Helium Rain and The State of Water Ice in Giant Planets Predicted with Ab Initio Simulations

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1. Introduction to Simulations
2. Helium rain on Jupiter
3. Phase diagram of water ice
4. Erosion of icy and rocky materials in cores in giant planets
5. Do iron and rocks ever mix in planetary interiors

Supported by NASA and NSF.
I. Ab Initio Simulations of Materials at High Pressure
Focus: Characterization of the Interior of Solar and Extrasolar Giant Planets

Solar GP: Jupiter, Saturn

Temperature (K) vs. Density (g cm$^{-3}$)

- Plasma
- Atomic Fluid
- Molecular Fluid
- Molecular Solid
- Metallic Fluid
- Metallic Solid

- $n=10^{18}$ cm$^{-3}$
- $n=10^{26}$ cm$^{-3}$

n=10$^{18}$ cm$^{-3}$
1) Path integral Monte Carlo for $T > 5000\text{K}$
1) Path integral Monte Carlo for T>5000K
2) Density functional molecular dynamics below

Born-Oppenheimer approx. MD with classical nuclei:

\[ F = m \cdot a \]

Forces derived DFT with electrons in the instantaneous ground state.
What is meant by first-principles simulations?

Schrödinger equation:

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

Look for an antisymmetric solution (Pauli exclusion):

\[
\Psi(x_1, x_2, \ldots, x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix}
\chi_1(x_1) & \chi_2(x_1) & \cdots & \chi_N(x_1) \\
\chi_1(x_2) & \chi_2(x_2) & \cdots & \chi_N(x_2) \\
\vdots & \vdots & \ddots & \vdots \\
\chi_1(x_N) & \chi_2(x_N) & \cdots & \chi_N(x_N)
\end{vmatrix}
\]

Density functional theory:
- Local density approximation (LDA)
- Gen. Gradient approximation (GGA)
- Hybrid functionals
- Van der Waals functionals
- Quantum Monte Carlo

Simulation of molecular hydrogen

Methane – molecular orbitals
Quantum Monte Carlo Calculations of MgSiO$_3$ Perovskite and Post-Perovskite

Comparison of molecular and metallic hydrogen

Molecular hydrogen

Metallic hydrogen
Jupiter’s Composition

Composition on the surface (solar):

<table>
<thead>
<tr>
<th>H</th>
<th>0.742</th>
<th>0.736</th>
<th>Ne</th>
<th>0.00023(3)</th>
<th>0.0018</th>
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<tr>
<td>He</td>
<td>0.231(4)</td>
<td>0.249</td>
<td>P</td>
<td>&lt; 0.00007</td>
<td>0.00001</td>
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<tr>
<td>C</td>
<td>0.009(2)</td>
<td>0.0029</td>
<td>S</td>
<td>0.00091(6)</td>
<td>0.00050</td>
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<tr>
<td>N</td>
<td>&lt; 0.012</td>
<td>0.00085</td>
<td>Ar</td>
<td>&lt; 0.00015</td>
<td>0.00007</td>
</tr>
<tr>
<td>O</td>
<td>&lt; 0.0035</td>
<td>0.0057</td>
<td>“Z”</td>
<td>0.027</td>
<td>0.015</td>
</tr>
</tbody>
</table>

Guillot et al. (Jupiter book, 2002, chap.3)
The Size of Jupiter’s Core is uncertain

A) Typical models by Guillot et al.: $M_{\text{core}} = 0-7 \, M_E$

B) We derived a model: $M_{\text{core}} = 14-18 \, M_E$

Guillot et al. (Jupiter book, 2002, chap.3)
Juno Mission
launched successfully August 2011

My contribution:
• Equation of state calculations for hydrogen-helium mixtures
• Thermodynamics of heavier elements

Mission Timeline:
• Launch - August 2011
• Earth flyby gravity assist - October 2013
• Jupiter arrival - July 2016
• End of mission (deorbit) - October 2017
Jupiter’s Interior Temperature Profile

Temperature (K)

Pressure (GPa)

SC model (interpolated)

DFT-MD, no TDI, Militzer et al. (2008)

DFT-MD, no TDI, Nettelmann et al. (2008)

Jupiter’s core-mantle boundary
Jupiter’s Interior Temperature Profile

Interiors of Saturn and Jupiter are more dense

Militzer, Hubbard, Apj (2013)
Recalibration of Mass-Radius Relationship of Hot Jupiters

II. Helium Rain on Jupiter
Galileo Entry Probe found: **Helium and Neon depleted in Jupiter’s Atmosphere**
Can hydrogen and helium become immiscible? Helium rain inside Saturn?

Mixing free energy $\Delta G_{\text{mix}}(P,T)$:
$$\Delta G_{\text{mix}}(x) = G(x) - x G_{\text{He}} - (1-x) G_{\text{H}}$$

$G(P,T)=E+PV-TS$ Main difficulty is to calculate the mixing entropy!
Neon depletion is consistent with helium depletion in Jupiter

Quantitative agreement between:
- 1.2% reduction in helium from solar.
- 9-fold reduction in neon from solar.
- $\Delta G = -2.35\text{eV}$ at 5000K
Why grew the giant plants so large while all terrestrial planets stayed small? Because they form beyond the ice line.
III. New Phases of Water Ice
Phase Diagram of water ice

Ice Ih has negative Clapeyron slope:

$$\frac{dT_{melt}}{dP} = \frac{V_{\text{liquid}} - V_{\text{solid}}}{S_{\text{liquid}} - S_{\text{solid}}} = \frac{\Delta V}{\Delta S} < 0 < 0$$

$$G(P,T) = E + PV - TS$$
Phase Diagram of water ice

Ice X: the highest pressure phase seen in experiments.
Phase Diagram of water ice

\[ \text{Pbcm phase predicted with ab initio simulations by Benoit et al. (1996)} \]
Phonon instability leads to new phase of water ice at 7.6 megabar

Militzer and Wilson, *PRL* 105 (2010) 195701
2013: Ab Initio Structure Search Methods predict Two New Ice Structures at Megabar Pressure

<table>
<thead>
<tr>
<th>Name/Symmetry</th>
<th>Author, Year</th>
<th>Pressure (Mbar)</th>
<th>#mol.</th>
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<tbody>
<tr>
<td>Ice X (Pn-3m)</td>
<td>Polian, 1984</td>
<td>0.44</td>
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<tr>
<td>Pbcm</td>
<td>Benoit, 1996</td>
<td>3</td>
<td>4</td>
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<tr>
<td>Pbca</td>
<td>Militzer, Wilson, 2010</td>
<td>7.7</td>
<td>8</td>
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<tr>
<td>P3_121</td>
<td>Pickard, Needs, 2013</td>
<td>8.1</td>
<td>12</td>
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<tr>
<td>Pcca</td>
<td>Pickard, Needs, 2013</td>
<td>14.4</td>
<td>12</td>
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<tr>
<td>P2_1/c</td>
<td>Ji, 2011</td>
<td>19.6</td>
<td>8</td>
</tr>
<tr>
<td>C2/m (metallic)</td>
<td>McMahon, 2011</td>
<td>56.2</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>Hermann, 2011</td>
<td>60</td>
<td>2</td>
</tr>
<tr>
<td>H_2O_2</td>
<td>Pickard, Needs 2013</td>
<td>~50</td>
<td></td>
</tr>
<tr>
<td>H_4O</td>
<td>Zhang, Militzer, 2013</td>
<td>~50</td>
<td></td>
</tr>
</tbody>
</table>

**References**

Pickard, Needs **110** (2013) 245701

IV. Is Ice Stable in Cores of Giant Planets?
Is the interface between ice and metallic hydrogen stable in giant planet cores?

Analysis of Gibbs Free Energy differences shows ice erosion is an entropy driven process

Predict core erosion in both Saturn and Jupiter

Computer simulations predict erosion of icy cores in Saturn and Jupiter

Predict core erosion in both Saturn and Jupiter

Conclusions

- Indirect evidence for **helium rain on Jupiter** based on low neon abundances in atmosphere
- **Superionic H\textsubscript{2}O water** could be relevant for Uranus and Neptune
- **All core materials** such as ices, rocks and iron are **thermodynamically unstable** – core erosion timescale unclear
- **Iron and rocks mix** at temperatures 4,000-10,000 K.
The End