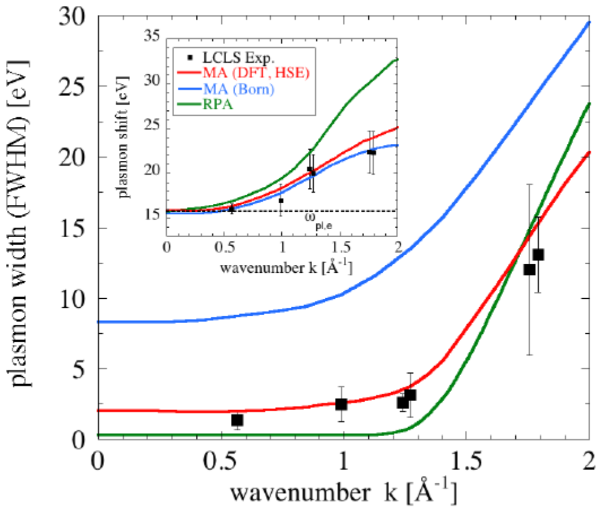
Full XRTS spectrum calculated with DFT-MD simulations:

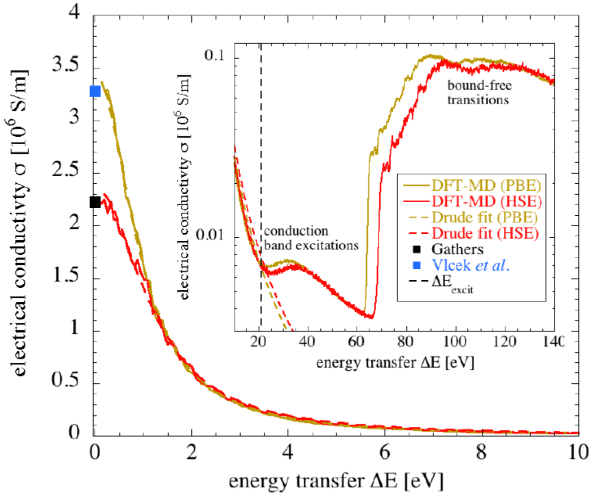
1. Excellent agreement with high-resolution LCLS experiments.

2. Plasmon dispersion (shift and width) in agreement with experiment.

3. HSE superior to PBE XC functional in the DFT calculations.

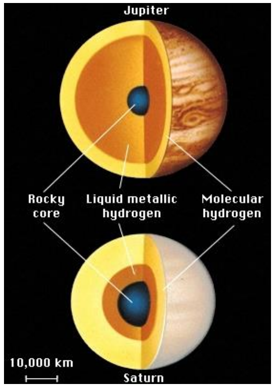
4. Non-Drude electrical conductivity derived from f-f transitions (Cooper minimum).

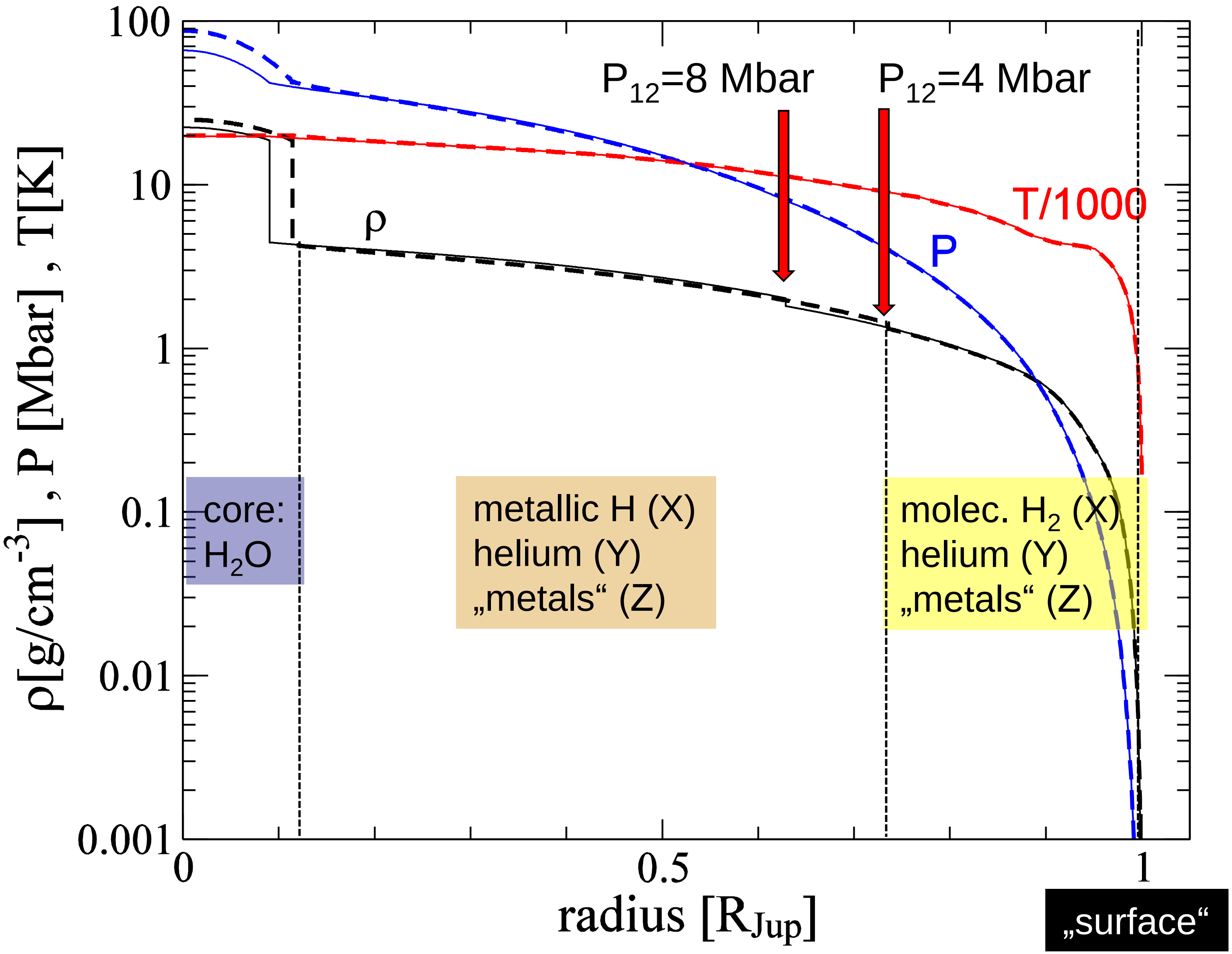




Jupiter`s Interior with LM-REOS (H-He-H_2O)

Assuming a three-layer structure

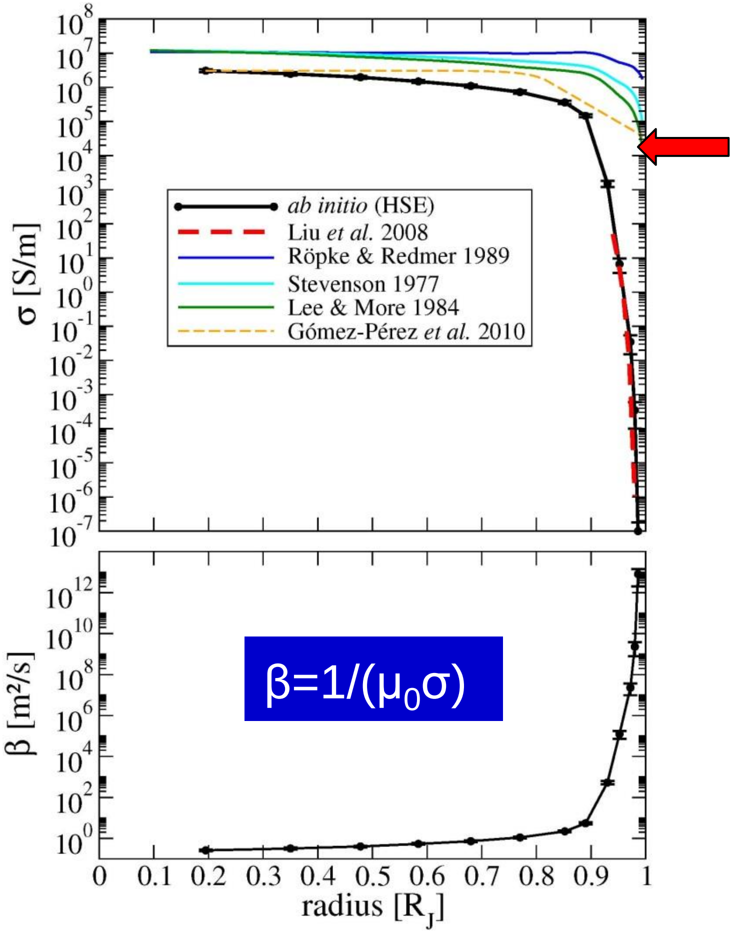




N. Nettelmann et al., ApJ **750**, 52 (2012), M. French et al., ApJS **202**, 5 (2012)

Material Properties along Jupiter`s Isentrope

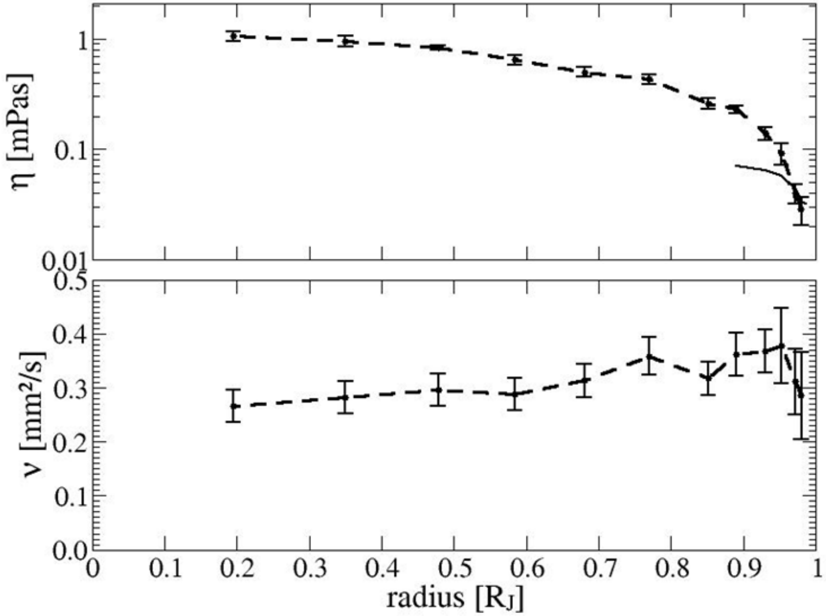
M. French et al., ApJS **202**, 5 (2012): self-consistent EOS and material data from DFT-MD.
Used for planetary modeling (interior, dynamo, evolution)



MIT

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

$\eta(H_2O@20^{o}C)$ = 1 mPas



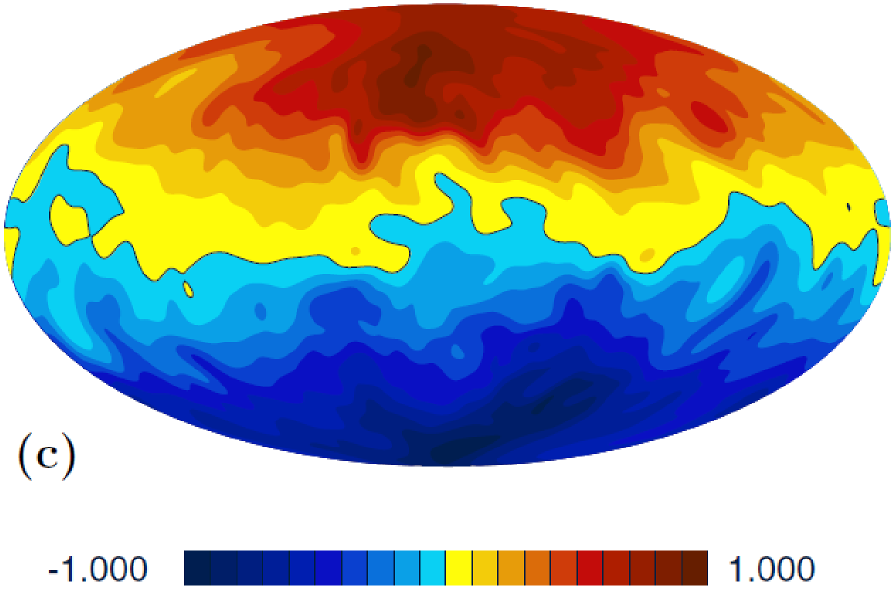
Dynamic (η) and kinematic (ν=η/ρ) viscosity along Jupiter`s isentrope.

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

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

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.

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

DFG SPP 1488 Planetary Magnetism (2011-2016):

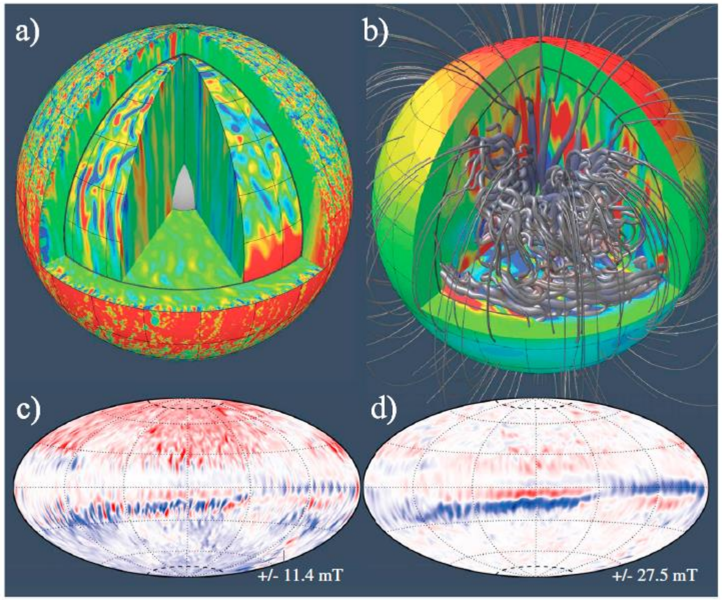


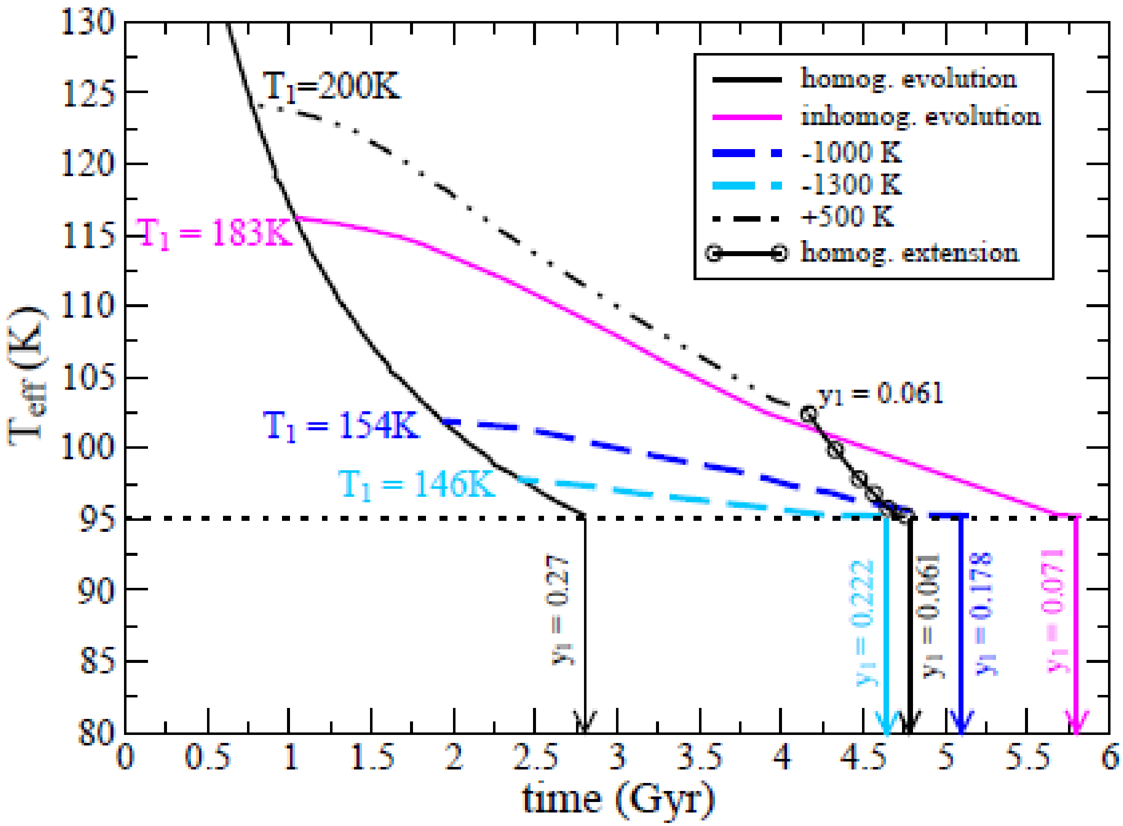
Figure 2. (a) The azimuthal flow component on the outer surface and the right cut, and the radial flow component in the equatorial and left cuts. The inset sphere slices visualize the weaker flow at greater depths. The right inset shows the azimuthal flow amplified by a factor of 10, and the left inset shows the radial flow amplified by a factor of 2.5. The flow amplitude strongly increases with radius, while the length scale decreases. (b) The radial magnetic field on the outer surface and the left cut. The surface field has been amplified by a factor of 10. The right and horizontal cuts (at −10°) show the azimuthal magnetic field. The thickness of the magnetic field lines has been scaled with the third root of the local magnetic field strength. (c and d) The radial and azimuthal magnetic fields at the transition radius 0.87 r_o that is marked with a dark grey line in Figures 2a and 2b. Yellow/red (blue) indicates outward (inward) or eastward (westward) directions.

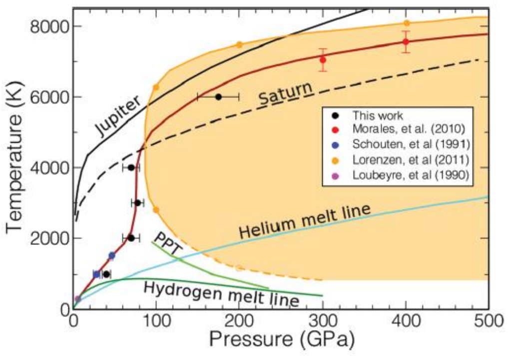
T. Gastine et al., GRL **41**, 5410 (2014)

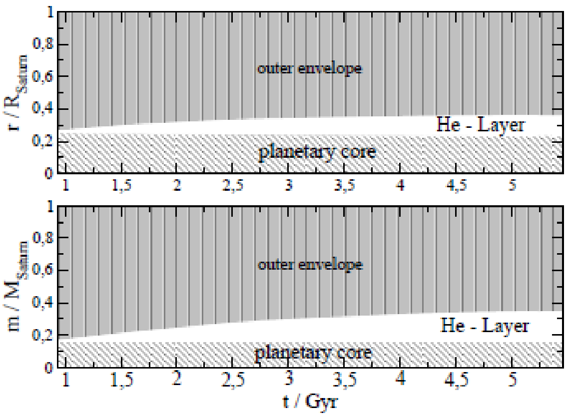
Saturn Cooling Curves using the 2009 Lorenzen et al. H-He Phase Diagram

Lorenzen H-He EOS with demixing available for all He concentrations.

Shifts by $\Delta T = -1300$ K and $\Delta T = +500$ K yield the correct cooling time.







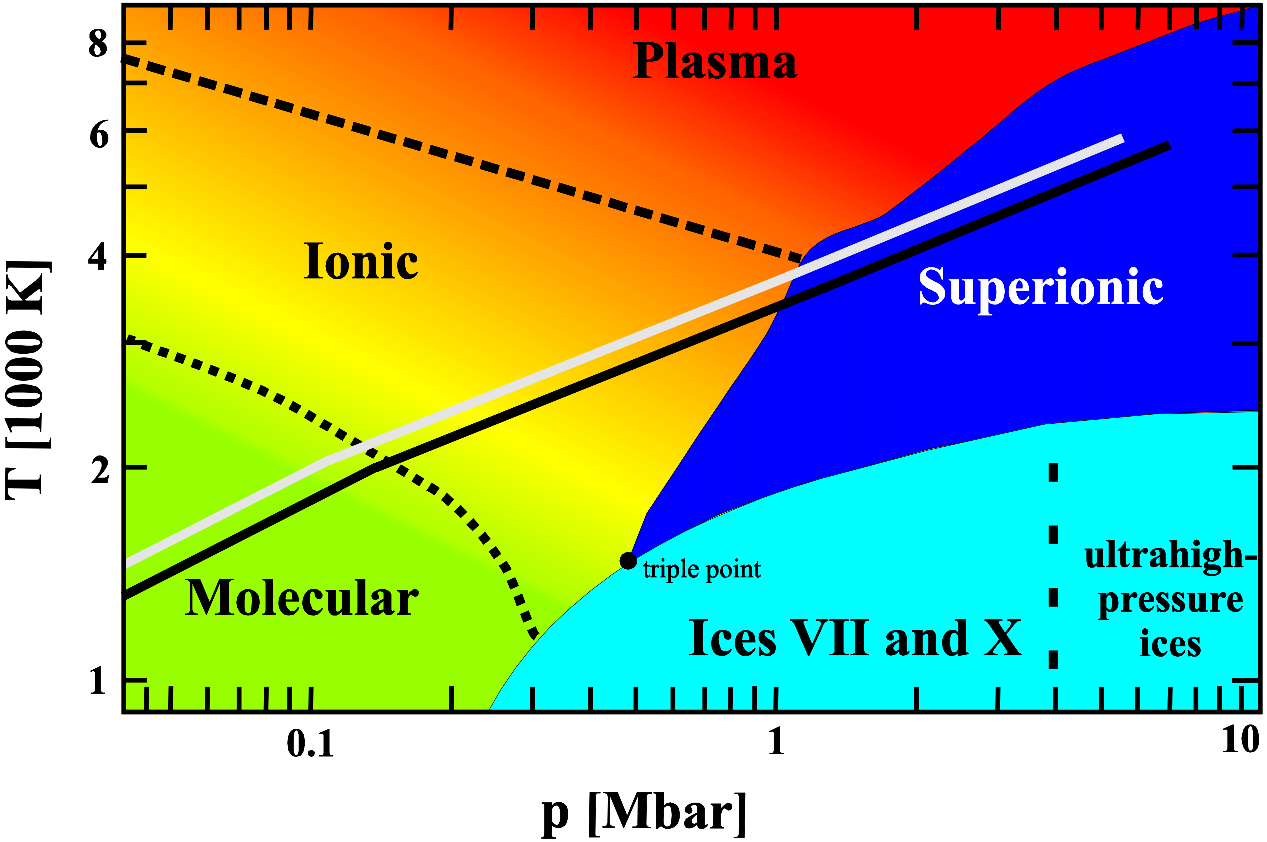
R. Püstow, N. Nettelmann, W. Lorenzen, RR, Icarus **267**, 323 (2016).

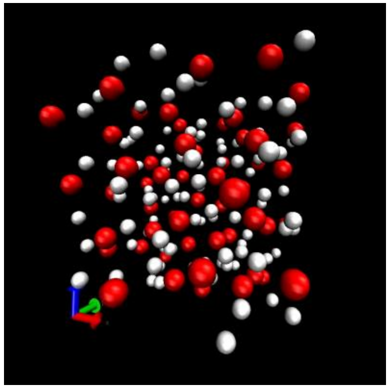
New calculations based on vdW-DF H-He EOS for interior and evolution are on the way.

Ice Giants – High Pressure Phase Diagram for C-N-O-H: H_2O

RR et al., Icarus **211**, 798 (2011)

Uranus (white)
Neptune (black)





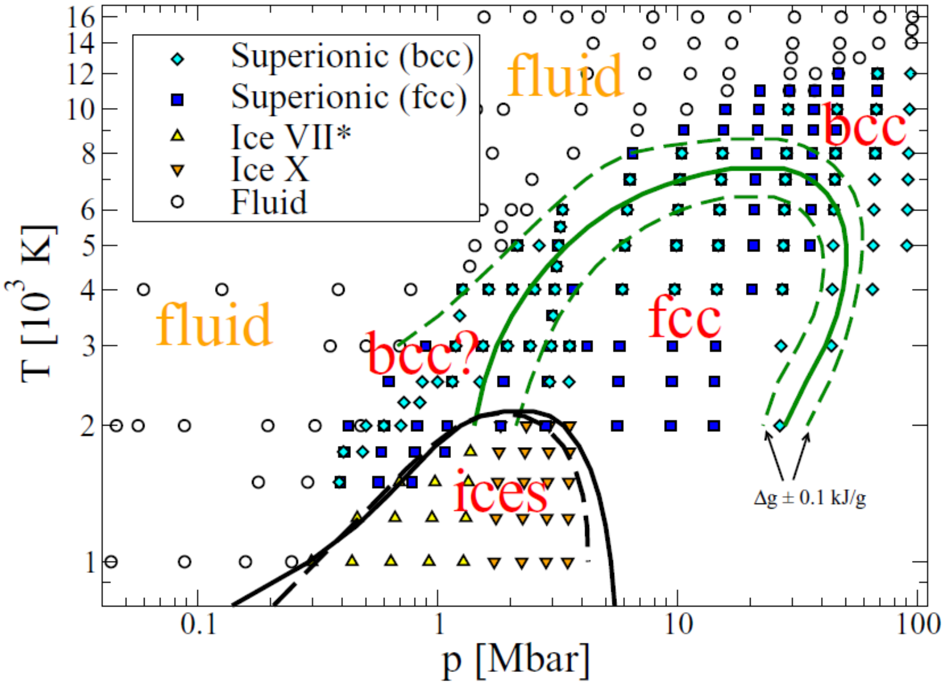
C. Cavazzoni et al.,
Science **283**, 44 (1999)
T.R. Mattsson et al.,
PRL **97**, 017801 (2006)
E. Schwegler et al.,
PNAS **105**, 14779 (2008)
H.F. Wilson et al.,
PRL **110**, 151102 (2013)

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

Water ices VII and X:
M. French, RR, PRB **91**, 014308 (2015)
Superionic bcc and fcc phases:
M. French et al., PRB **93**, 022140 (2016)

H_2O: Superionic Phases and Conductivity

Dynamo (deep interior) and Ohmic dissipation (atmosphere)

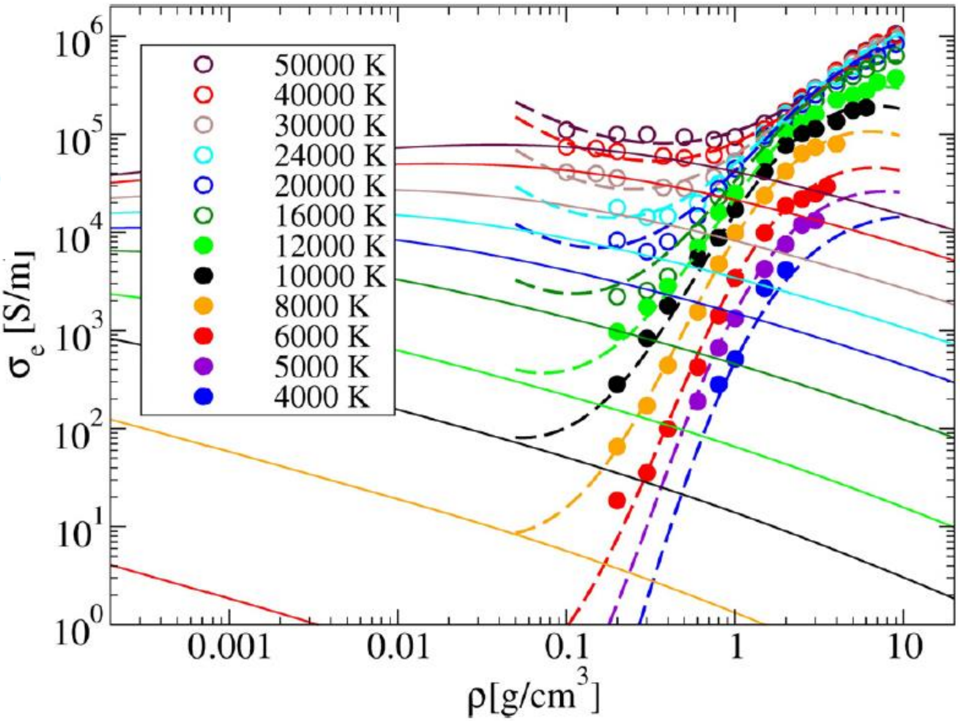


M. French, RR, PRE **93**, 022140 (2016)

Free energy functional for the EOS of ice VII and X.
Small differences between EOS data for fcc and bcc SI.

DFT data from Kubo-Greenwood formula.
Dashed lines: fit function.
Solid lines: multi-component conductivity model for low-density fluid.

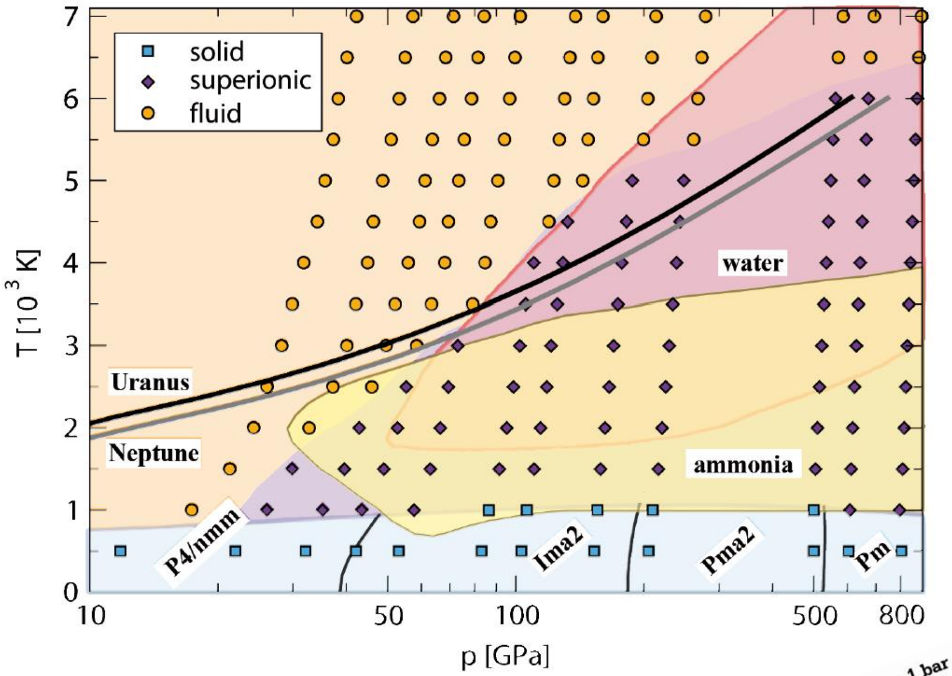
M. French, RR, PoP **24**, 092306 (2017)



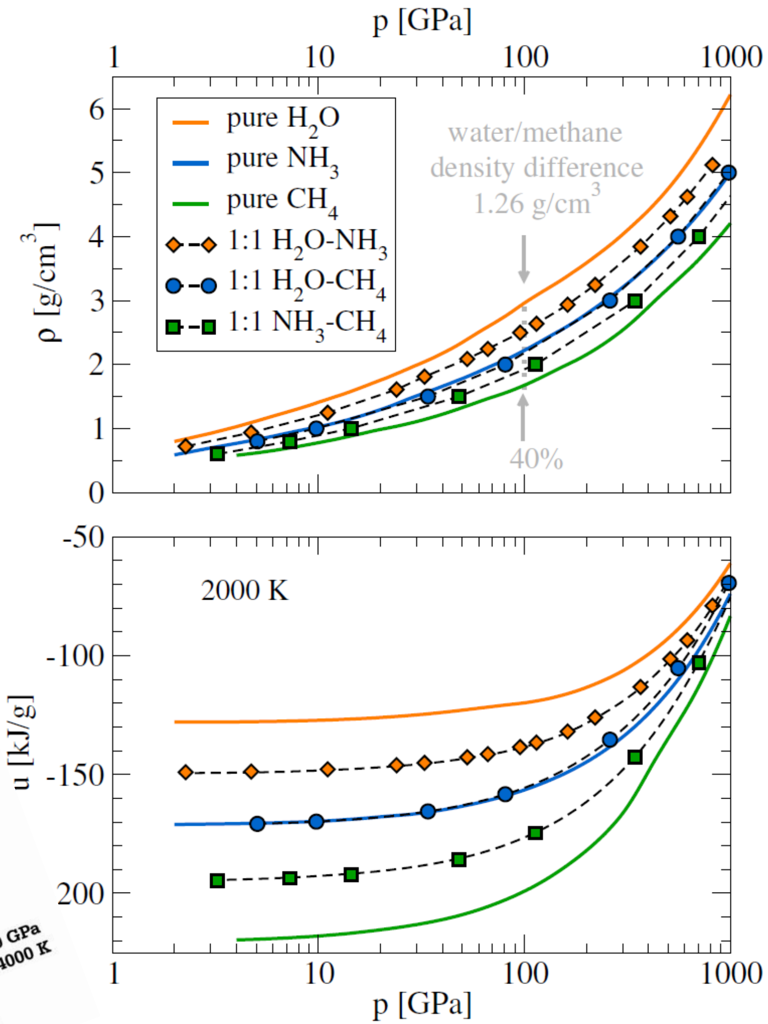
Uranus and Neptune: C-N-O-H

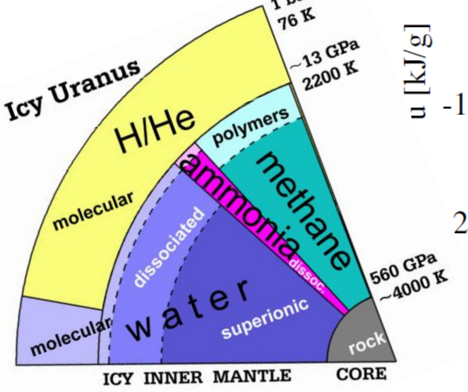
$H_2O:NH_3$ = 1:1 mixture:
Superionic phase occurs as in H_2O, NH_3!

Validity of linear mixing for C-N-O-H:
Amagat`s law works well!



M. Bethkenhagen et al.,
JPCA **199**, 10582 (2016)





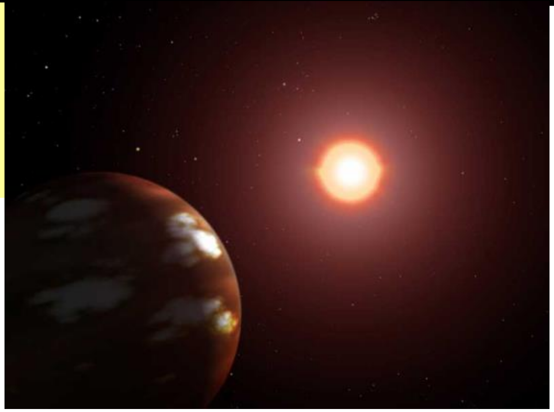
M. Bethkenhagen et al., ApJ **848**, 67 (2017)

Neptune-sized Exoplanet GJ 436b

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

	Neptune	**GJ 436b**
mass [$M_\oplus$]	17.13	22.2 ± 1
radius [$R_\oplus$]	3.86	4.327 ± 0.183
surface temperatur [K]	70 (at 1 bar)	712 ± 36
semi major axis [AU]	30	0.0291 ± 0.0004
period	165 years	2.6439 days

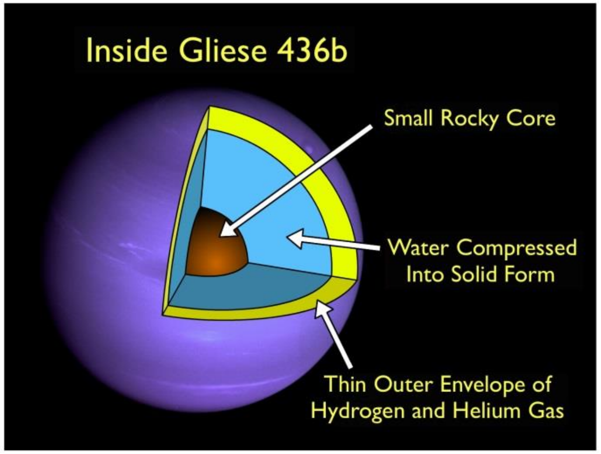
Host star is M Dwarf with T_{eff}=3350 K and
M=0.44 M_{Sun}, 33 Ly away (Leo)
H.L. Maness et al., PASP **119**, 90 (2007)



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

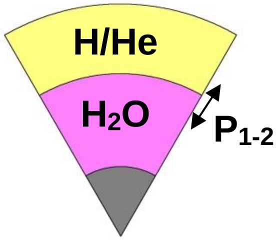
GJ 436b: Neptune-like or Super-Earth?

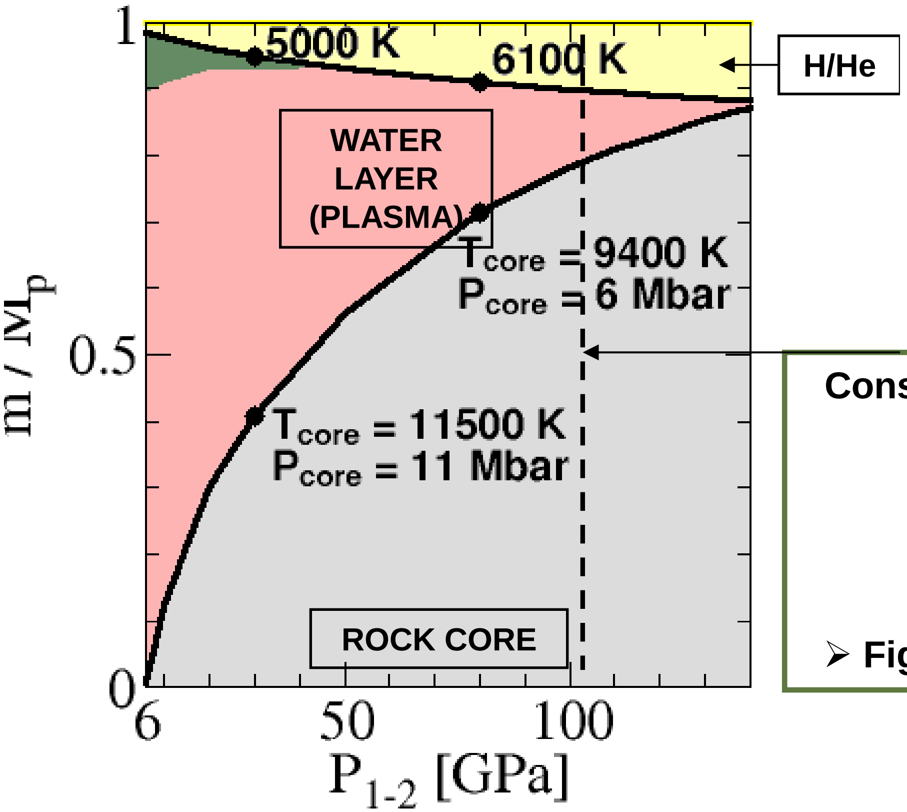
J. Wright: exoplanets.eu (2007)



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%

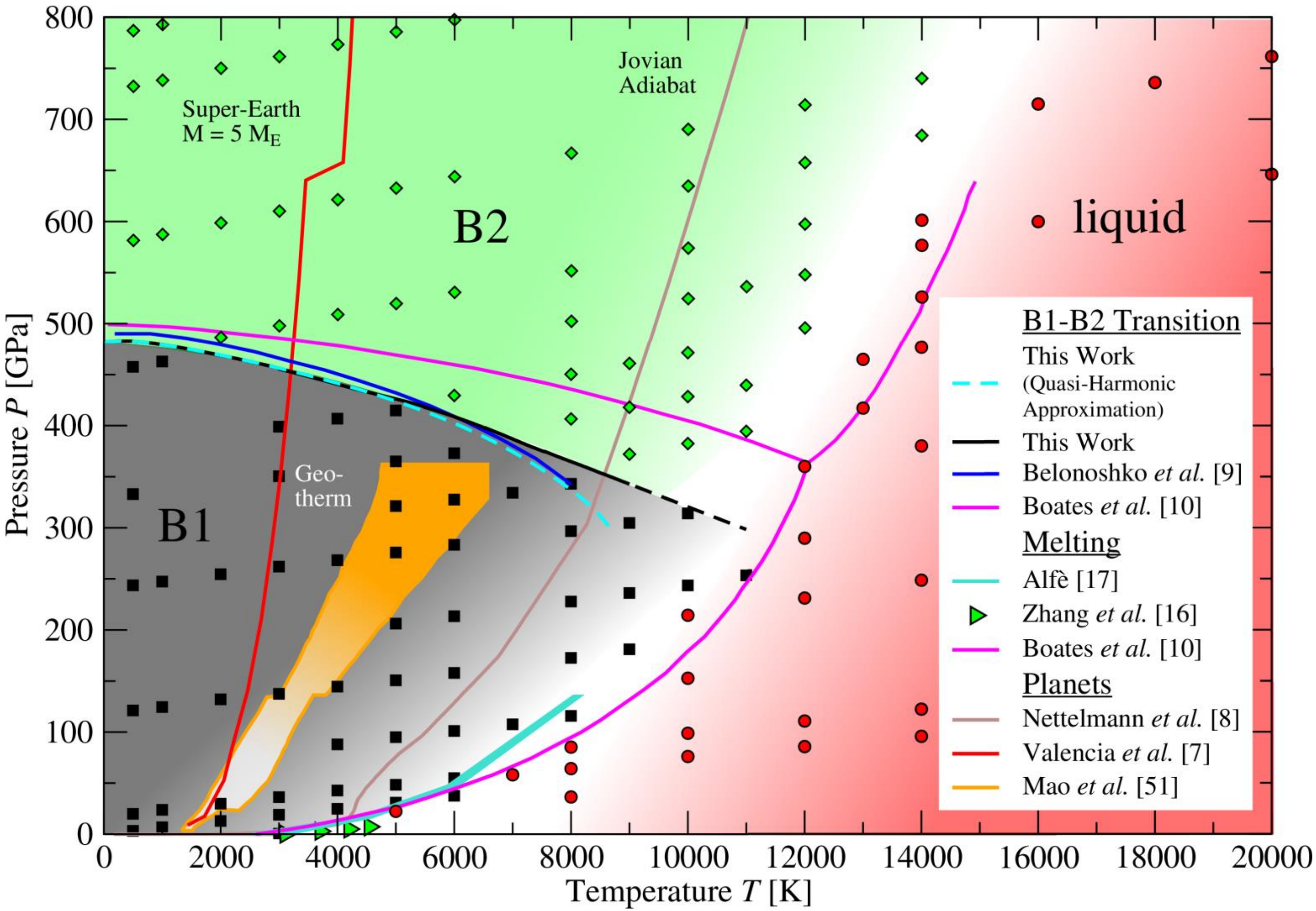
- **Figueira et al., A&A (2009)**

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

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

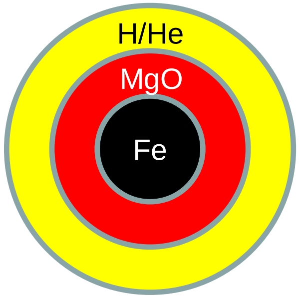
High Pressure Phase Diagram for MgO-FeO-SiO_2 – Earth, super-Earths

MgO: D. Cebulla, RR, PRB **89**, 134107 (2014)



Dynamic compression experiments:
McWilliams et al. (2012), Coppari et al. (2013), Root et al. (2015).

M-R Relation and Interior Models for Super-Earth Kepler 10b

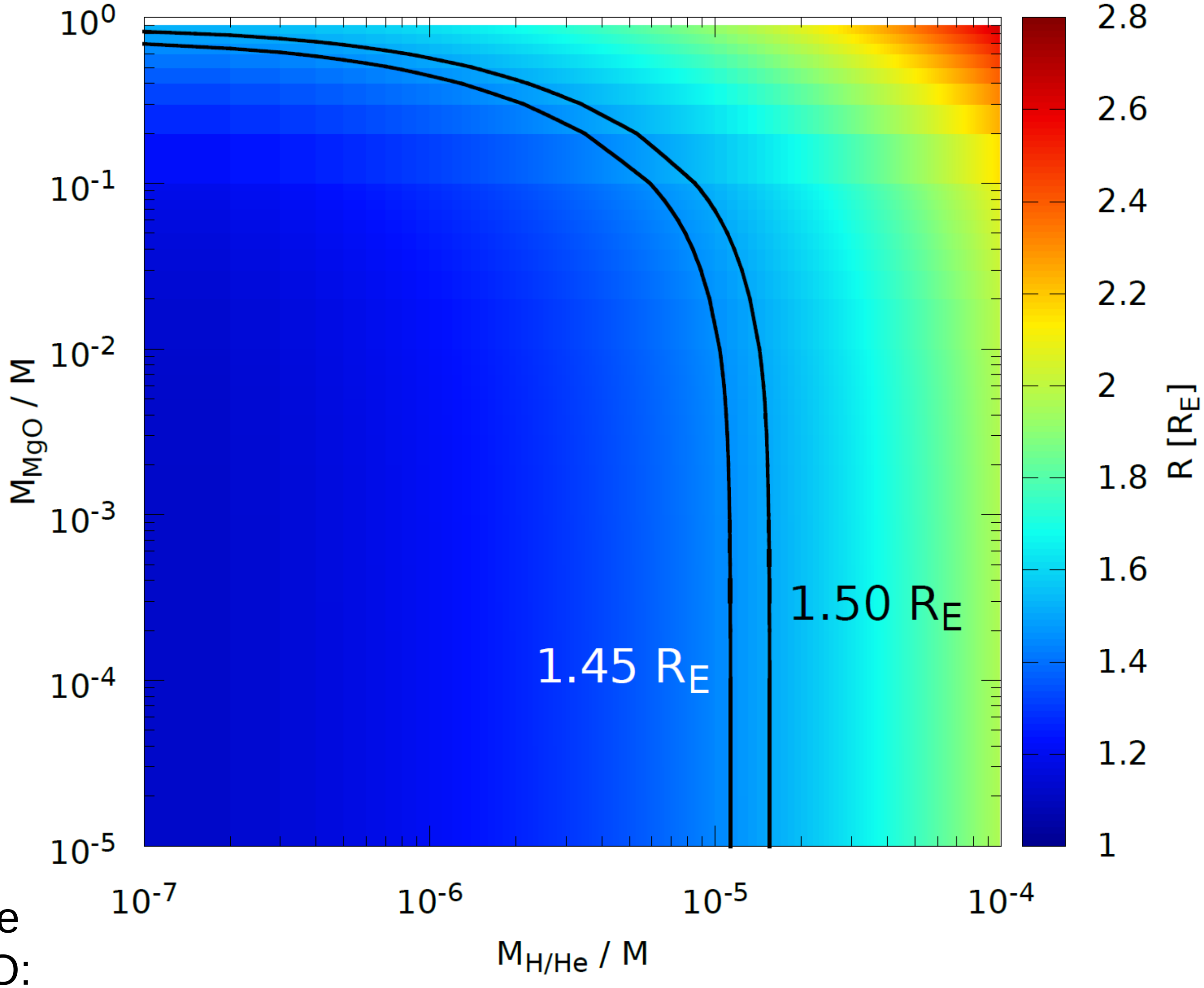


G star 560 Ly away

Kepler 10b:
R~1.475 R_E
M~4.6 M_E
a=0.01864 AU
T=0.8375 d

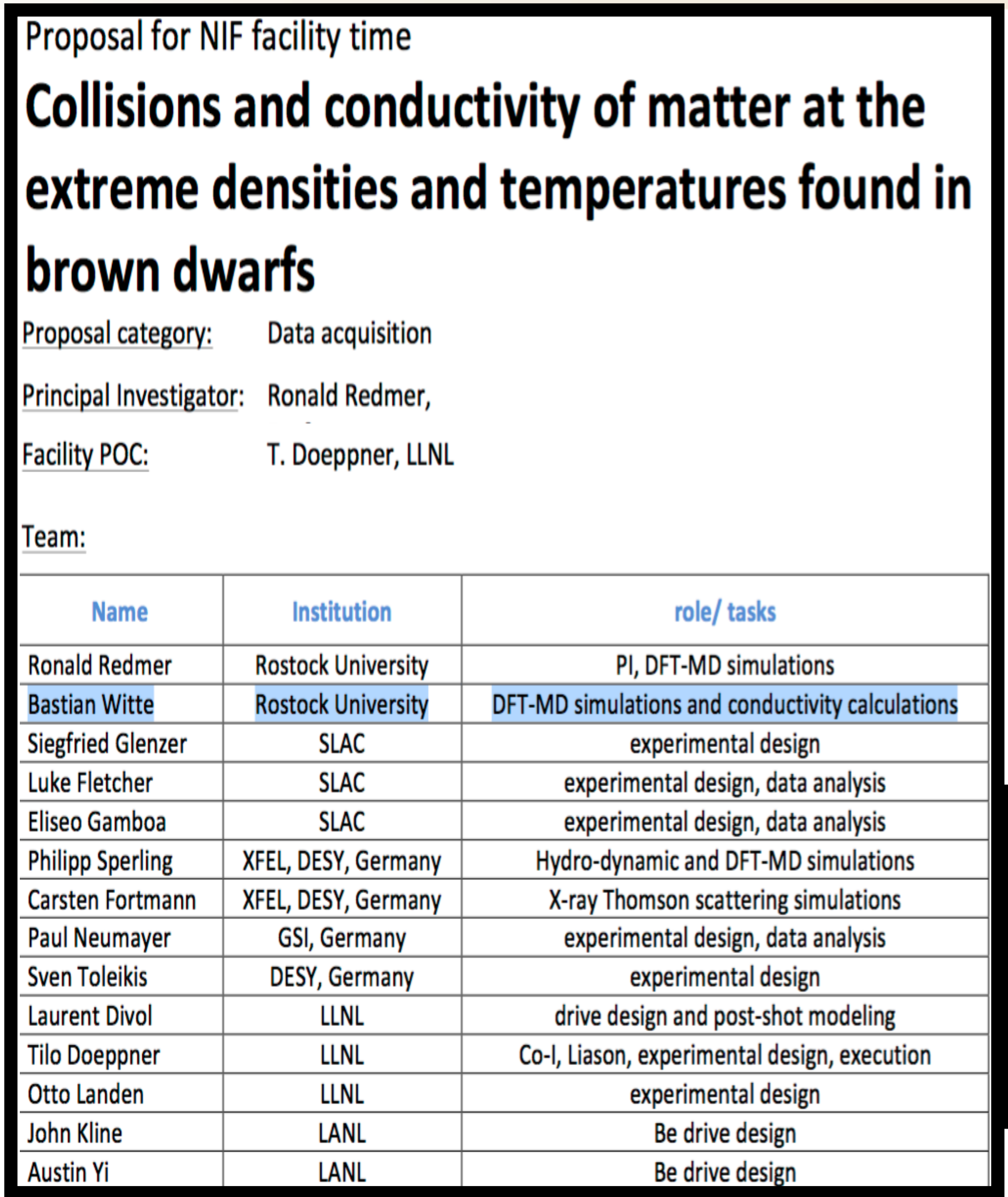
Kepler 10c:
R~2.35 R_E
M~17.2 M_E
a=0.241 AU
T=45.3 d

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



C. Kellermann, RR (submitted)

Discovery Science proposal: 3 NIF shot days granted - D_WDM_XRTS_Be 2017/11/07-08



Proposal for NIF facility time

Collisions and conductivity of matter at the extreme densities and temperatures found in brown dwarfs

Proposal category: Data acquisition

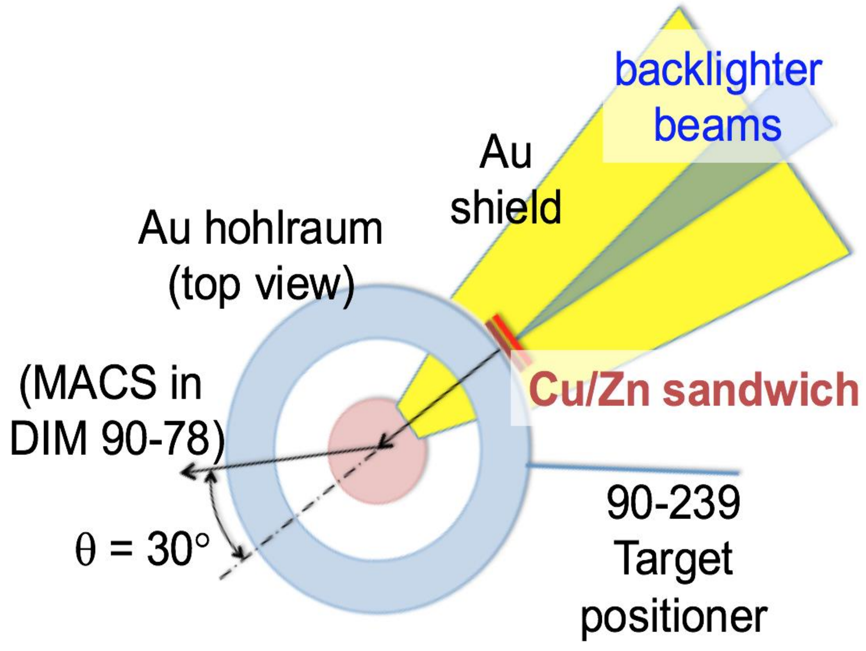
Principal Investigator: Ronald Redmer,

Facility POC: T. Doeppner, LLNL

Team:

Name	Institution	role/ tasks
Ronald Redmer	Rostock University	PI, DFT-MD simulations
Bastian Witte	Rostock University	DFT-MD simulations and conductivity calculations
Siegfried Glenzer	SLAC	experimental design
Luke Fletcher	SLAC	experimental design, data analysis
Eliseo Gamboa	SLAC	experimental design, data analysis
Philipp Sperling	XFEL, DESY, Germany	Hydro-dynamic and DFT-MD simulations
Carsten Fortmann	XFEL, DESY, Germany	X-ray Thomson scattering simulations
Paul Neumayer	GSI, Germany	experimental design, data analysis
Sven Toleikis	DESY, Germany	experimental design
Laurent Divol	LLNL	drive design and post-shot modeling
Tilo Doeppner	LLNL	Co-I, Liason, experimental design, execution
Otto Landen	LLNL	experimental design
John Kline	LANL	Be drive design
Austin Yi	LANL	Be drive design

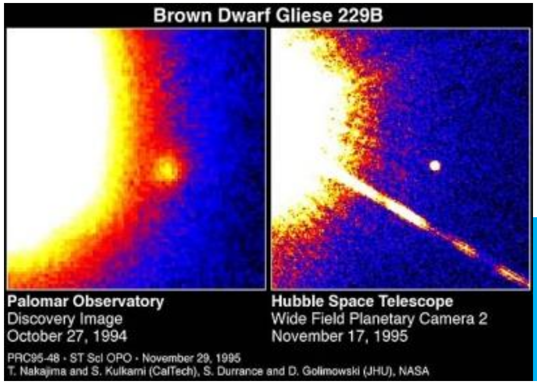
Collective XRTS with Be at 40 g/cm^3



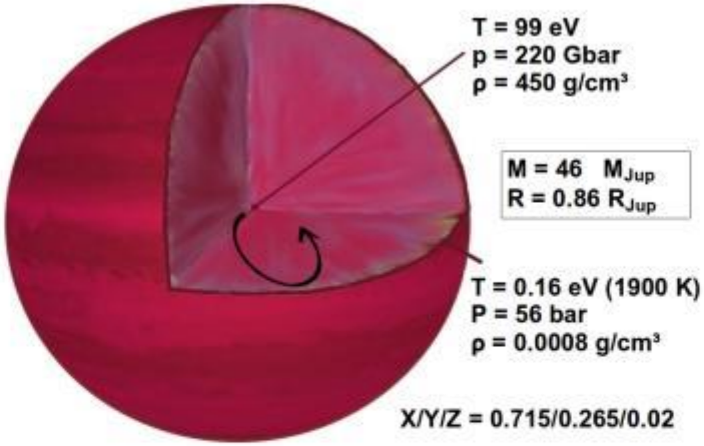
- Number of beams:	192
- Total energy:	≤ 0.9 MJ
- Total peak power:	200TW
- per beam:	< 1.1 TW (except backlighter beams)

Physics of Brown Dwarfs

- **Jupiter-sized: 13 M_{Jup} < M < 75 M_{Jup}**
- **Degenerate H-He matter**
- **Interior – evolution – dynamo ?**
- **Fully convective layer ?**

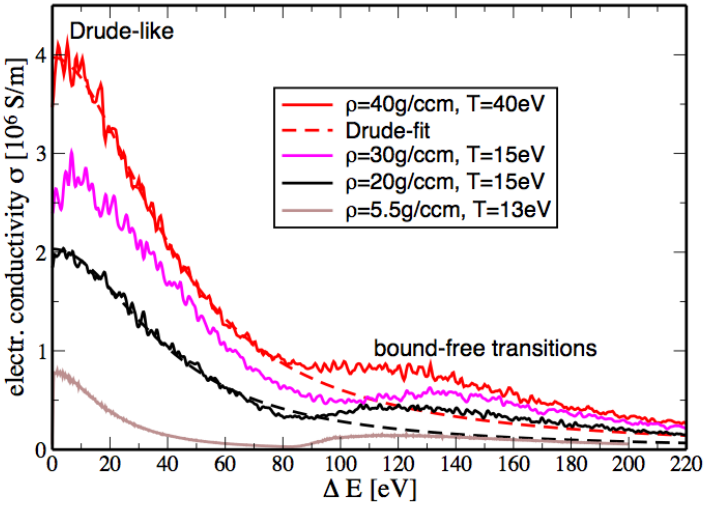


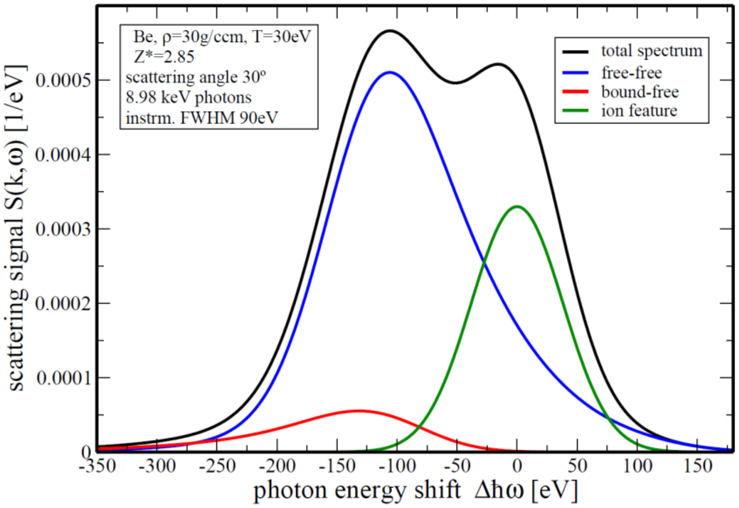
Gliese 229 B
1995, 18.8 Ly
M1 + T6 (50 AU)



A. Becker et al., ApJS **215**, 21 (2014):
H-He EOS and one-layer interior models

NIF shots will demonstrate
collective XRTS in dense Be





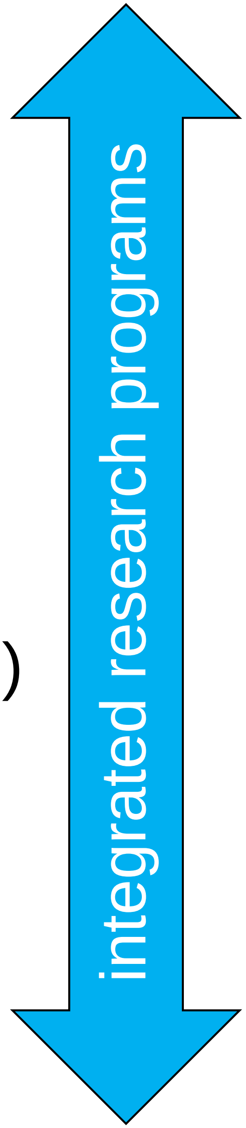
DFT-MD: B. Witte

Summary & Outlook

- **Fundamental properties of WDM:**
  → ab initio simulations are an essential tool for
  - **EOS data and high-pressure phase diagram**
  - **conductivities, viscosity**
  - **highly resolved XRTS spectra**

- **Plasma diagnostics: infer plasma properties**
  → analyze DAC and shock wave experiments
  → analyze XRTS experiments (LCLS, European XFEL)

- **Application: planetary physics - understand**
  → diversity of solar/extrasolar planets
  → interior, evolution, magnetic field (dynamo)
  → **BDs: NIF shots D_WDM_XRTS_Be (17/11/07-08)**

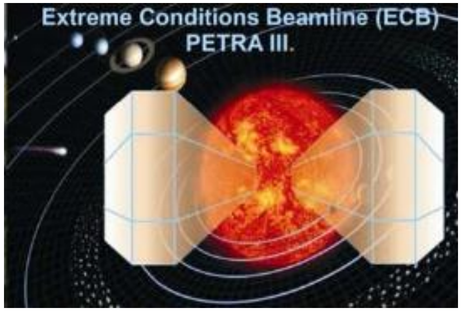

integrated research programs

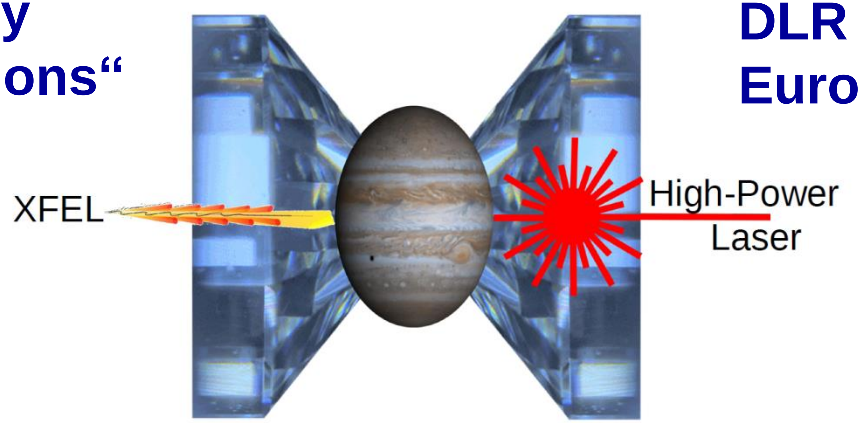
Upcoming Workshops & Conferences

16th International Conference on the Physics of Nonideal Plasmas (PNP-16)
September 24-28, 2018, Saint Malo

7th Joint Workshop on High Pressure, Planetary, and Plasma Physics (HP4)
October 10-12, 2018, DLR Berlin

FOR 2440 „Matter Under Planetary Interior Conditions“





U Rostock
BGI Bayreuth
DESY
DLR Berlin
European XFEL

Many thanks to

Paul Grabowski
and HEDSC Team
for the invitation
and hospitality

Tilo Döppner and
the NIF Team for
the great shot day

All – for coming
and the interest