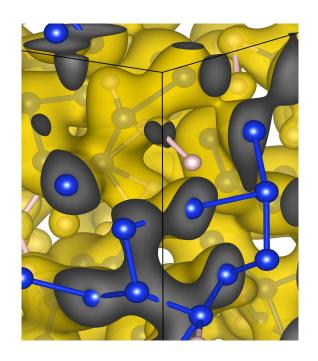
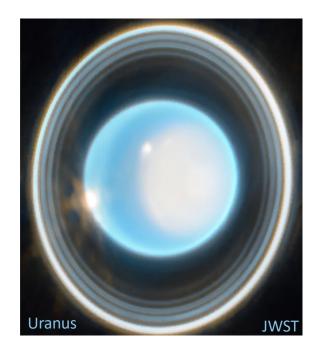
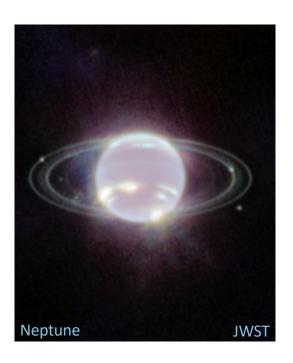
Interior Structure of Uranus and Neptune – Why Don't These Planets Generate Dipolar Magnetic Fields?







Burkhard Militzer

University of California, Berkeley

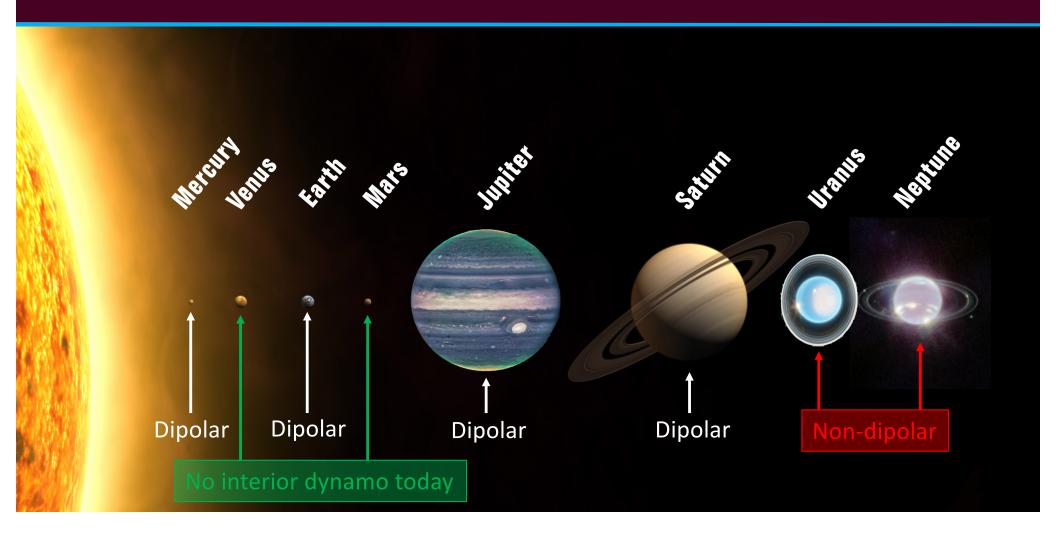
Big Questions that my Group Helps Address

- 1. How did our solar system form?
- 2. What are giant planets made of?
- 3. How do materials behave at high pressure?

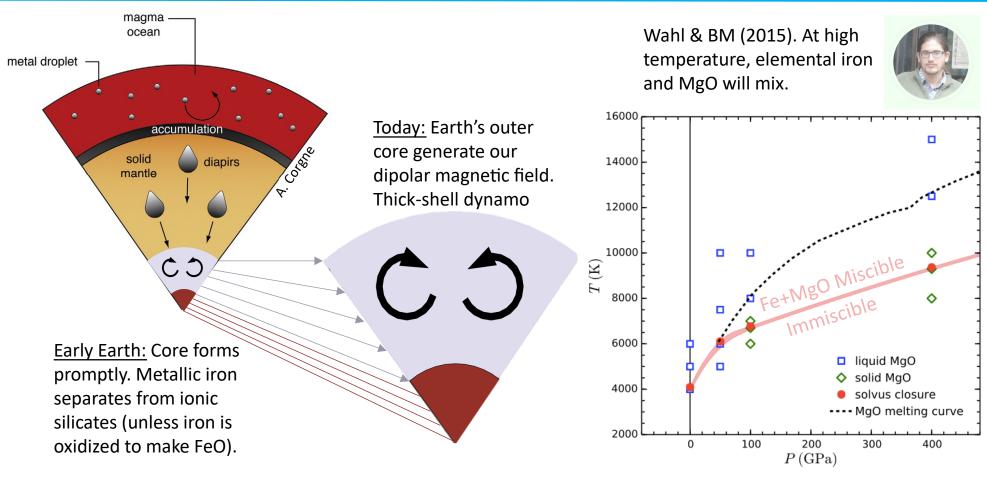




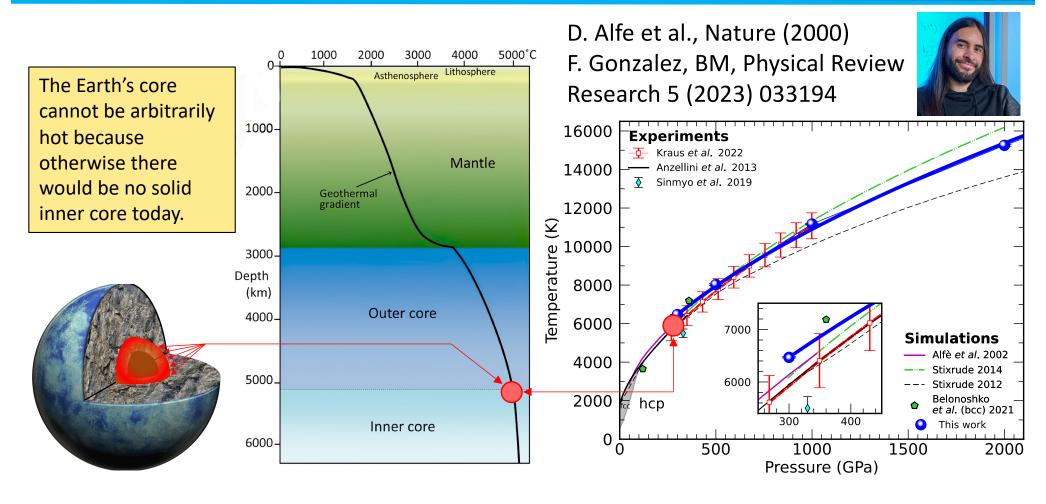
Magnetic Fields in our Solar System



Earth cores forms because iron and silicates are immiscible. Magnetic Field in Liquid Outer Core

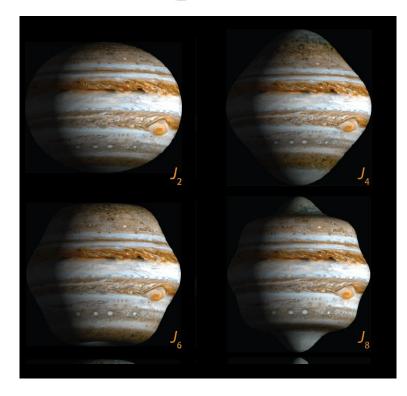


Earth has a solid inner core. So the Melting Temperature of Iron Constrains the Temperature of Earth's Core.



Gravity Field Measurements represented by harmonics J_n

$$V(r, \mu) = \frac{GM}{r} \left[1 - \sum_{n=1}^{\infty} \left(\frac{a}{r} \right)^{2n} J_{2n} P_{2n}(\mu) \right]$$



Difference in Precision between single Flyby and Orbiting Mission

Pioneer+Voyager Jupiter flybys

Voyager Uranus flyby

$$J_2 = 14697 \pm 1$$
 $J_2 = 3510 \pm 0.72$
 $J_4 = -584 \pm 5$ $J_4 = -33.61 \pm 1$
 $J_6 = 31 \pm 20$ $J_6 = ?$

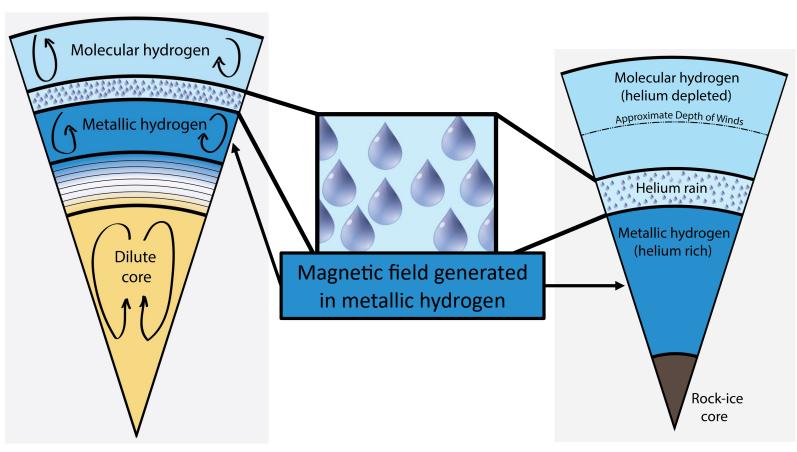
Measurements of Juno orbiter

$$J_2 = 14696.5735 \pm 0.0017$$

 $J_4 = -586.6085 \pm 0.0024$
 $J_6 = 34.2007 \pm 0.0067$

Uranus orbiter would increase gravity precision by factor 1000.

Models with Helium Rain for Jupiter and Saturn



Jupiter's interior with dilute core (Militzer et al., 2022)

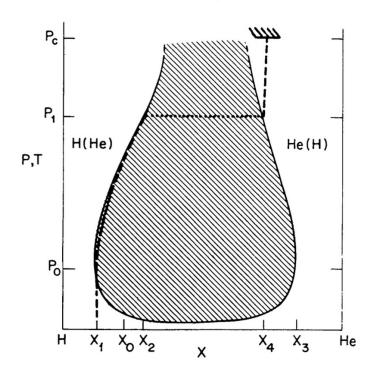
Saturn's interior

Stevenson & Salpeter (1977): Helium Rain Hypothesis to Explain Excess in Saturn's Thermal Emission

THE DYNAMICS AND HELIUM DISTRIBUTION IN HYDROGEN-HELIUM FLUID PLANETS

D. J. STEVENSON* AND E. E. SALPETER

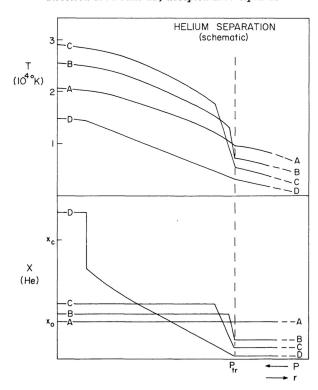
Center for Radiophysics and Space Research and Physics Department, Cornell University Received 1976 June 23; accepted 1977 April 13



THE PHASE DIAGRAM AND TRANSPORT PROPERTIES FOR HYDROGEN-HELIUM FLUID PLANETS

D. J. STEVENSON AND E. E. SALPETER

Center for Radiophysics and Space Research and Physics Department, Cornell University Received 1976 June 23; accepted 1977 April 13

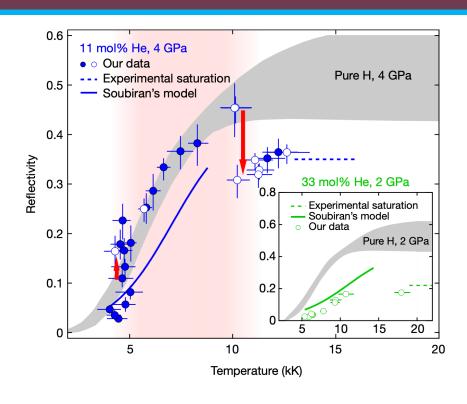


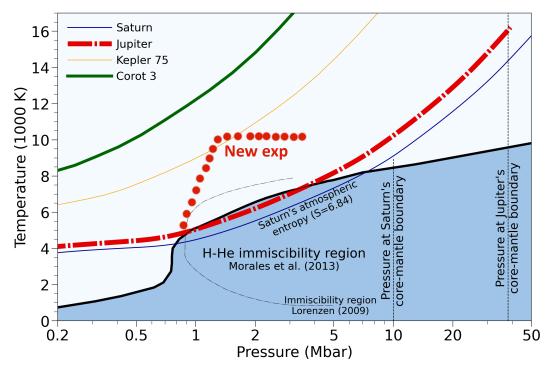
Evidence of hydrogen-helium immiscibility at Jupiter-interior conditions

https://doi.org/10.1038/s41586-021-03516-0

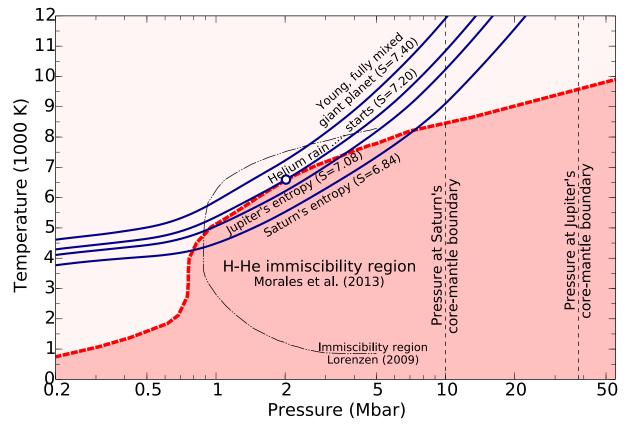
Received: 13 October 2015

S. Brygoo $^{1\boxtimes}$, P. Loubeyre $^{1\boxtimes}$, M. Millot 2 , J. R. Rygg 3 , P. M. Celliers 2 , J. H. Eggert 2 , R. Jeanloz 4 & G. W. Collins 3





Planets cool convectively: So we assume most of their interior layers are isentropic and homogeneous





One enjoyable way to observe convection: Ordering miso soup in a sushi restaurant

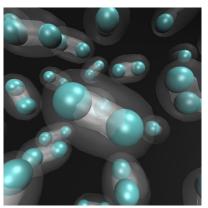
What are ab initio simulations?

Schrödinger equation:

$$-\frac{\hbar^2}{2m} \vec{\nabla}^2 \psi(\vec{r}) + V(\vec{r}) \psi(\vec{r}) = E \psi(\vec{r})$$

Look for an antisymmetric solution (Pauli exclusion):

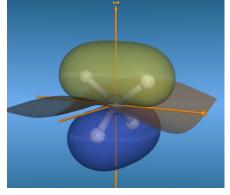
$$\Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \chi_1(\mathbf{x}_1) & \chi_2(\mathbf{x}_1) & \cdots & \chi_N(\mathbf{x}_1) \\ \chi_1(\mathbf{x}_2) & \chi_2(\mathbf{x}_2) & \cdots & \chi_N(\mathbf{x}_2) \\ \vdots & \vdots & & \vdots \\ \chi_1(\mathbf{x}_N) & \chi_2(\mathbf{x}_N) & \cdots & \chi_N(\mathbf{x}_N) \end{vmatrix}$$



Density functional theory:

Generalized Gradient approximation (PBE)
Hybrid functionals (HSE for conductivity)

Quantum Monte Carlo



Methane - molecular orbitals

Simulation of molecular hydrogen

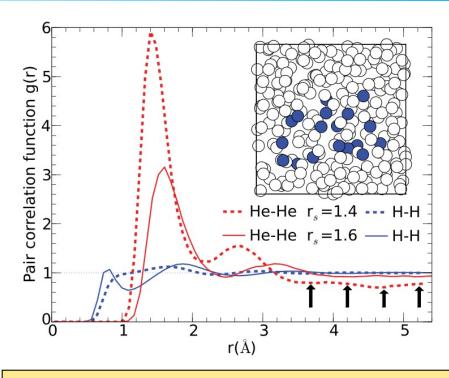
Calculate Free Energies and Entropy with Thermodynamic Integration. Here Applied to Molecular Hydrogen

For fixed NVT
$$F_B - F_A = \int_0^1 d\lambda \, \langle U_B - U_A \rangle_\lambda$$

$$V_{\lambda} = \lambda V_{\text{KS}} + (1 - \lambda) V_{\text{cl}},$$

$$V = \sum_{i,j,i>j} g_{ij} V_{\text{mol}}(r_{ij}) + (1 - g_{ij}) V_{\text{inter}}(r_{ij})$$

Provides access to entropy and free energies that cannot be derived from standard MD simulations. For hydrogen, see BM, Phys. Rev. B 87 (2013) 014202.



Inside the immiscibility region, the simulations may spontaneously phase separate. Look for drop in g(r) at large distances.

Determine Phase Transformations Either Dynamically or Thermodynamically

Perform MD simulations and wait for the system change to a new phase

- Heat until it melts
- Heat until it mixes
- Two-phase simulations
- Spontaneous phase separation

Gibbs free energy calculations

$$F_B - F_A = \int_0^1 d\lambda \, \langle U_B - U_A \rangle_{\lambda}$$

$$U(\lambda) = U_A + \lambda(U_B - U_A)$$

$$G_{DFT} = F_{DFT} + P_{DFT}V$$

Gibbs free energy (Which is more stable?)

$$TS_{DFT} = U_{DFT} - F_{DFT}$$

Entropy (ionic & electronic) (Construct isentropes)

Uranus

Mass = 14.5 Earths

Radius = 4.0 Earths

Density = 1.3 gram/cm³

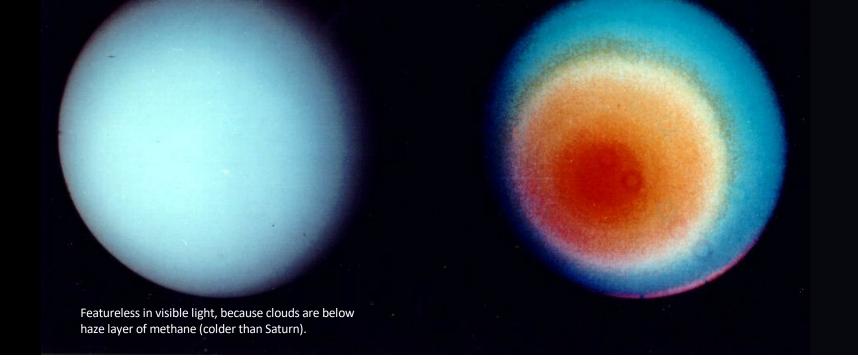
Distance: 19.2 AU

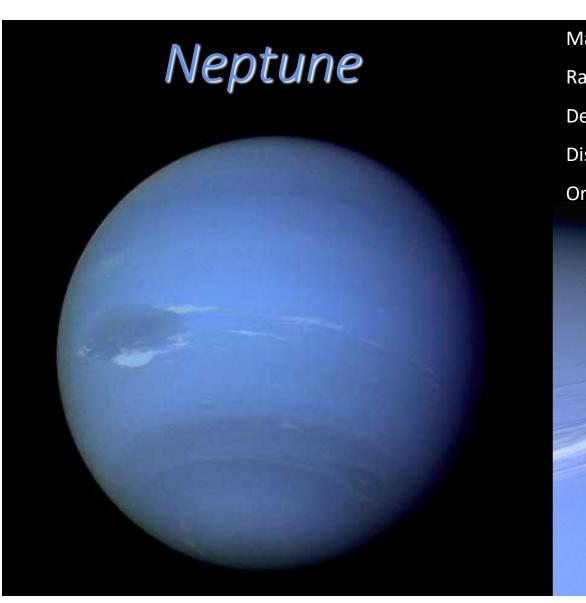
Orbital Period: 84 years

Rotation period: 17.2 hours.

Visible Light:

Infrared Light (almost no thermal emission):





Mass = 17 Earths

Radius = 3.9 Earths

Density = 1.76 x water

Distance: 30 AU

Orbital Period: 163 years

Cyclonic storms.

Uranus Neptune

Open questions:

- Tilt of Uranus' rotation axis (giant impact hypothesis)
- Different CH₄ abundances (Uranus: 2.3 %, Neptune 1.4%)
- Uranus has almost no intrinsic heat flux (thermal boundary layer?)
- Uranus has a regular set of satellites. Neptune has only two in inclined orbits. (Triton is almost planet-like.)
- Interior composition uncertain ("Ice giants" misnomer)
- Unusual magnetic fields

Disclaimer: Due to lack of time, the following innovative papers cannot be discussed in this talk

- M Podolak, A Weizman, M Marley, Comparative models of Uranus and Neptune. Planet. Space Sci. 43, 1517–1522 (1995).
- K Soderlund, M Heimpel, E King, J Aurnou, Turbulent models of ice giant internal dynamics: Dynamos, heat transfer, and zonal flows. Icarus 224, 97–113 (2013).
- R Helled, P Bodenheimer, The formation of Uranus and Neptune: Challenges and implications for intermediate-mass exoplanets. The Astrophys. J. 789, 69 (2014).
- K Soderlund, S Stanley, The underexplored frontier of ice giant dynamos. Philos. Trans. Royal Soc. A 378, 20190479 (2020).
- E Bailey, DJ Stevenson, Thermodynamically governed interior models of Uranus and Neptune. The Planet. Sci. J. 2, 64 (2021).
- L Stixrude, S Baroni, F Grasselli, Thermal and tidal evolution of Uranus with a growing frozen core. The Planet. Sci. J. 2, 222 (2021).
- N Movshovitz, JJ Fortney, The promise and limitations of precision gravity: Application to the interior structure of Uranus and Neptune. The Planet. Sci. J. 3, 88 (2022).

1986: Voyager 2 arrives at Uranus and finds it has no strong dipolar field. Why might that be?

Podolak, Hubbard, Stevenson write in "Uranus" edited by Bergstrahl et al.

The most obvious and most popular explanation of the unusual field geometry is that we arrived at Uranus during a reversal. Indeed, the observed field geometry has some similarities to that inferred for Earth during geomagnetic reversals: a tilted dipole and an unusually large quadrupole (Merrill and McElhinny 1983). The problem with this explanation is that if Uranus is similar to Earth, then the probability of encountering the planet during a reversal event is only about 1% (the Earth's field takes a few thousand years to reverse, yet the time between reversals is very long, typically a few hundred thousand years). If we accept the reversal explanation, then we must either accept an improbable chance or say that Uranus differs from the Earth in some very substantial way. The latter explanation seems attractive but dif-

1986: Voyager 2 arrives at Uranus and finds it has no strong dipolar field. Why might that be?

1989: Voyager 2 arrives at Neptune and determined that dred thousand years). If we accept the reversal explanation, then we must either accept an improbable chance or say that Uranus differs from the Earth in some very substantial way. The latter explanation seems attractive but dif-

Ruzmaikin & Starchenko (1991): U+N generate their magnetic fields in a THIN SHELL

On the Origin of Uranus and Neptune Magnetic Fields

A. A. RUZMAIKIN

Institute of Terrestrial Magnetism, Ionosphere and Radio Wave Propagation, Troitsk, Moscow Region, USSR

AND

S. V. STARCHENKO

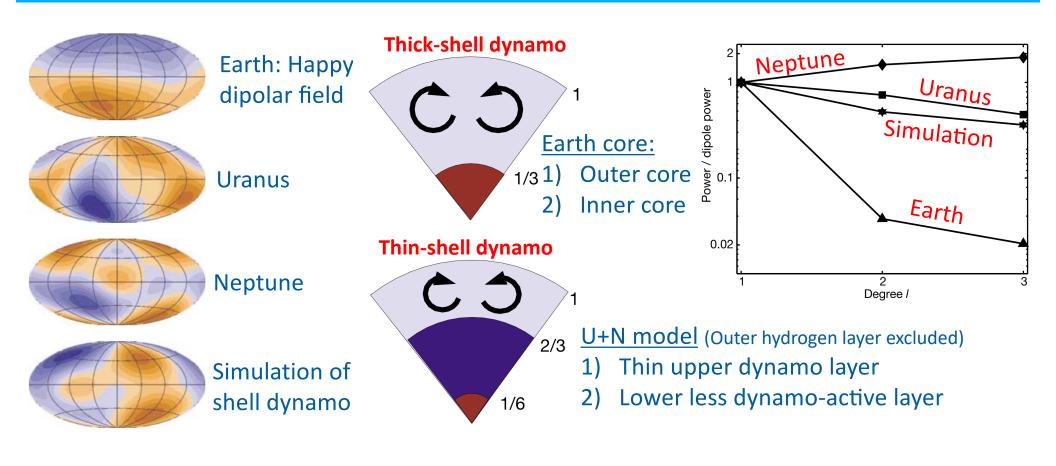
Schmidt Institute of Physics of the Earth, Moscow, USSR

Received July 6, 1990; revised April 9, 1991

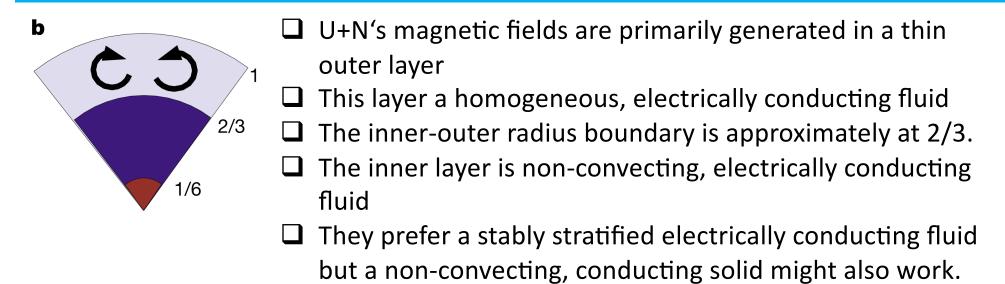
The Uranus and Neptune magnetic fields discovered by Voyager 2 can be explained by a dynamo acting in a thin conductive convective shell existing at the bottom of the icy oceans of the planets. The main helicity and differential rotation are the source for the dynamo which effectively excites nonaxisymmetric modes of the mean magnetic field. Estimates of the magnetic field amplitude in the nonlinear regime and of the inclination between the magnetic moment and the rotation axis are given. © 1991 Academic Press, Inc.

In this paper a model for the generation of the mean magnetic fields of Uranus and Neptune by action of the mean helicity of the convective motions and differential rotation is constructed. The field is generated in a thin shell where the conditions for self-excitation and the rates of growth for the axisymmetric and nonaxisymmetric modes are closed. One result in particular is that axisymmetric and nonaxisymmetric components of the dipole magnetic field are of the same order. The sum of these

Stanley & Bloxham (2004): Numerical Simulations of Thin-Shell Dynamos matched Observed Fields



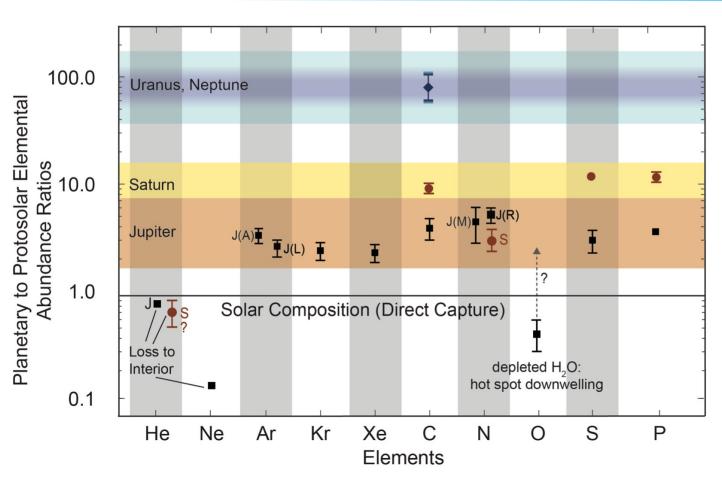
Stanley & Bloxham (2004 and 2006): Most preferred Interior Structure Model



Open questions:

- 1) What is the composition of the upper layer?
- 2) What is the composition of the lower layer?
- 3) Why is the lower layer not convecting?

Atmospheres of Uranus and Neptune are Rich in Carbon (CH₄ was detected)



U+N: $40...100 \times solar$

Saturn: 9 × solar

Jupiter: $4 \times \text{solar}$

Atreya et al. (2016) Sromovsky et al. (2011) Voyager occultation, CH₄ clouds

M. Ross in Nature in 1981: Diamond Rain in U+N

The ice layer in Uranus and Neptune—diamonds in the sky?

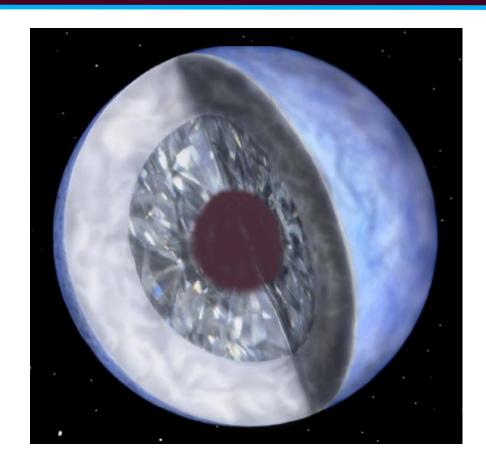
Marvin Ross

University of California, Lawrence Livermore National Laboratory, Livermore, California 94550, USA

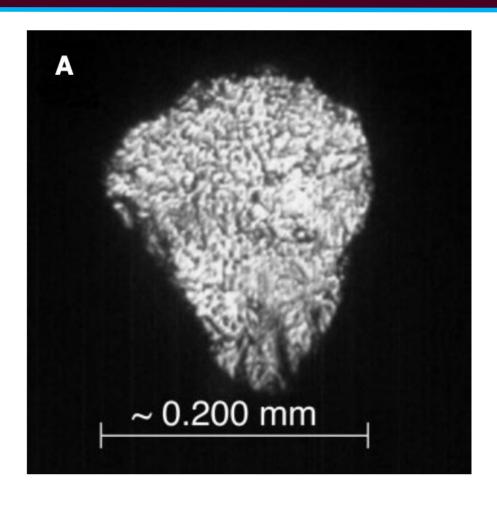
Many of the current models of Uranus and Neptune postulate a three-layer structure, consisting of an inner rocky core, a middle 'ice' layer of fluid, H₂O, CH₄, NH₃ and an outer hydrogenhelium layer of solar composition¹. The estimated pressures and temperatures of the ice layer ranges from about 6 Mbar and 7.000 K at the inner core-ice houndary, to ~0.2 Mbar and 2,200 K at the outer ice/hydrogen-helium boundary. I point out here that shockwave experiments on these liquids²⁻⁵, as well as theoretical studies⁵⁻⁷, imply that the H₂O and NH₃ in the ice layer are almost totally ionized and the CH₄ has been pyrolysed to carbon, possibly in the metallic or diamond form^{8,9}.

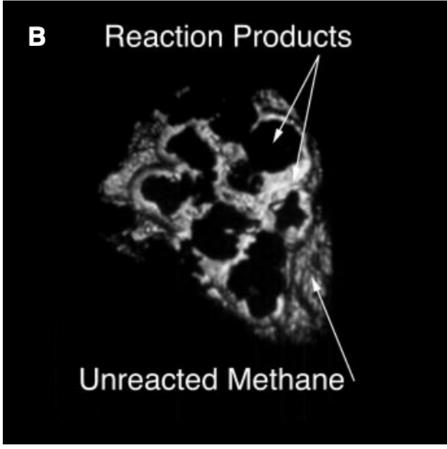
In recent years shock-wave experiments have been carried

which predicted that above 0.20 Mbar and 2,000 K, methane is converted into elemental carbon and molecular hydrogen.



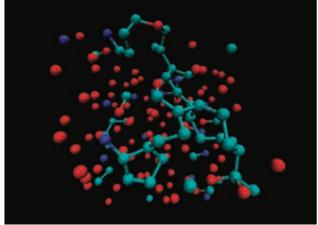
Benedetti et al. (1999): Laser Heated CH₄ forms Diamonds at 10-50 GPa and 2000-3000 K

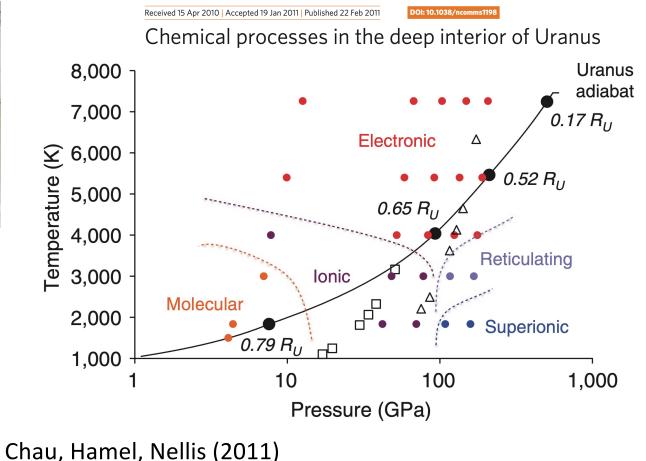




Experimental and Theoretical Work on "Synthetic Uranus" Mixture of H:O:C:N = 28:7:4:1





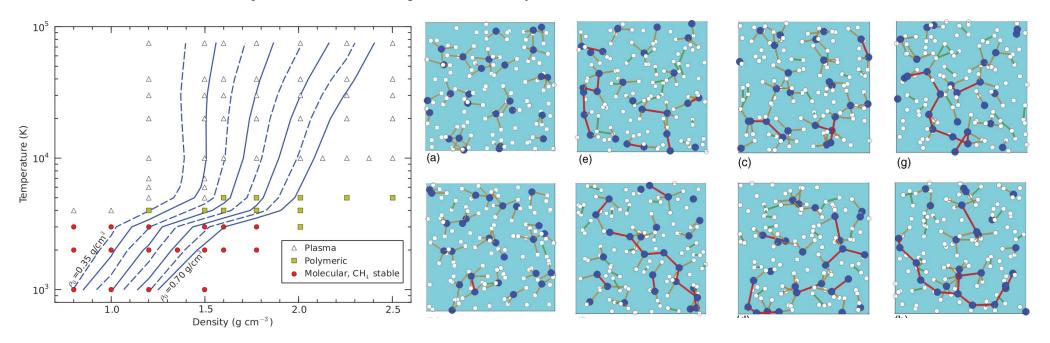


Our paper on polymeric state of methane under shock conditions (2012)

PHYSICAL REVIEW B 86, 224113 (2012)

Ab initio simulations of hot dense methane during shock experiments

Benjamin L. Sherman, Hugh F. Wilson, Dayanthie Weeraratne, and Burkhard Militzer^{2,3}



From my 2013-2016 NSF proposal

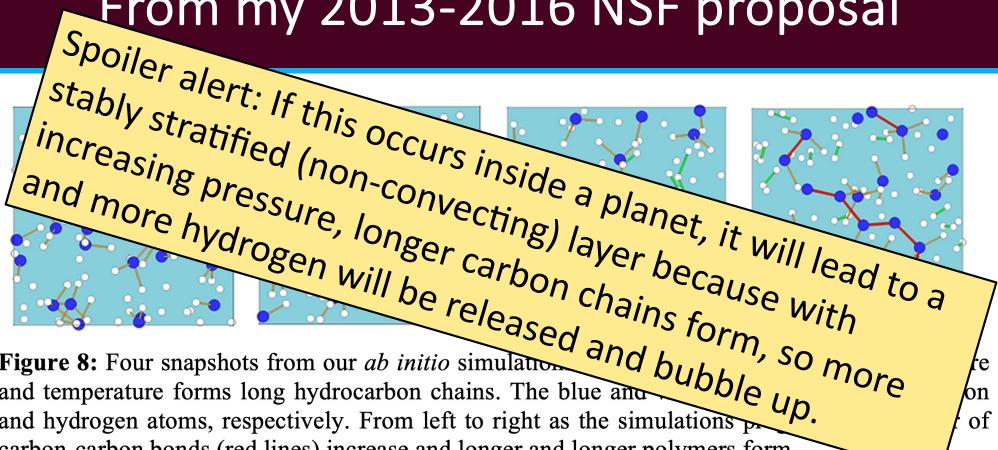


Figure 8: Four snapshots from our ab initio simulation. 6n and temperature forms long hydrocarbon chains. The blue and and hydrogen atoms, respectively. From left to right as the simulations carbon-carbon bonds (red lines) increase and longer and longer polymers form.

From my 2013-2016 NSF proposal

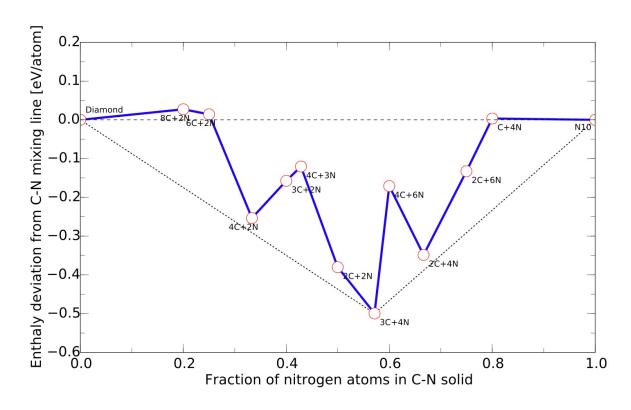
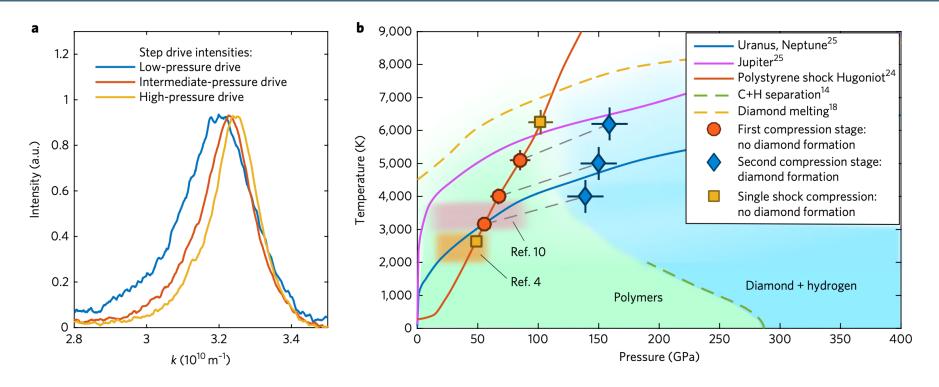


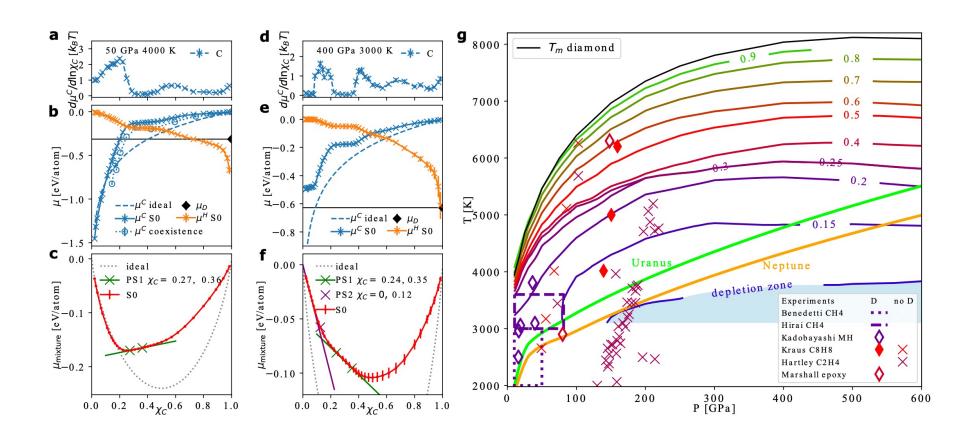
Figure 10: Convex hull diagram from our crystal of C-N structure search compounds at 3 Mbar that identified C₃N₄ as the most stable compound besides diamond and an N_{10} structure.

Kraus et al. (2017): Laser Compressed Hydrocarbons form Diamonds at High Pressure and Temperature

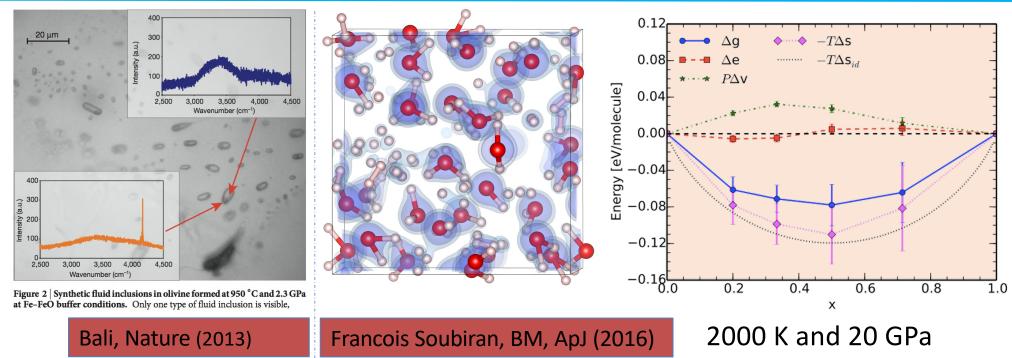
NATURE ASTRONOMY LETTERS



Cheng, Hamel, Bethkenhagen (2022): Diamond Formation from Hydrocarbon Mixtures



Simulations Predict H₂O and H₂ are miscible. Experiments do not under some conditions.

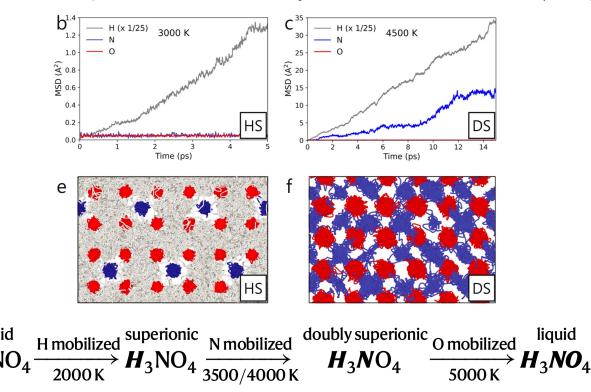


Simulations predict H₂O and H₂ to be miscible in U+N's interior.

Doubly Superionic State of C-N-O-H Compounds: Hydrogen and nitrogen mobile while oxygen is not.



Kyla de Villa, F. Gonzalez, BM, Nat. Comm. 14 (2023) 7580 Heated up structures from Conway et al. and Naumova et al. (2021)



http://arxiv.org/abs/2410.17499 How to detect DSI with experiments? Shock+XRD

Can Superionic Water explain the nondipolar fields?

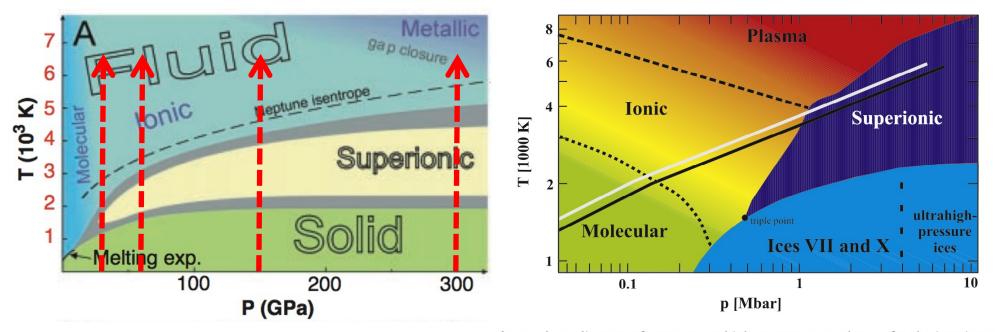
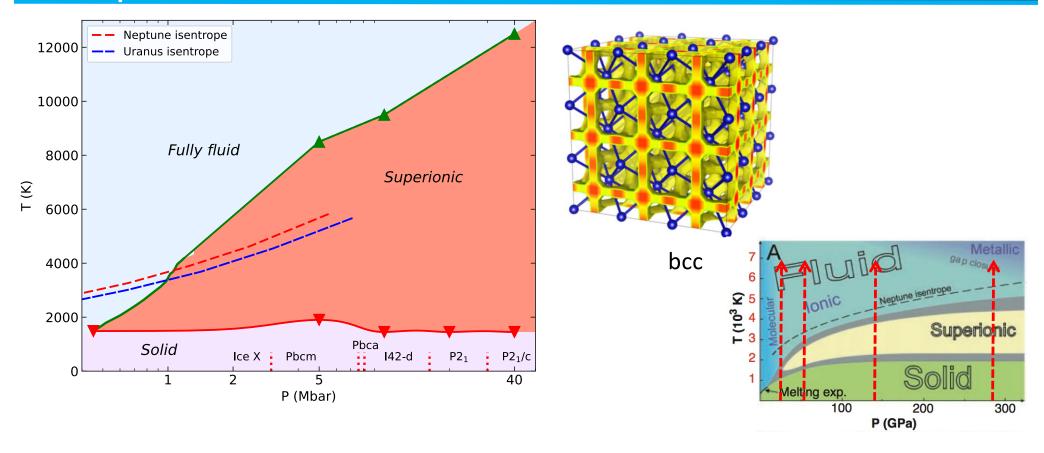


Fig. 1. Phase diagram of water up to high pressures as relevant for the interiors of Uranus and Neptune. The solid (ice VII and X), fluid (molecular, ionic, plasma), and

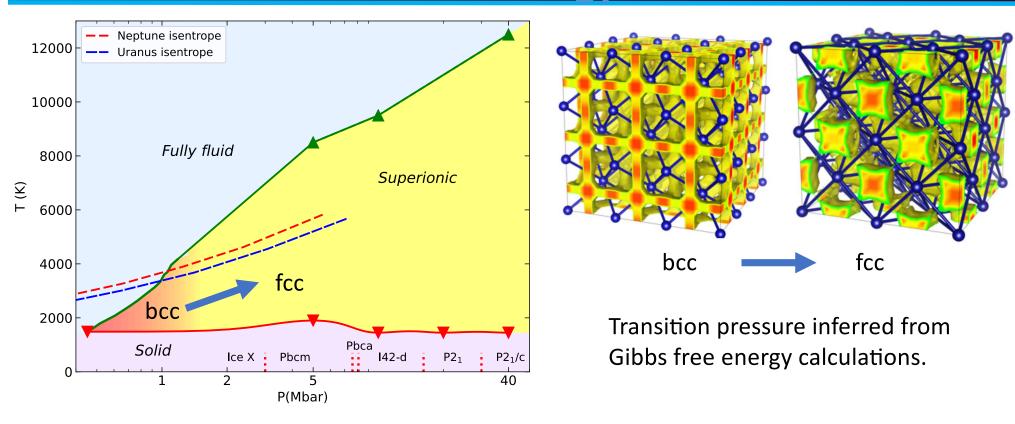
Cavazoni et al. (1999)

Redmer at al (2011)

Because Cavazoni had started from ice X, all superionic calculations assumed a bcc structure

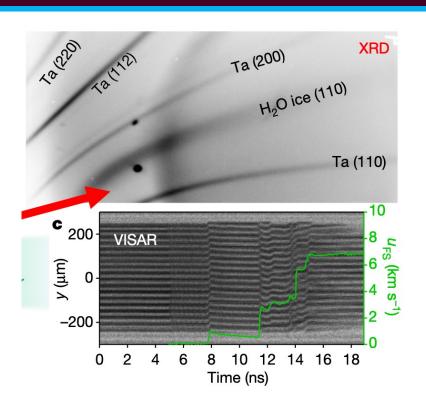


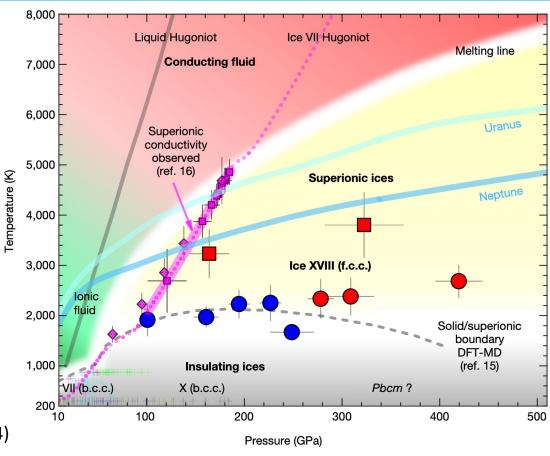
Bcc-to-fcc transition of Superionic Water Predicted with Gibbs Free Energy Calculations



H. F. Wilson, M. L. Wong, B. Militzer, Physical Review Letters 110 (2013) 151102

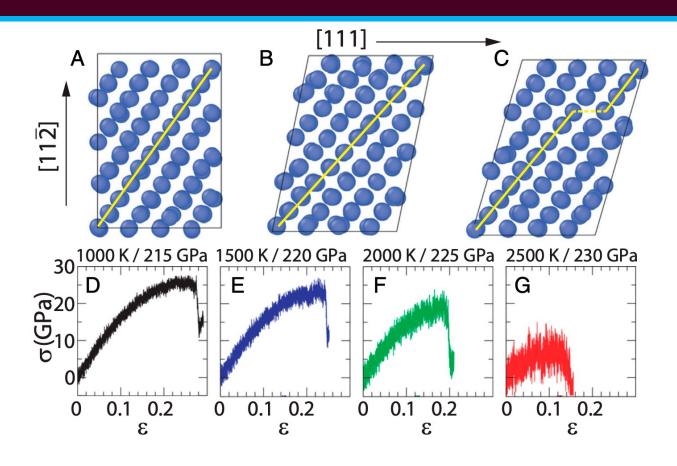
Millot et al. 2019: FCC Superionic ice generated with laser shock experiments





Stay tuned for results from D. Kraus (Gordon conf, 2024)

Matsulema et al. 2022: Superionic ice flows easily



Nettelmann et al. (2016): Thermal boundary layer to explain Uranus' low luminosity

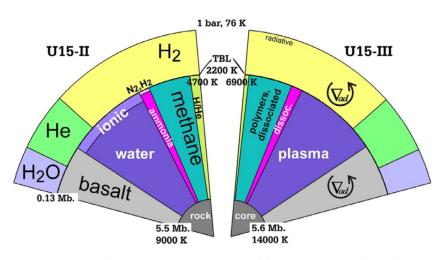
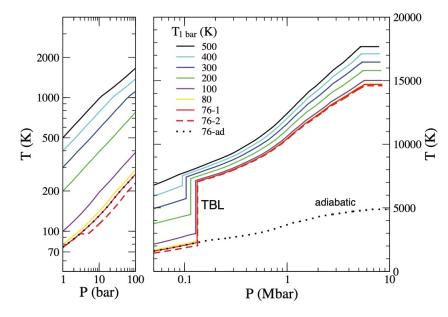


Fig. 9. Uranus three-layer structure models with thermal boundary layer that fit the gravity data and the luminosity. (*Left*) Model U15-II, with a maximum change of

Ice mixture H_2O : CH_4 : $NH_3 \approx 7.7:4:1$



Nonadiabatic models combine compositional gradients and much higher interior temperatures

Helled et al. (2020): Three layer: H, H₂O and rock; sharp and fuzzy boundaries

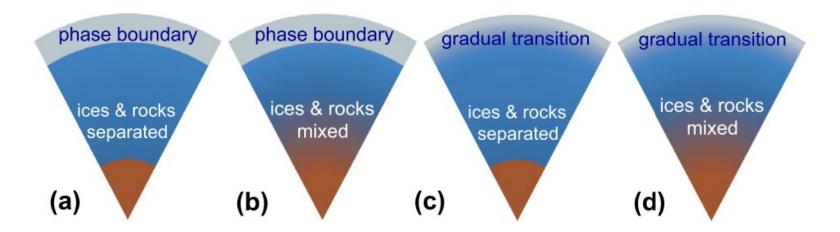
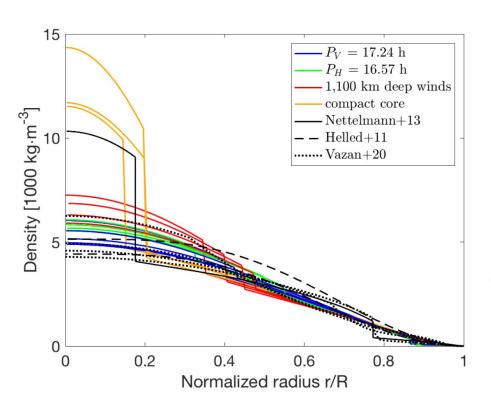
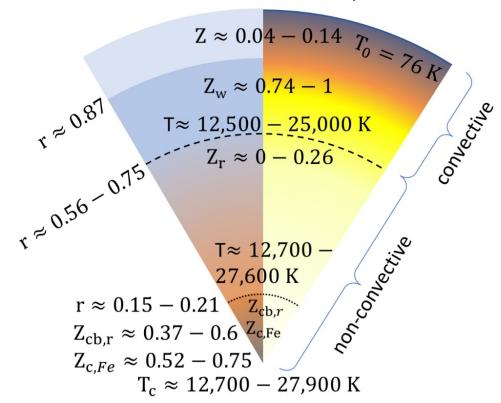


Fig. 4 Sketches of the possible internal structures of an ice giant. It is unclear whether Uranus and Neptune are differentiated and whether the transition between the different layers are distinct or gradual: (a) separation

Neuenschwander et al. (2024): Convective/Non-convective models with high interior temperatures



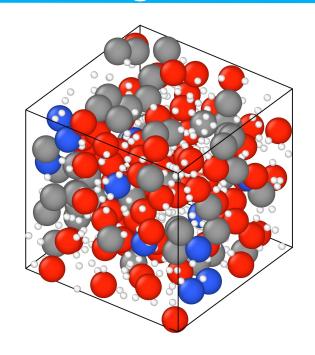
H-He, water, rock & iron, $P_V = 17.24 \text{ h}$



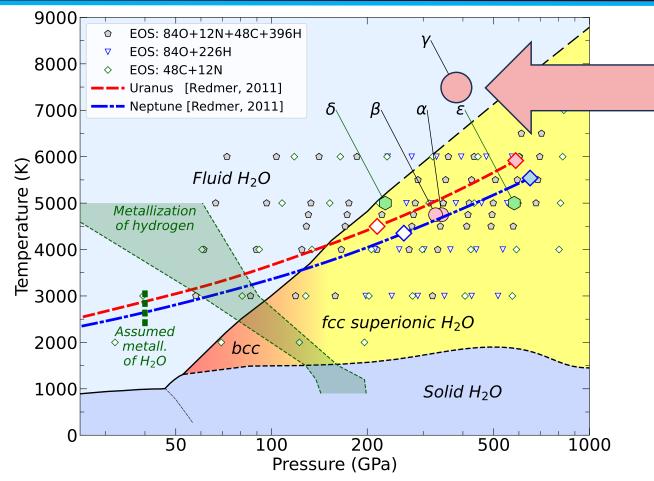


Machine learning becomes popular. These methods learn forces from ab initio simulations and then makes them much faster

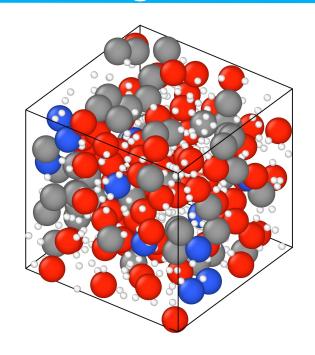
Performed much bigger simulations with Machine-Learning Accelerated Ab initio Simulations: 540 atoms



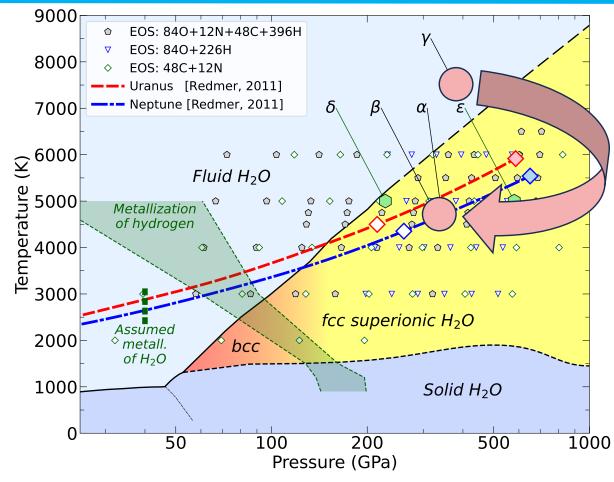
540 atoms: 84O+48C+12N+396H = $12 \times [7H_2O + 4CH_4 + NH_3]$ O:C:N = 7:4:1



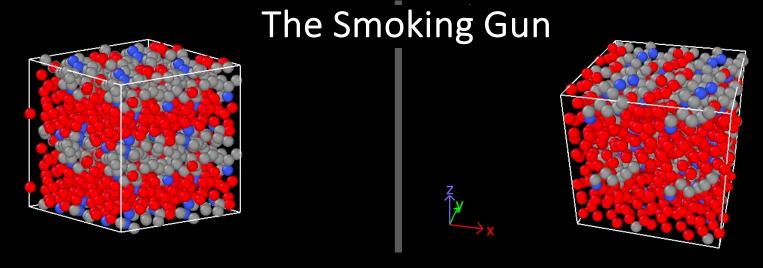
Performed much bigger simulations with Machine-Learning Accelerated Ab initio Simulations: 540 atoms



540 atoms: 84O+12N+48C+396H = $12 \times [7H_2O + 4CH_4 + NH_3]$ O:C:N = 7:4:1



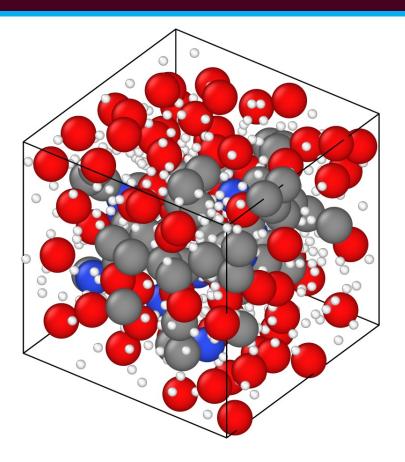
Smoking gun came from simulation with 84O+12N+48C+396H = $12 \times [7H_2O + 4CH_4 + NH_3]$

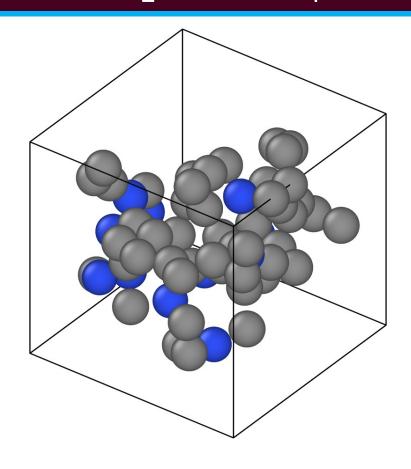


Is this real?

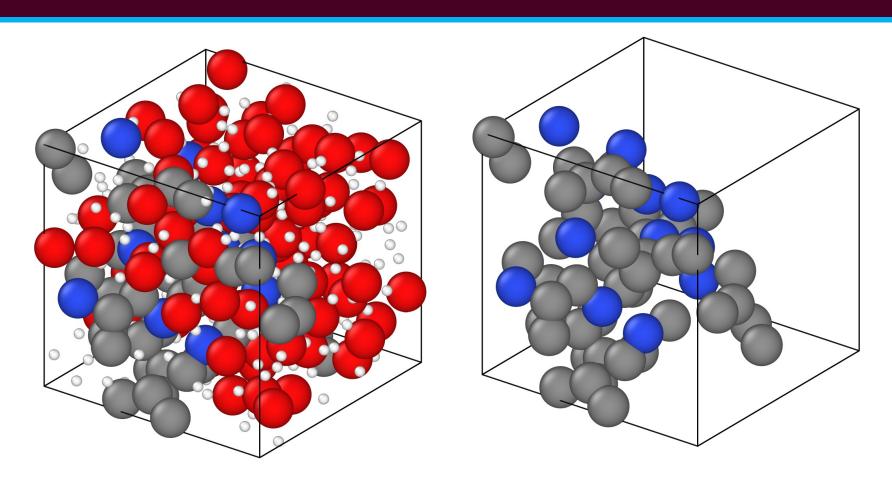
- 1) Would anyone confirm this result with ab initio simulations? So we turned off all machine learning and reconfirmed the findings!
- 2) Can this be confirmed with laboratory experiments?
- 3) Will a Uranus orbiter detect a signature in the planet?

Phase separation in simulation with $840+12N+48C+396H = 12 \times [7H_2O + 4CH_4 + NH_3]$

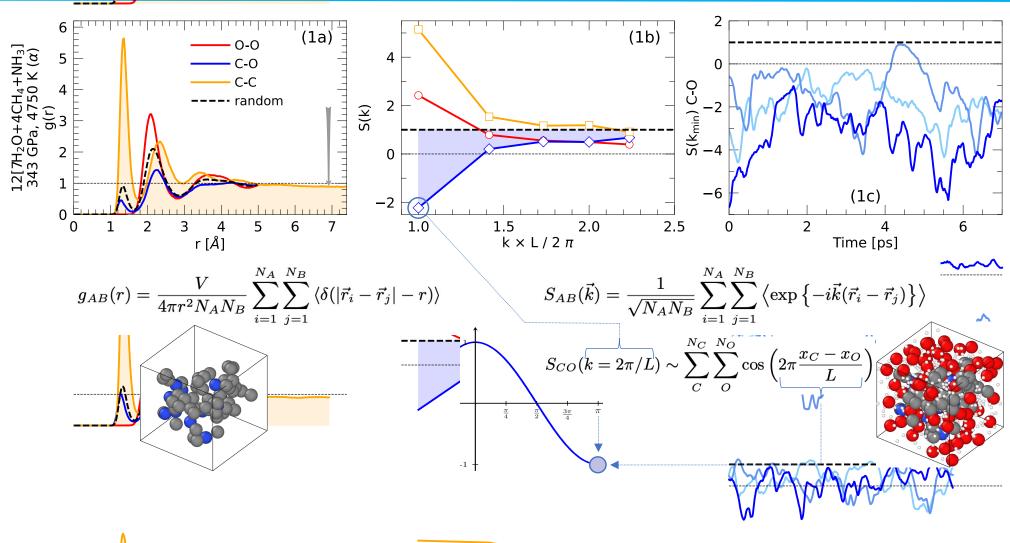




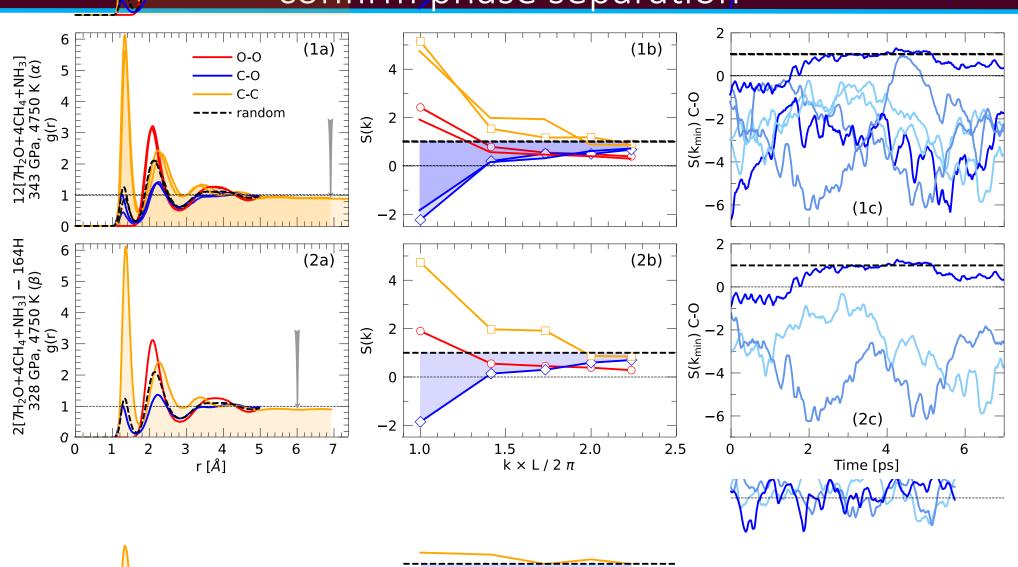
Phase Separation Confirmed with H-depleted simulations 84O+12N+48C+232H (164 H atoms were removed)

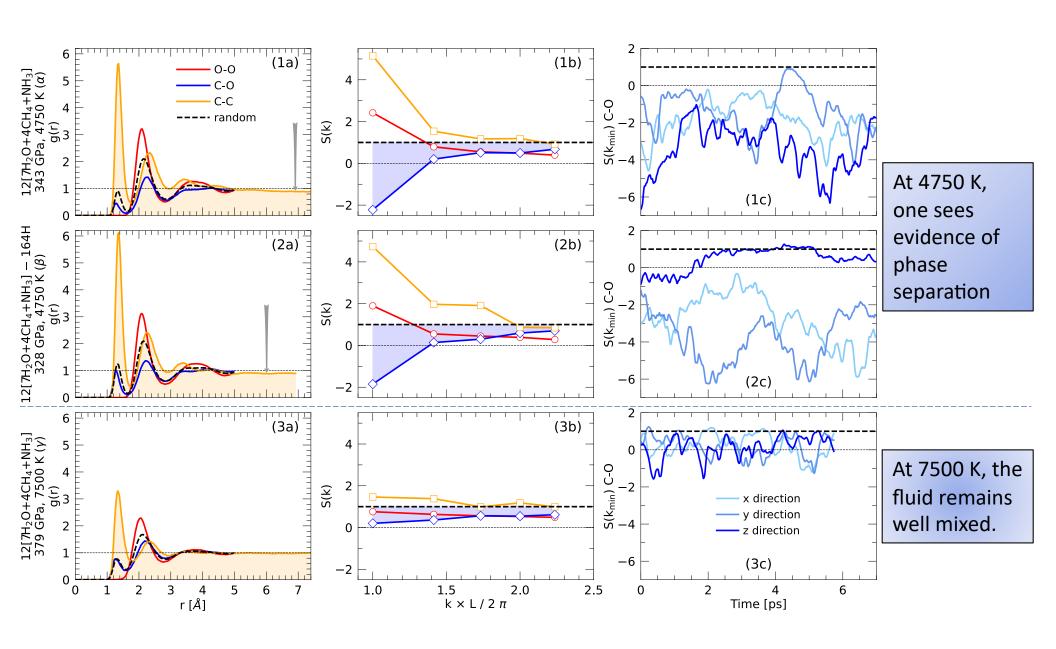


Pair Correlation g(r) and Structure S(k) confirm phase separation



Pair Correlation g(r) and Structure S(k) confirm phase separation

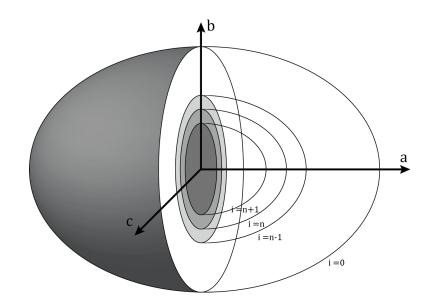


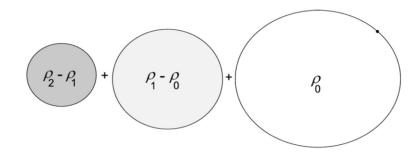


Concentric Maclaurin Spheroid (CMS) theory for rotating bodies in hydrostatic equilibrium

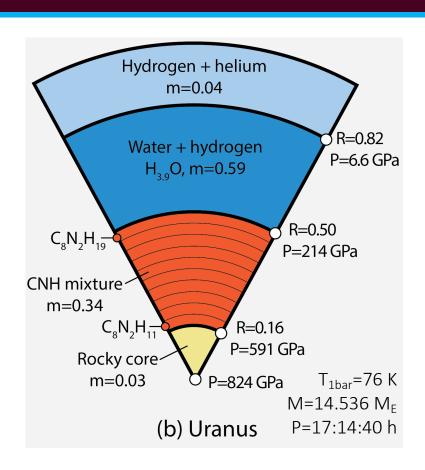
Model parameters:

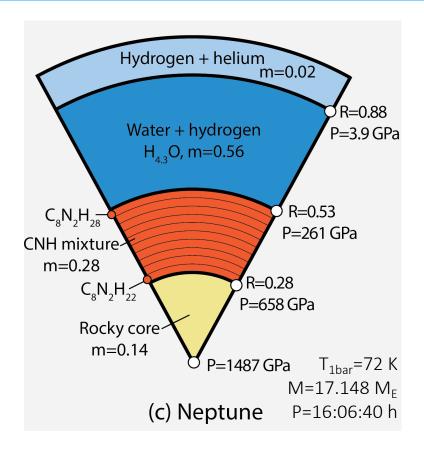
- EOS from ab initio simulations:
 - $\rho = \rho(P, T, composition)$
- Locations of the boundaries between the four layers
- Hydrogen fraction in the H₂O+H layer
- Hydrogen fraction in the C-N-H layer
- Use CMS to compute R, M, J_2 , J_4 , J_6 with high accuracy.
- Concentric Maclaurin Spheroid method Hubbard, ApJ (2013)
- Accelerated CMS method, Militzer et al., ApJ (2019)





Currently Favored Interior Models

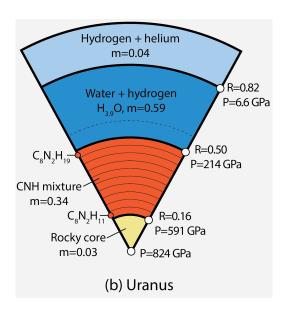




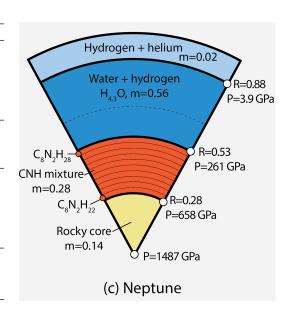
Assumptions for Interior Structure Models

Simplifying model assumptions

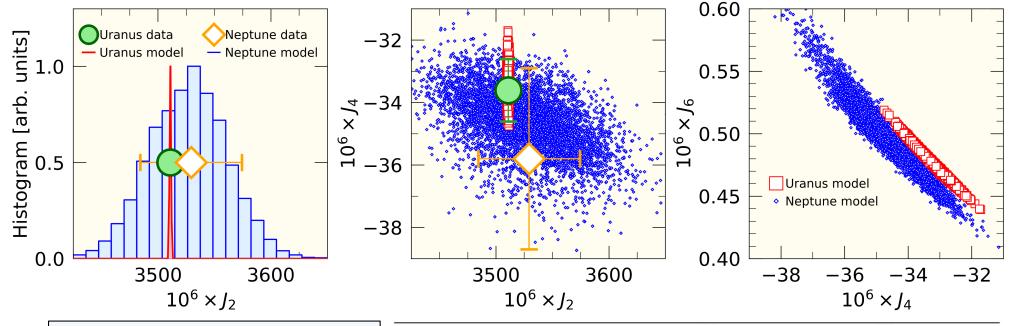
- 1) Complete phase separation between H₂O-rich layer and C-N-H layer
- 2) H₂O and H₂ mix and form a homogeneous and convecting layer
- 3) H_2O -rich layer is on top of C-N-H layer (So oil does not always float on top of water.)
- 4) H₂O-rich layer received its **extra hydrogen** from C-N-H but may not have absorbed it all.



	Uranus	Neptune
Measured $J_2 imes 10^6$	3510.99 ± 0.72	3529 ± 45
Model $J_2 imes 10^6$	3510.99	3529.40
Measured $J_4 imes 10^6$	-33.61 ± 1	-35.8 ± 2.9
Model $J_4 imes 10^6$	-33.61	-35.80
Model $J_6 imes 10^6$	0.4859	0.5314
H_1	1.923 ≈ H _{3.8} O	$2.245 \approx H_{4.5}O$
H_2	$0.5015\approx C_8 N_2 H_{19}$	$0.4418 \approx C_8 N_2 H_{17}$
H_3	$0.2053 \approx C_8 N_2 H_8$	$0.1055 \approx C_8N_2H_4$
r_1 [PU]	0.8156	0.8858
r_2 [PU]	0.4897	0.5232
r_3 [PU]	0.1471	0.2159
r_2/r_1 (volumetric radii)	0.6010	0.5915
$r_2/r_{ m 40GPa}$ (volumetric radii)	0.6680	0.6613
$\left(rac{M_C+M_N}{M_O+M_C+M_N} ight)$	0.373	0.400
$M_{ m Habsorbed}$ [PU]	0.05606	0.06902
$M_{ m Hreleased}$ [PU]	0.05607	0.06906

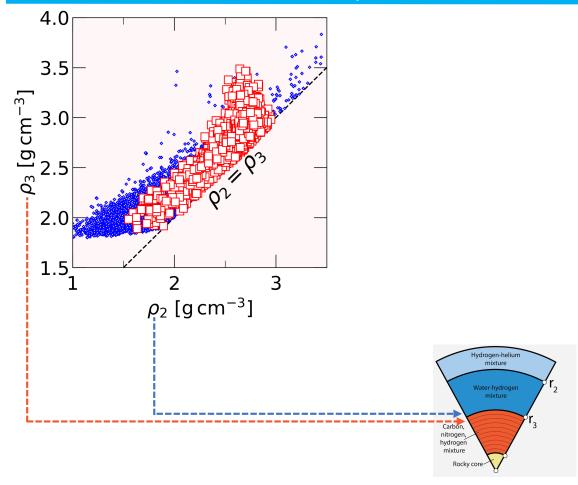


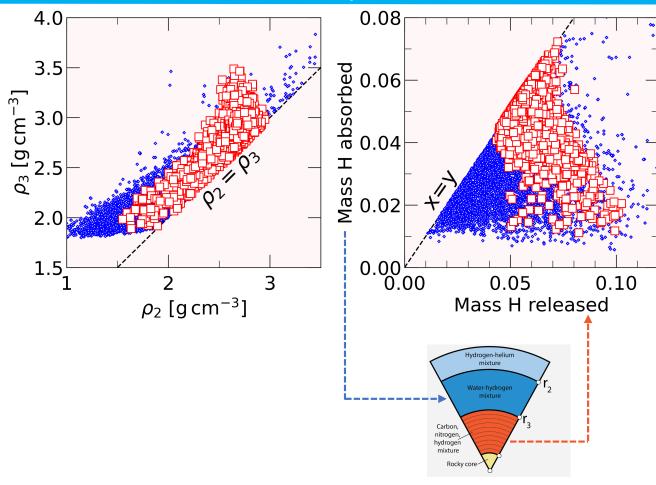
Monte Carlo Ensembles of U+N models that match the Gravity Measurements

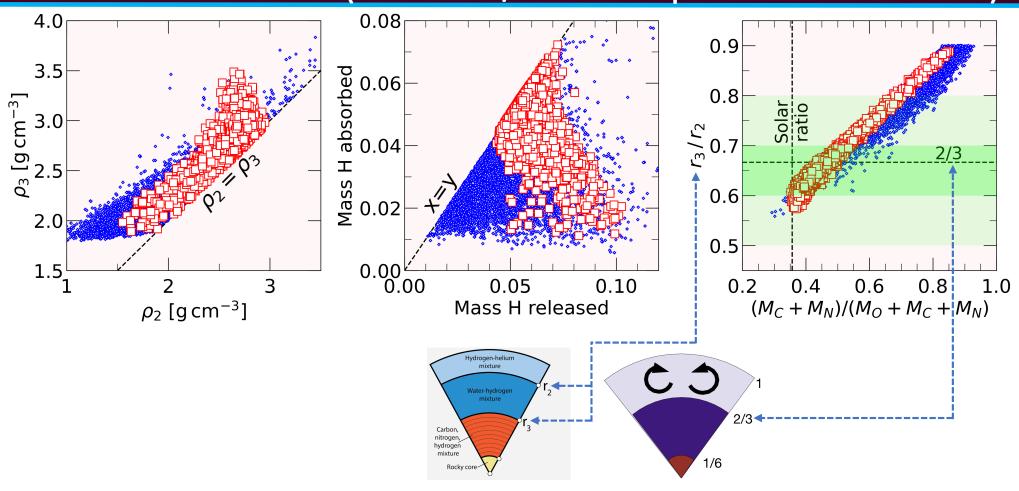


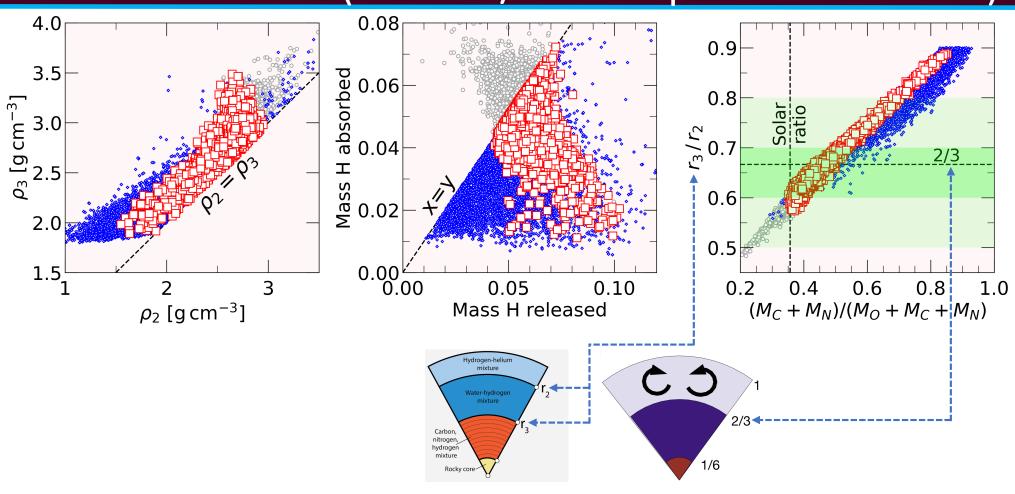
B. Militzer
Astrophysical J. 953 (2023) 111
Open QMC source code:
http://militzer.berkeley.edu/QMC
10.5281/zenodo.8038144

	Uranus	Neptune
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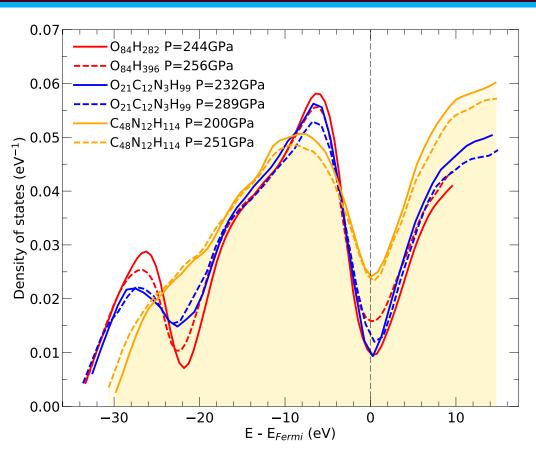








Are the different materials electrical conductors? Yes, all three are good "metals"



 $O_{21}N_3C_{12}H_{99}$ mixture

7000 or 11000 S/cm (derived with HSE)

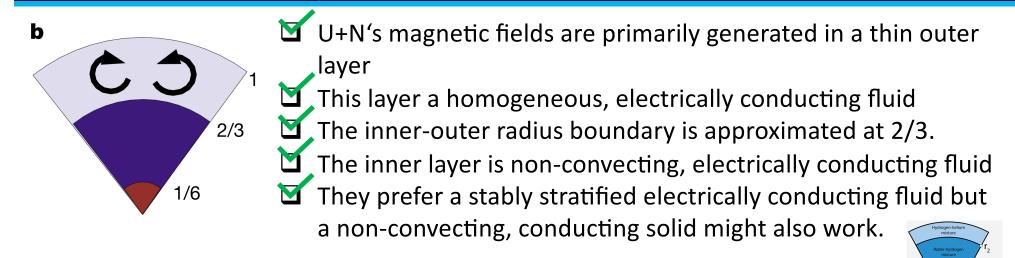
Water-hydrogen mixture O₈₄H₂₂₈ and O₈₄H₃₉₆

8000 or 21000 S/cm

Carbon-nitrogen-hydrogen mixture C₄₈N₁₂H₁₁₄

31000 and 35000 S/cm

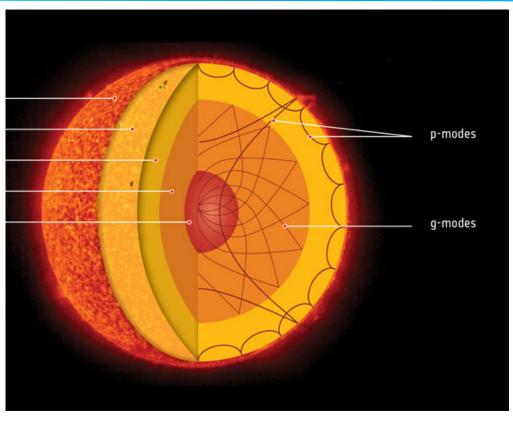
Our Model for U+N's Interior Structure is Consistent with Stanley & Bloxham's Predictions

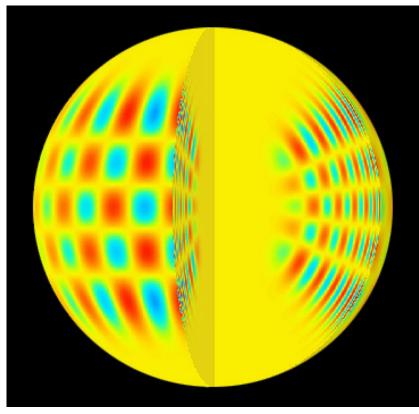


Open questions:

- 1) What is the composition of the upper layer? A conducting, fluid mixture of H₂O and H₂
- 2) What is the composition of the lower layer? Conducting carbon-nitrogen-hydrogen fluid
- 3) Why is the lower layer not convective? The amount of hydrogen varies with depth. Leading to density stratification that prevents convection.

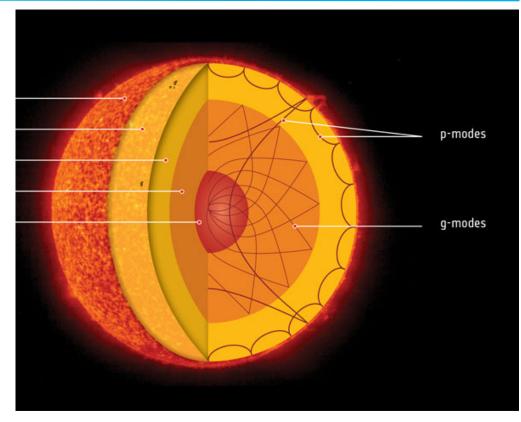
Helioseismology



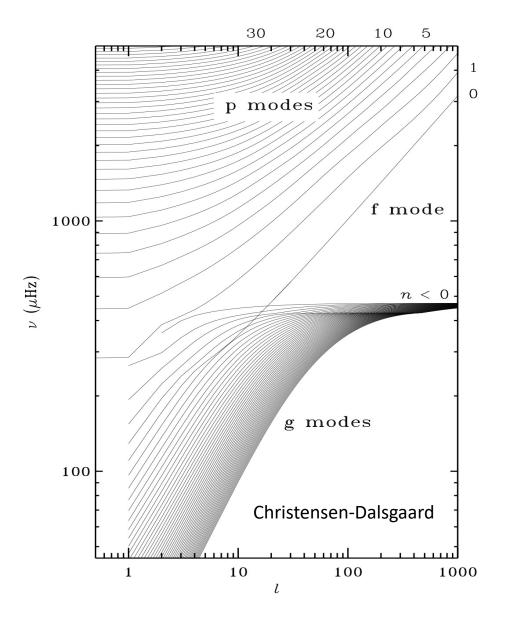


NASA SOHO P modes

Helioseismology



NASA SOHO

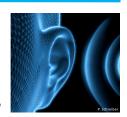


Helioseismology

P modes: "Pressure" waves

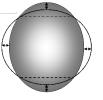
Primary restoring force is pressure

High-frequency limit: acoustic waves



F modes: "Fundamental" modes

• Are the limit of p modes as radial order n goes to zero (long-wavelength limit)



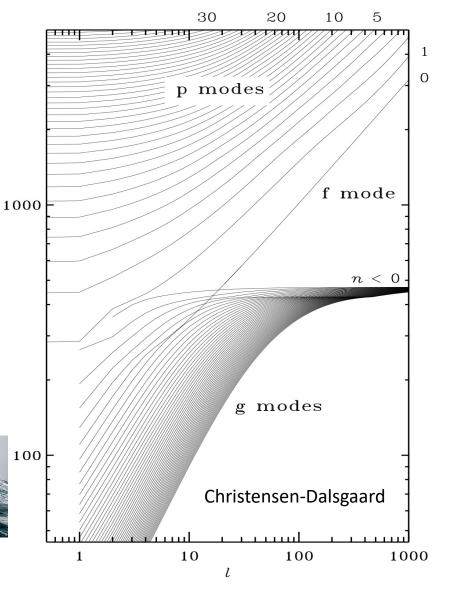
 ν (μ Hz)

- Also known as surface gravity wave, no nodes in interior. Deforms like a soccer ball
- No compression involved.

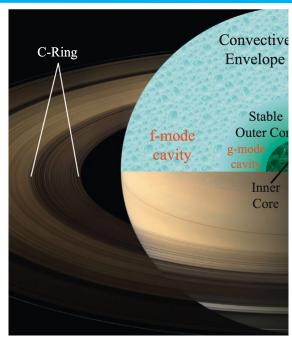
G Modes: "Gravity" waves

- Low frequency waves
- Primary restoring force is buoyancy
- Requires stable stratification, no convection

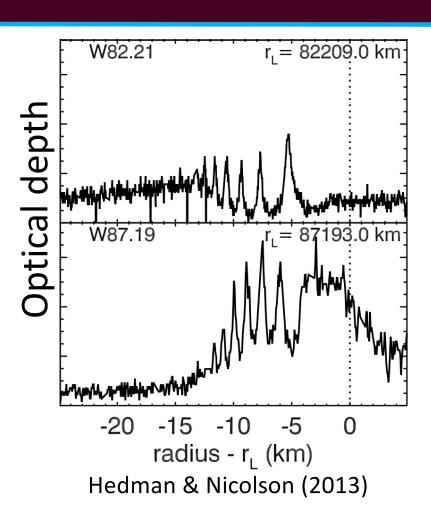




Saturn's Rings are a Seismometer, Spiral Density Waves



Fuller (2014)



Take-Away Points

- Ab initio simulations predict a O-C-N-H mixture to phase separated into a O-H and a C-N-H fluid at high pressure
- Constructed planet model for Uranus and Neptune.
 Their icy mantles of have two layers: an upper H₂O-H₂ layer and lower stably stratified C-N-H layer
- 3. Under these assumptions we can match the gravity and magnetic field measurements
- 4. A Uranus spacecraft should bring a **Doppler imager.**