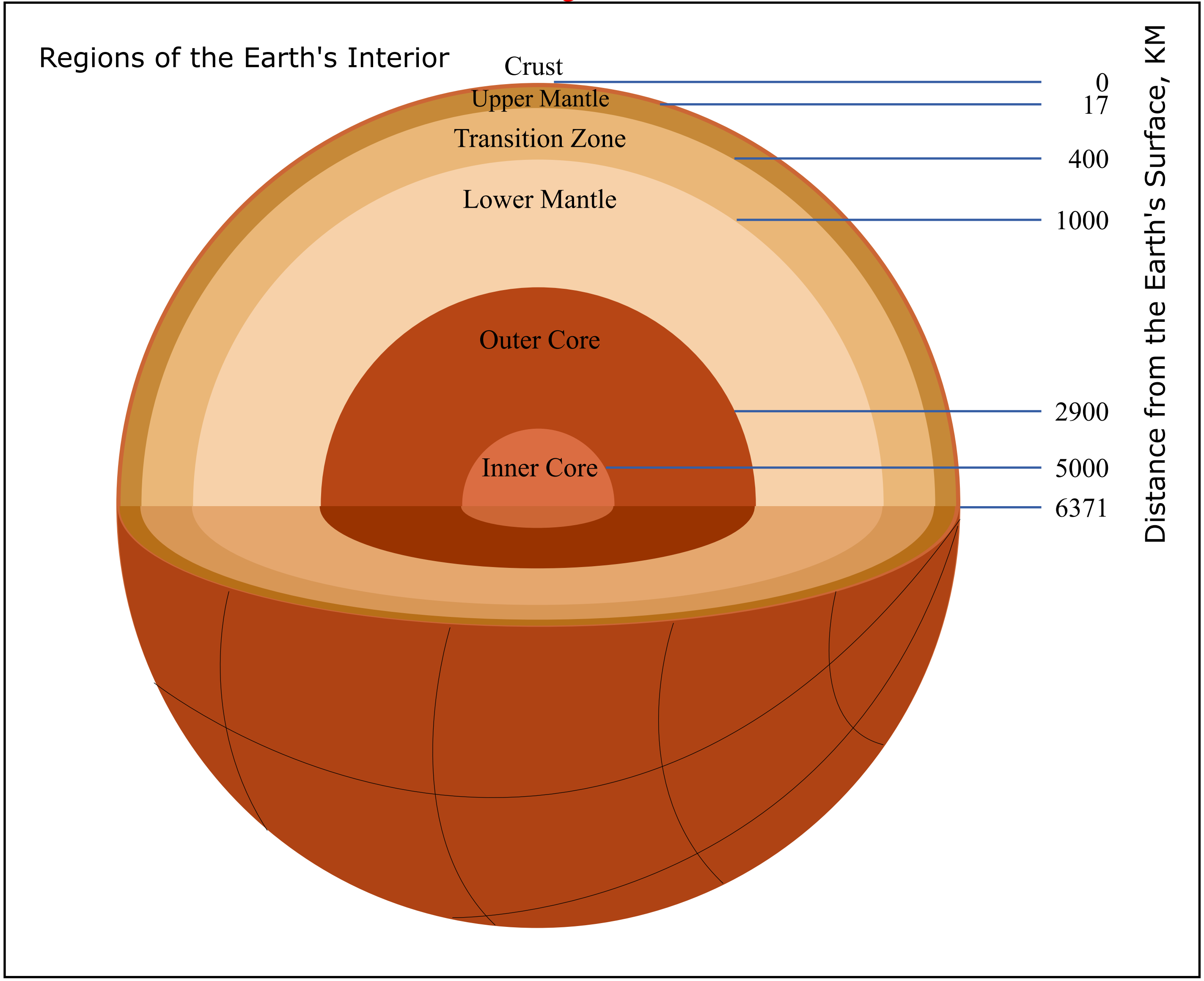
3.320: Final Lecture (May 10 2005)

JOURNEY TO THE CENTRE OF THE EARTH

Planetary Interiors



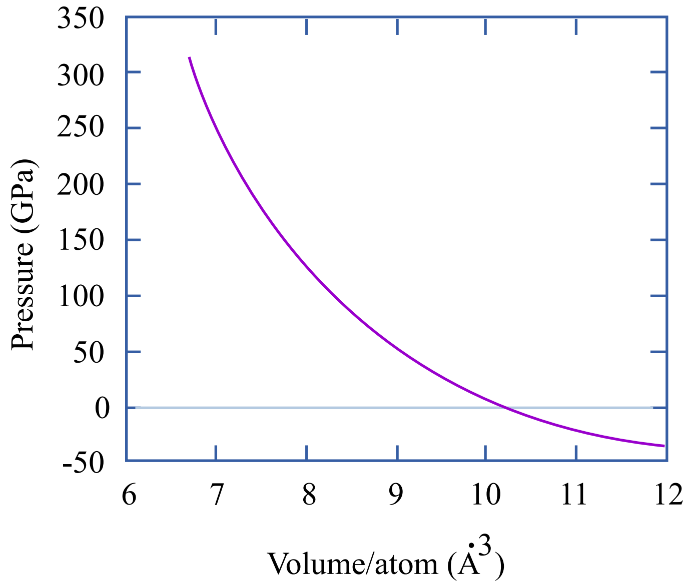
Alfe' and Gillan, Nature '98, '99, '00

Figure by MIT OCW.

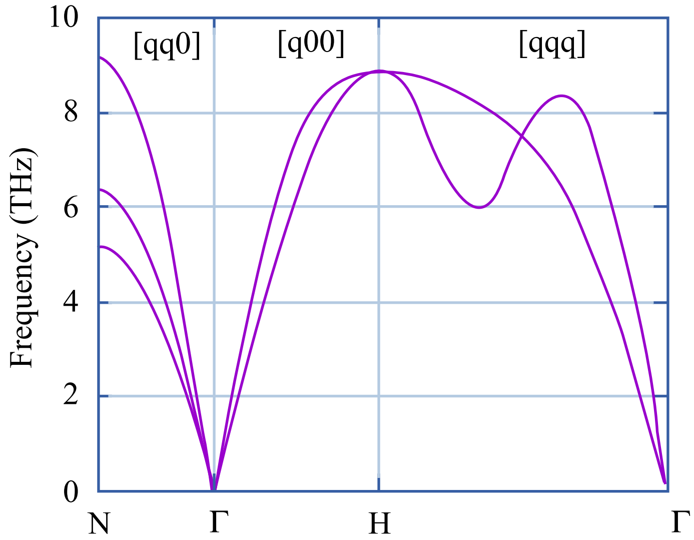
Earth's core

- 30% of mass of the planet
- Mainly iron (star nucleosynthesis) – the liquid outer core is slightly less dense (light impurities: S, O, Si, H ?)
- Pressure ranges 100-400 GPa, temperatures 3000-7000 K (?)
- Liquid-solid boundary: 330 Gpa (seismic waves)
- DAC: 300 GPa @ 300K, 200 Gpa @ 3700K

GGA-DFT Iron



Pressure as a function of atomic volume of hcp Fe.

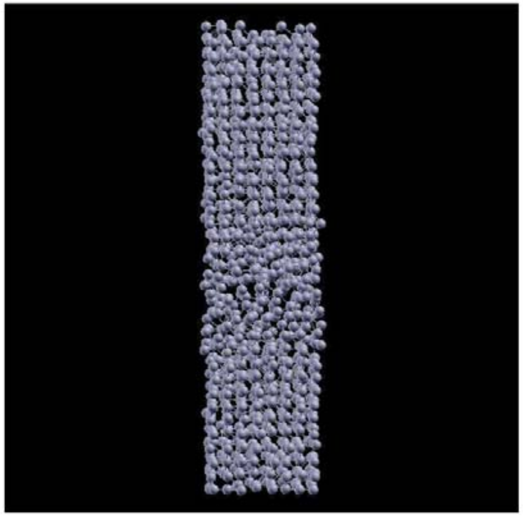


Phonon dispersion curves of ferromagnetic bcc Fe at Zero pressure along the [100], [110], and [111] directions.

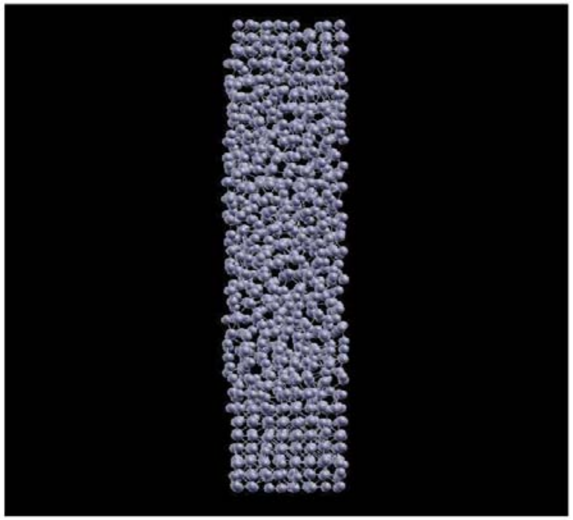
Figure by MIT OCW.

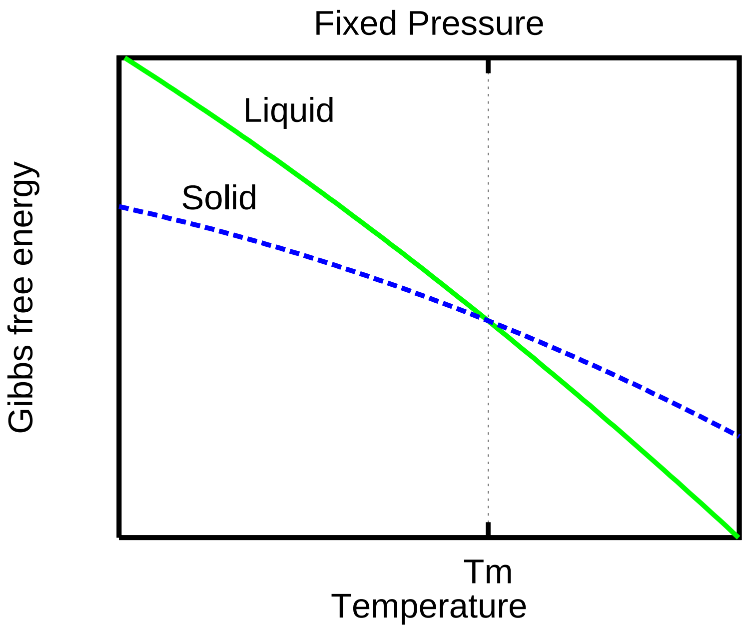
Melting Point

Initial T = 100 K, final T = 119.5 K.



Initial T = 130 K, final T = 120.9 K.





Thermodynamic integration (I)

$$\mathcal{U}(\lambda) = (1-\lambda)\mathcal{U}_{\mathrm{I}} + \lambda \mathcal{U}_{\mathrm{II}}$$

$$Q(N,V,T,\lambda) = \frac{1}{\Lambda^{3N} N!} \int d\mathbf{r}^N \exp[-\beta \mathcal{U}(\lambda)].$$

$$\begin{aligned}
\left(\frac{\partial F(\lambda)}{\partial \lambda}\right)_{N,V,T} &= -\frac{1}{\beta}\frac{\partial}{\partial \lambda} \ln Q(N,V,T,\lambda) = -\frac{1}{\beta Q(N,V,T,\lambda)} \frac{\partial Q(N,V,T,\lambda)}{\partial \lambda} \\
&= \frac{\int d\mathbf{r}^N (\partial \mathcal{U}(\lambda)/\partial \lambda) \exp[-\beta \mathcal{U}(\lambda)]}{\int d\mathbf{r}^N \exp[-\beta \mathcal{U}(\lambda)]} = \left\langle \frac{\partial \mathcal{U}(\lambda)}{\partial \lambda} \right\rangle_{\lambda}
\end{aligned}$$

Partitioning the free energy

$$F = -k_B T \ln\left\{ \frac{1}{N!\,\Lambda^{3N}} \int d\mathbf{R}_1 \ldots d\mathbf{R}_N \right.$$

$$\left. \times \exp[-\beta U(\mathbf{R}_1, \ldots \mathbf{R}_N; T_{el})] \right\},$$

$$U(R_1,\ldots,R_N;T_{el}) = U(R_1^0,\ldots R_N^0;T_{el}) + U_{vib}^{harm}(R_1,\ldots,R_N;T_{el}) + U_{vib}^{anharm}(R_1,\ldots,R_N;T_{el})$$

Harmonic Term

$$F_{\mathrm{harm}} = -k_{\mathrm{B}} T \ln\left\{ \frac{1}{\Lambda^{3N}} \int d\mathbf{R}_1 \ldots d\mathbf{R}_N \times \exp[-\beta U_{\mathrm{harm}}(\mathbf{R}_1, \ldots \mathbf{R}_N; T_{\mathrm{el}})] \right\},$$

$$U_{\mathrm{harm}} = \frac{1}{2} \sum_{ls\alpha, l'' t\beta} u_{ls\alpha} \Phi_{ls\alpha, l'' t\beta} u_{l'' t\beta} \quad \Rightarrow \quad F_{\mathrm{harm}} = \frac{3 k_{\mathrm{B}} T}{N_{\mathbf{k}s}} \sum_{\mathbf{k}s} \ln(\beta \hbar \omega_{\mathbf{k}s})$$

Anharmonic Term

$$F_{\text{anharm}} = (F_{\text{vib}} - F_{\text{ref}}) + (F_{\text{ref}} - F_{\text{harm}}),$$

$$F_{\text{vib}} - F_{\text{ref}} = \int_0^1 d\lambda \, \langle U_{\text{vib}} - U_{\text{ref}} \rangle_\lambda^{\text{vr}},$$

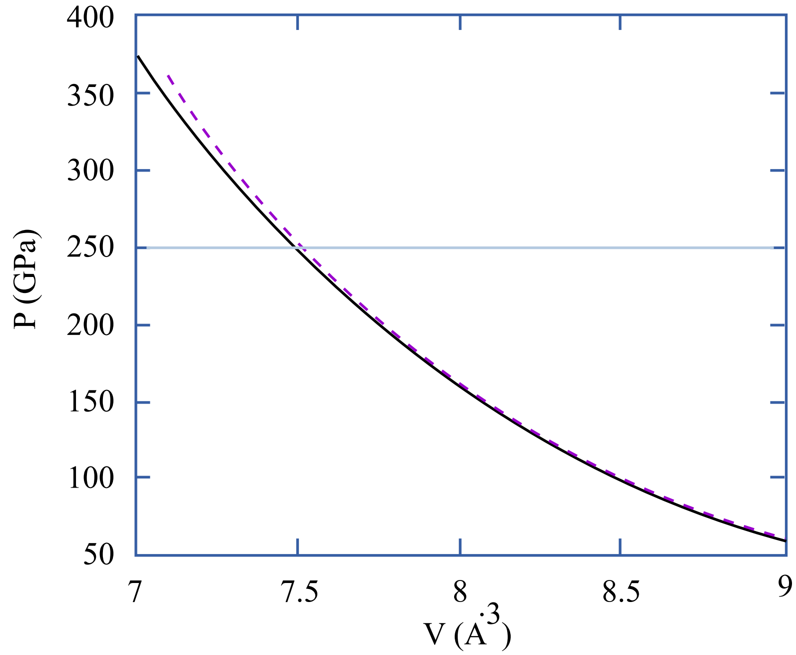
$$F_{\text{ref}} - F_{\text{harm}} = \int_0^1 d\lambda \, \langle U_{\text{ref}} - U_{\text{harm}} \rangle_\lambda^{\text{rh}}.$$

Reference System

$$U_{\mathrm{IP}} = \frac{1}{2} \sum_{I \neq J} \phi(|\mathbf{R}_I - \mathbf{R}_J|),$$

$$U_{\mathrm{ref}} = c_1 U_{\mathrm{harm}} + c_2 U_{\mathrm{IP}}.$$

Shock Hugoniot



Experimental and *ab initio* Hugoniot pressure *p* as a function of atomic volume *V*.

Figure by MIT OCW.

Taking the temperature…

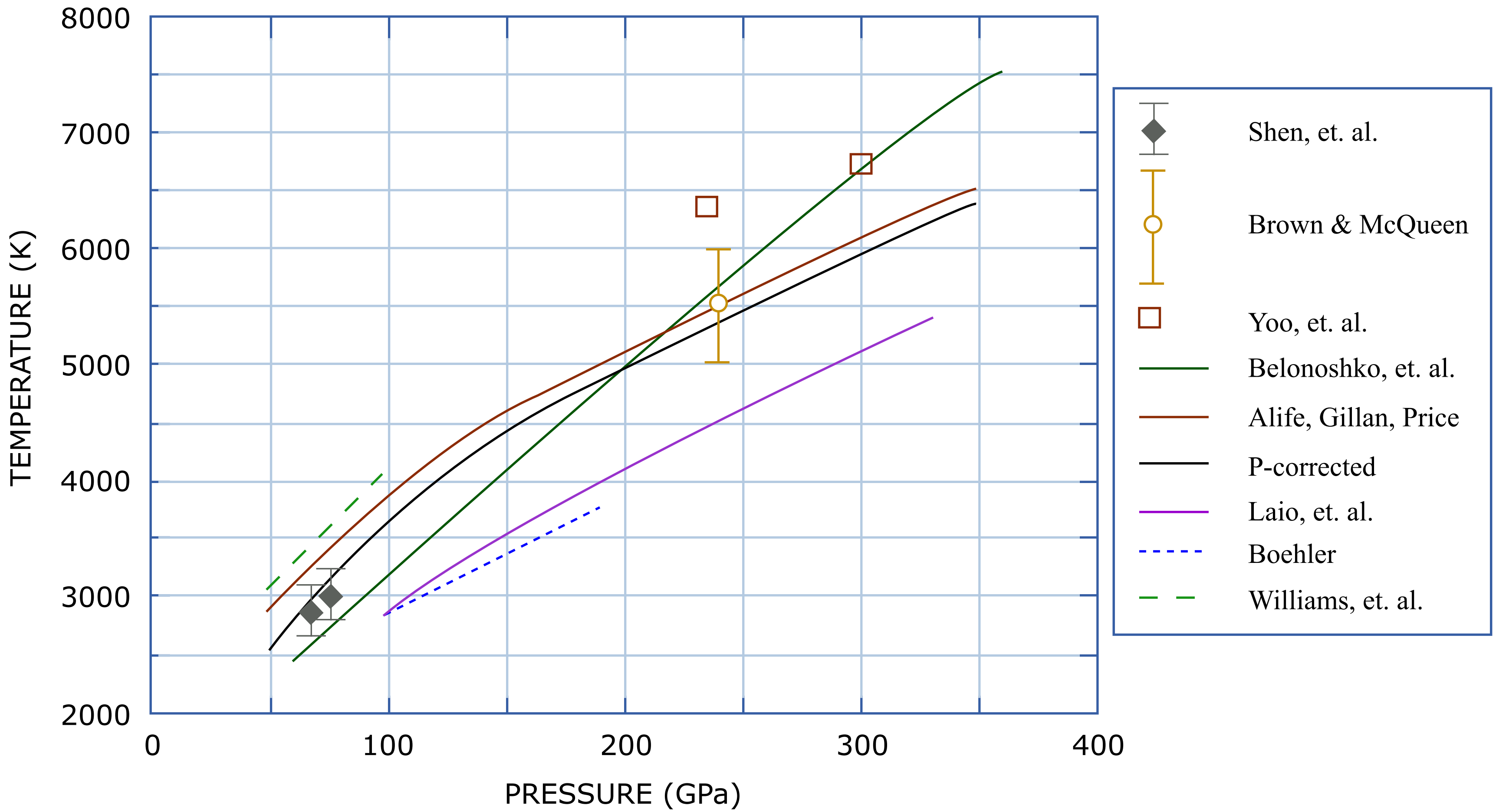


Figure by MIT OCW. After D. Alfe.

Force Matching Method

Laio et al, Science '00

Graph and diagram removed for copyright reasons.

Neptune and Uranus

Ancilotto et al, Science '97

- Middle ice layer: methane, ammonia, and water in solar proportions
- From 20 GPa/2000K to 600 Gpa/8000K

A rain of diamonds ?

Diagrams removed for copyright reasons.

Source: Figure 1 in Ancilotto, F., et al. "Dissociation of Methane into Hydrocarbons at Extreme (Planetary) Pressure and Temperature." *Science* 275, no. 5304 (Feb. 1997): 1288-1290 .

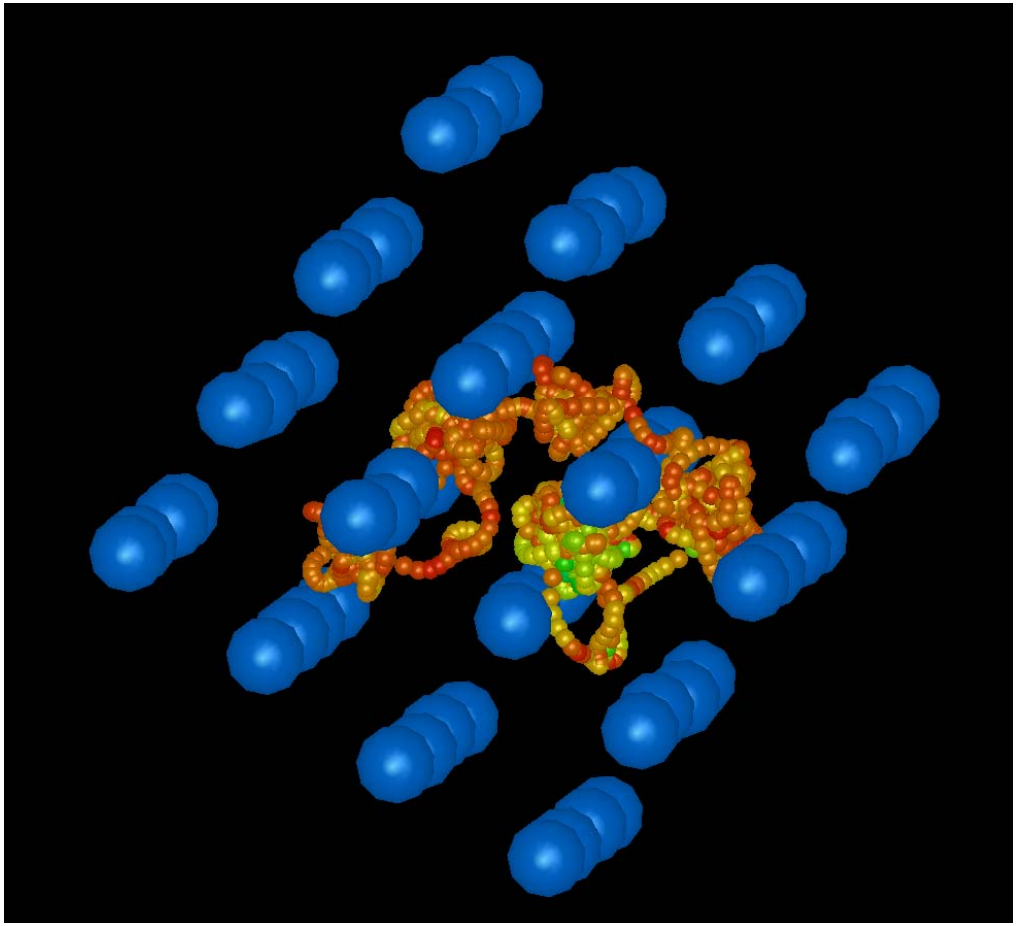
Image removed for copyright reasons.

From Benedetti et al, 1999.

Experimental confirmation that hydrocarbons and diamonds could both form methane at planetary conditions came from a diamond-anvil experiment at UC-Berkeley by Jeanloz et al.

Superprotonic Water

Cavazzoni et al, Science '99



Courtesy of Erio Tosatti. Used with permission.

Image removed for copyright reasons.

Scan of paper: Goncharov, A.F., et al. "Dynamic Ionization of Water under Extreme Conditions." *Physical Review Letters* 94 (April 1, 2005).

Pairing in dense alkali

Graph and diagram removed for copyright reasons.

Figure 5 in Neaton and Ashcroft, Nature 1999.