The Abdus Salam
International Centre for Theoretical Physics

2137-9

Joint ICTP-IAEA Advanced Workshop on Multi-Scale Modelling for Characterization and Basic Understanding of Radiation Damage Mechanisms in Materials

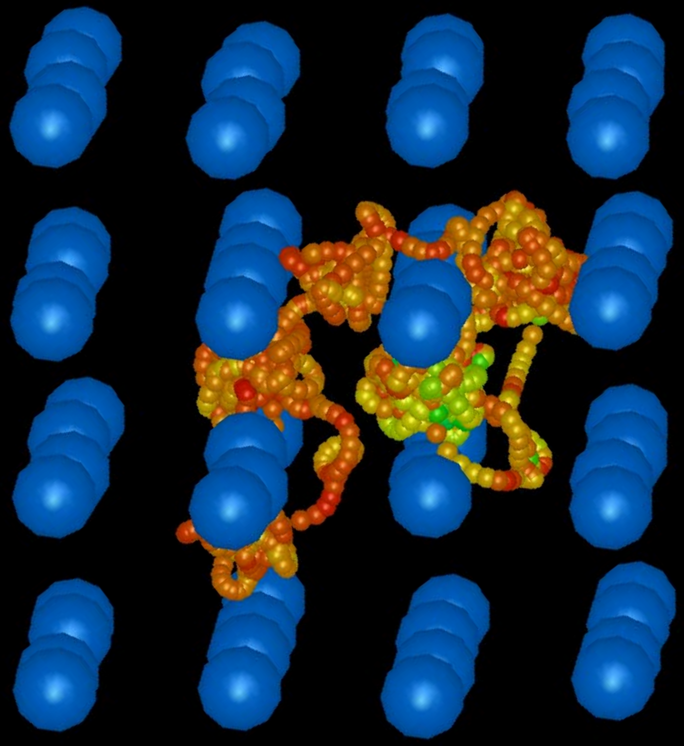
12 - 23 April 2010

ICTP Modeling at extreme conditions

S. Scandolo
ICTP
Trieste
Italy

Simulating matter at extreme conditions

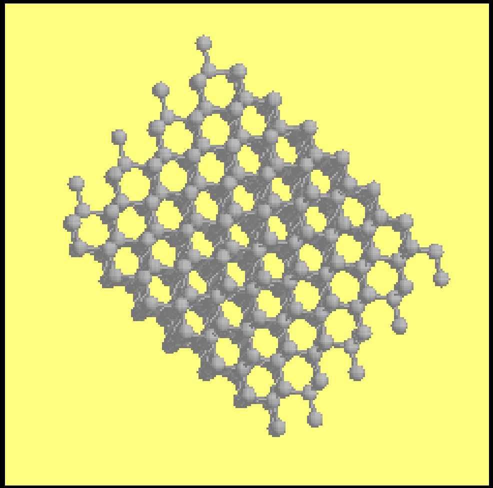
Sandro Scandolo
(the Abdus Salam ICTP,
Trieste, Italy)

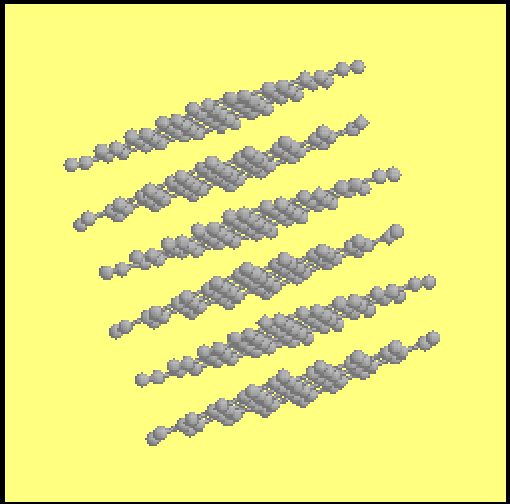


ICTP-IEAE Workshop
April 2010

Diamond

Graphite





High pressure in

Physics

nature

Melting hydrogen

A new superfluid awaits discovery

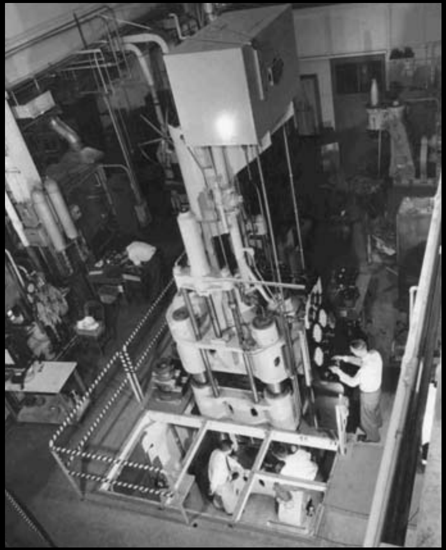
Redesigning life
Synthetic biology raises safety fears

Beta Pictoris
New planets in the ring

Influenza
Old pandemics never die...

1935: prediction of metallic hydrogen

Materials Science

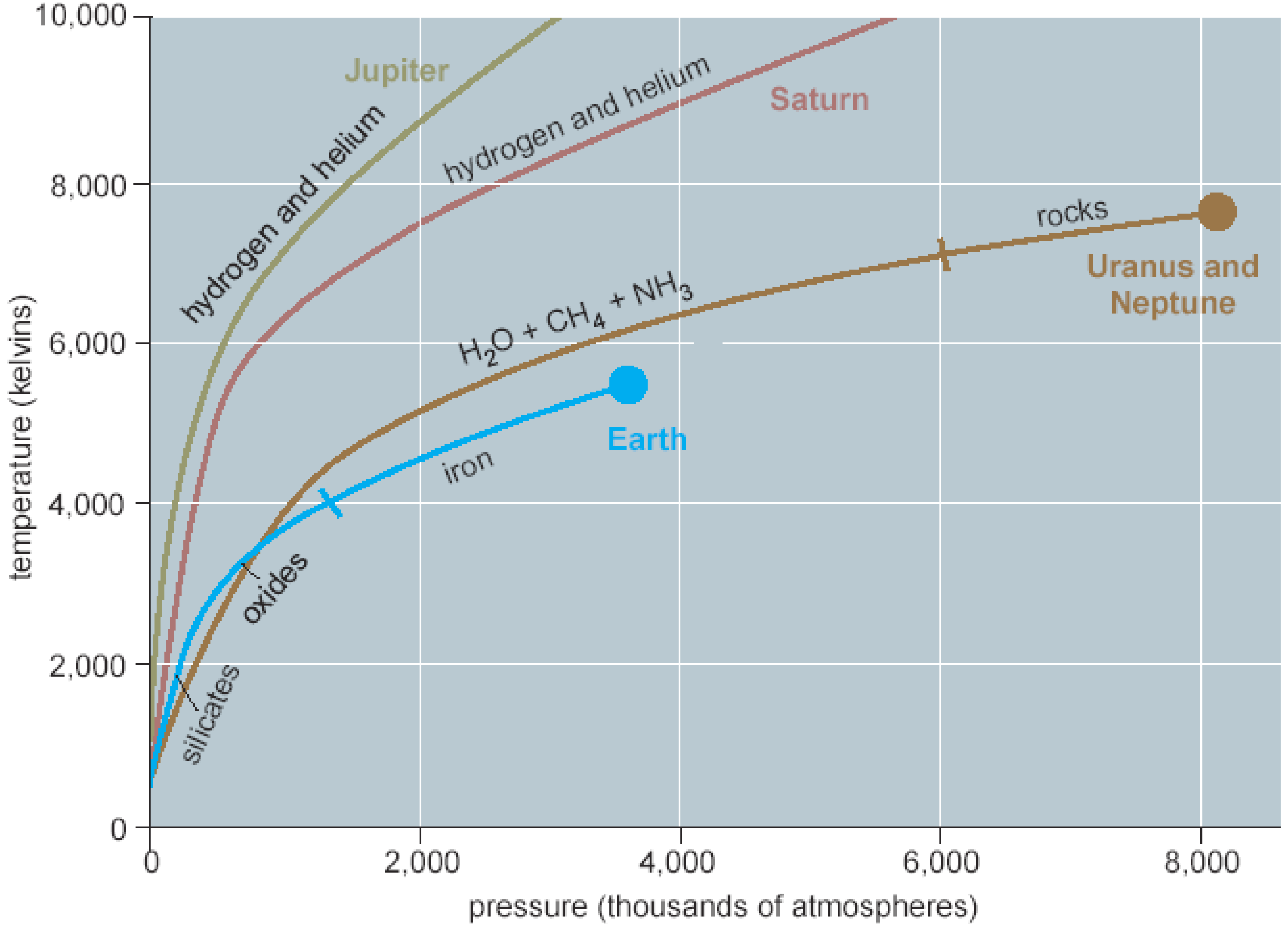


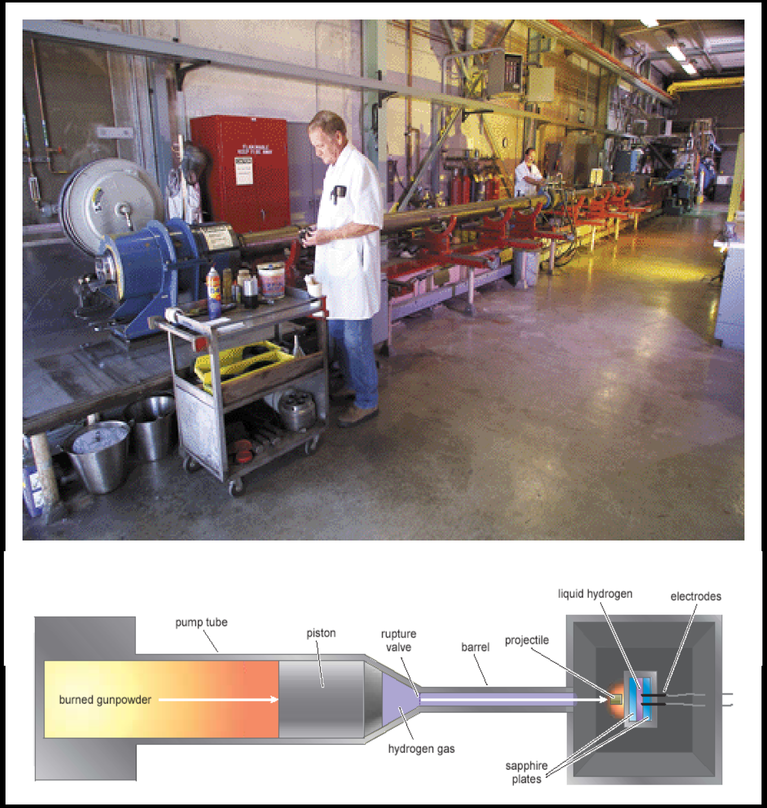
1951: the first man-made diamonds

Planetary Science

1991: Earth’s core conditions reproduced in the laboratory

Scandolo & Jeanloz, American Scientist (2003)

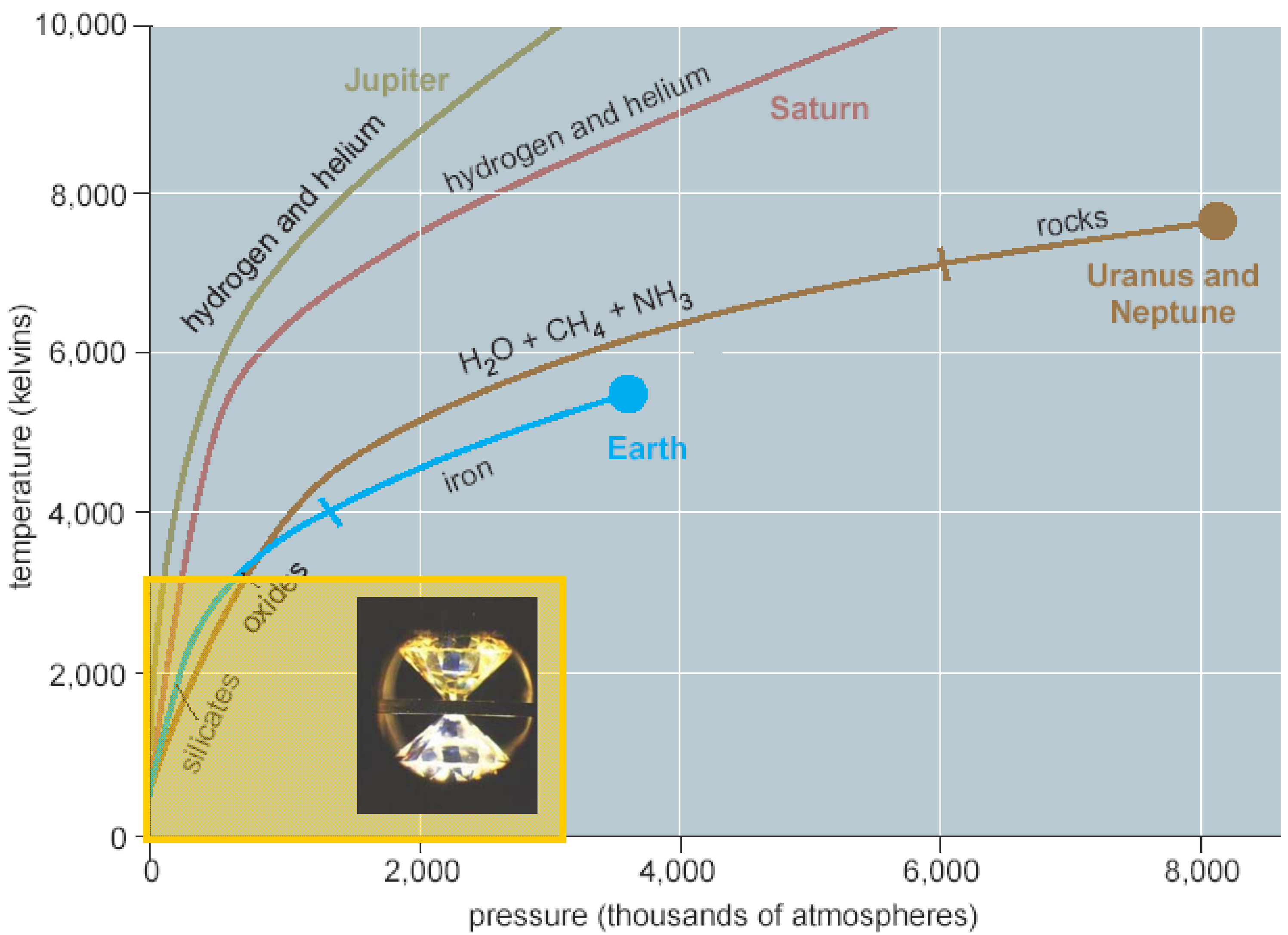




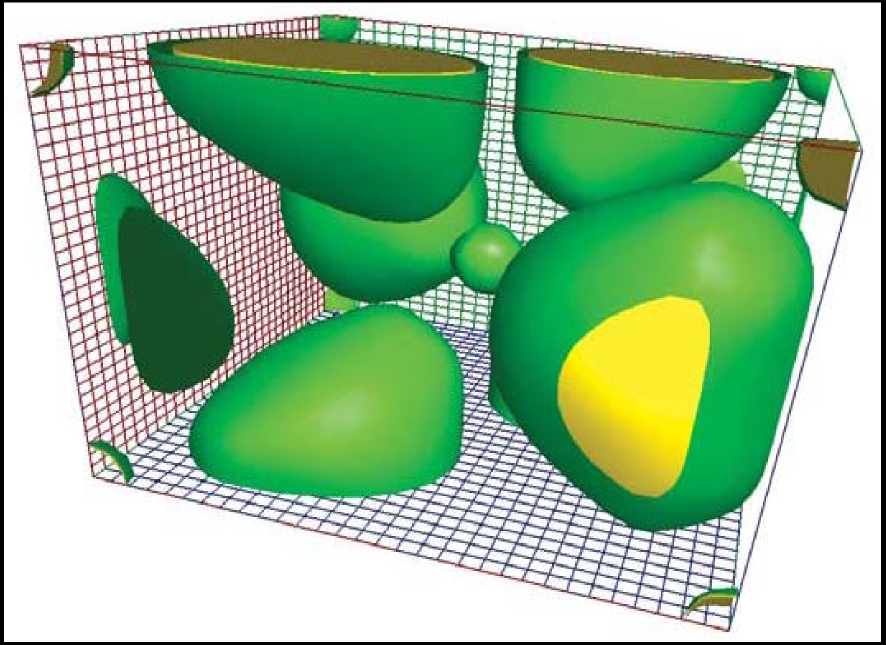
Shock waves

Diamond anvil cell

Scandolo & Jeanloz, American Scientist (2003)



Quantum simulations: The “standard model”



Electron charge density in SiO_2 stishovite

“Molecular dynamics”
for atoms

$$\mathrm{Ma} = \mathrm{F} = \boxed{-\mathrm{dE}}/\mathrm{dR}$$

Schroedinger equation
for electrons

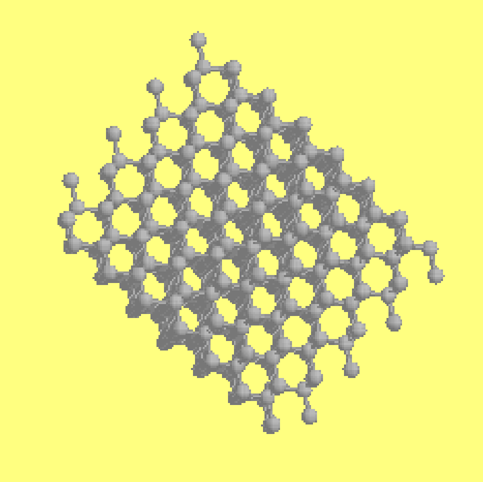
$$\mathrm{H}\psi = \boxed{\mathrm{E}\psi}$$

e^--e^- interactions:
 Density Functional Theory

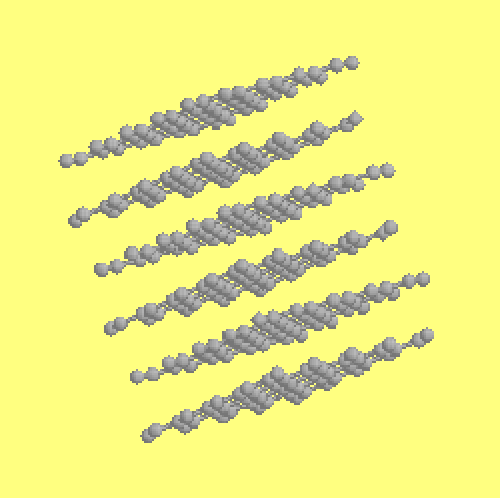
e^--nuclei interactions:
 Pseudopotentials

“Ab-initio” molecular dynamics = Classical molecular dynamics in the potential energy surface generated by the electrons in their quantum ground state

Diamond

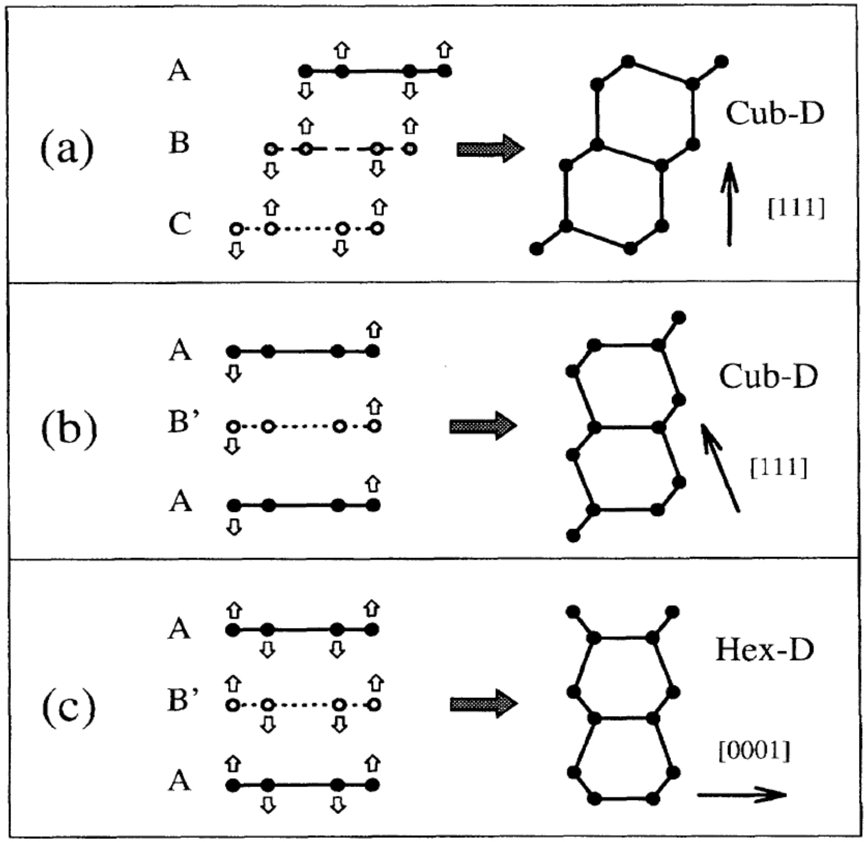


Graphite

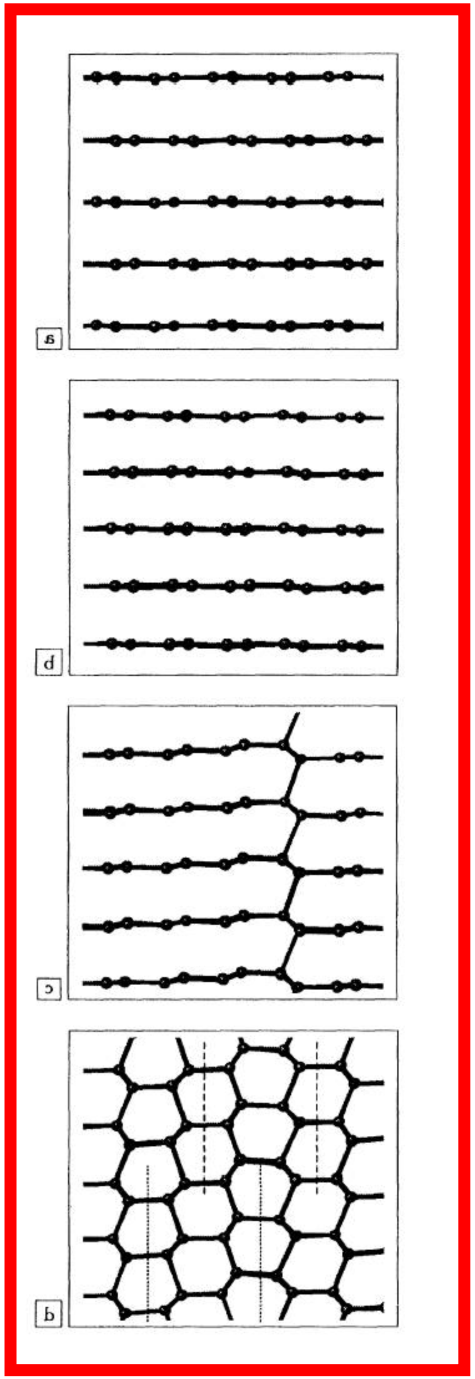


Atomistic mechanism of the graphite to diamond transition

Possible paths

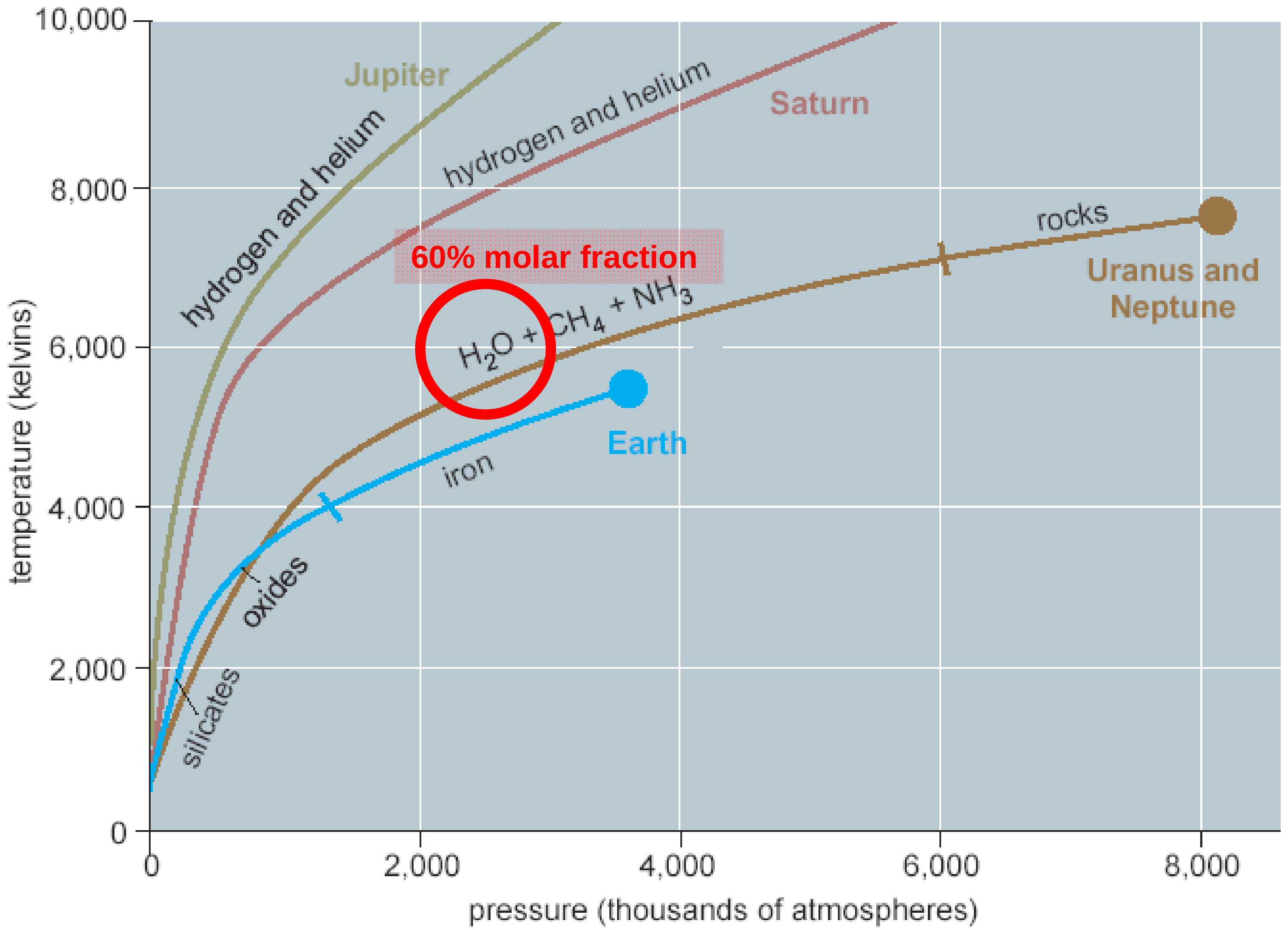


S. Scandolo et al., PRL 74, 4015 (1995)

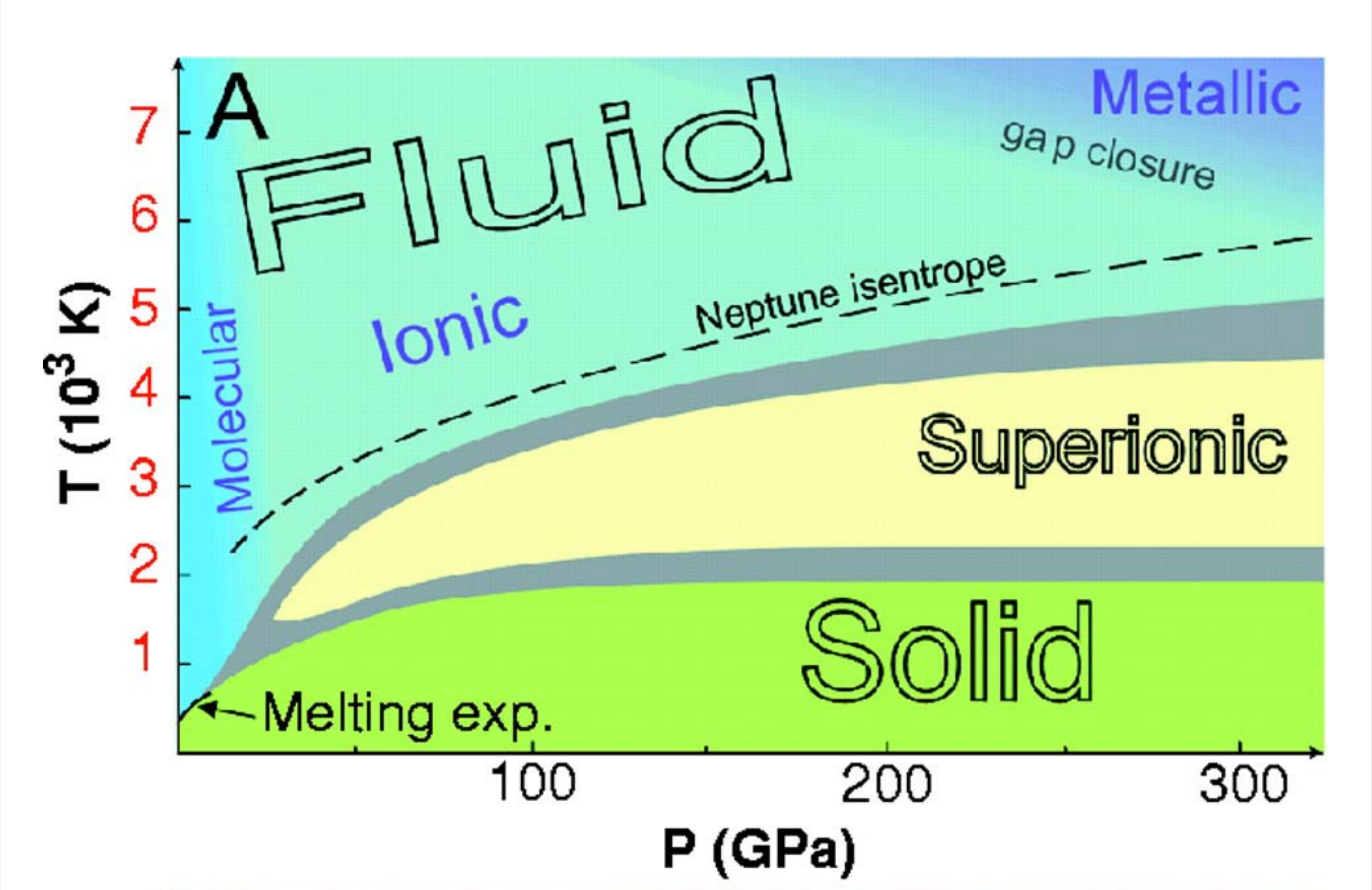


1 picosecond

Water and hydrogen at planetary conditions


10,000
8,000
6,000
4,000
2,000
0
0
2,000
4,000
6,000
8,000
temperature (kelvins)
pressure (thousands of atmospheres)
Jupiter
hydrogen and helium
hydrogen and helium
Saturn
60% molar fraction
$H_2O + CH_4 + NH_3$
rocks
Uranus and Neptune
Earth
iron
oxides
silicates

phase diagram of water from first principles



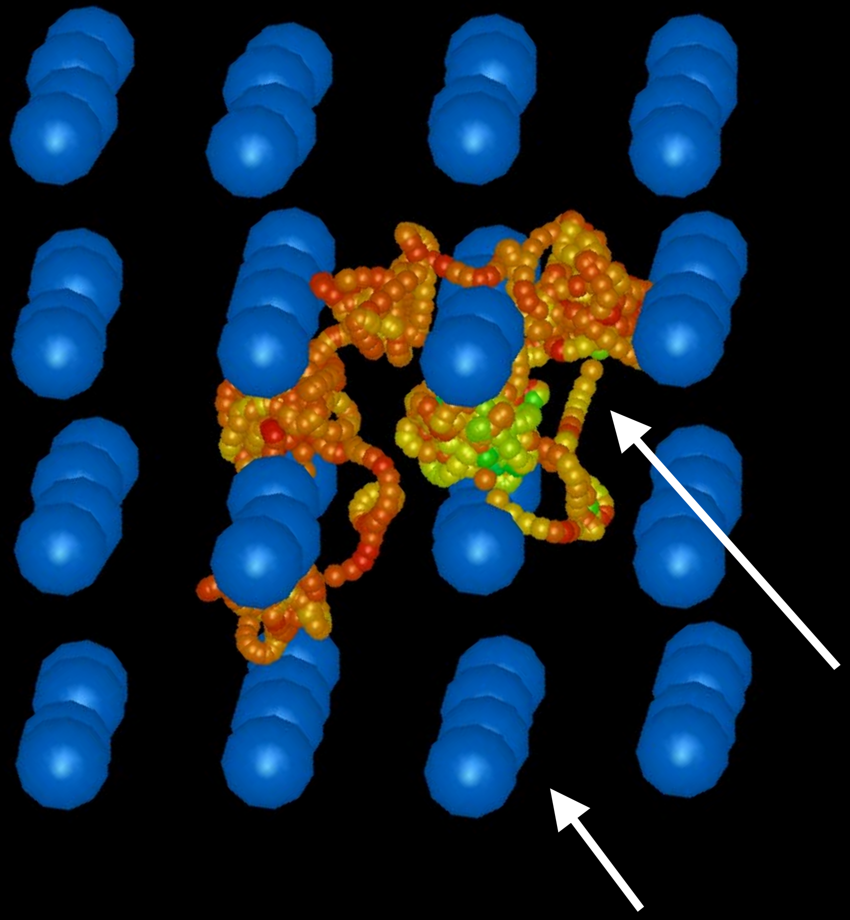
C. Cavazzoni et al., Science 283, 44 (1999)

**Experimental confirmation (?)
of superionic phase:
A. Goncharov et al.,
Phys. Rev. Lett. (2006)**

C. Cavazzoni et al., Science 283, 44 (1999)

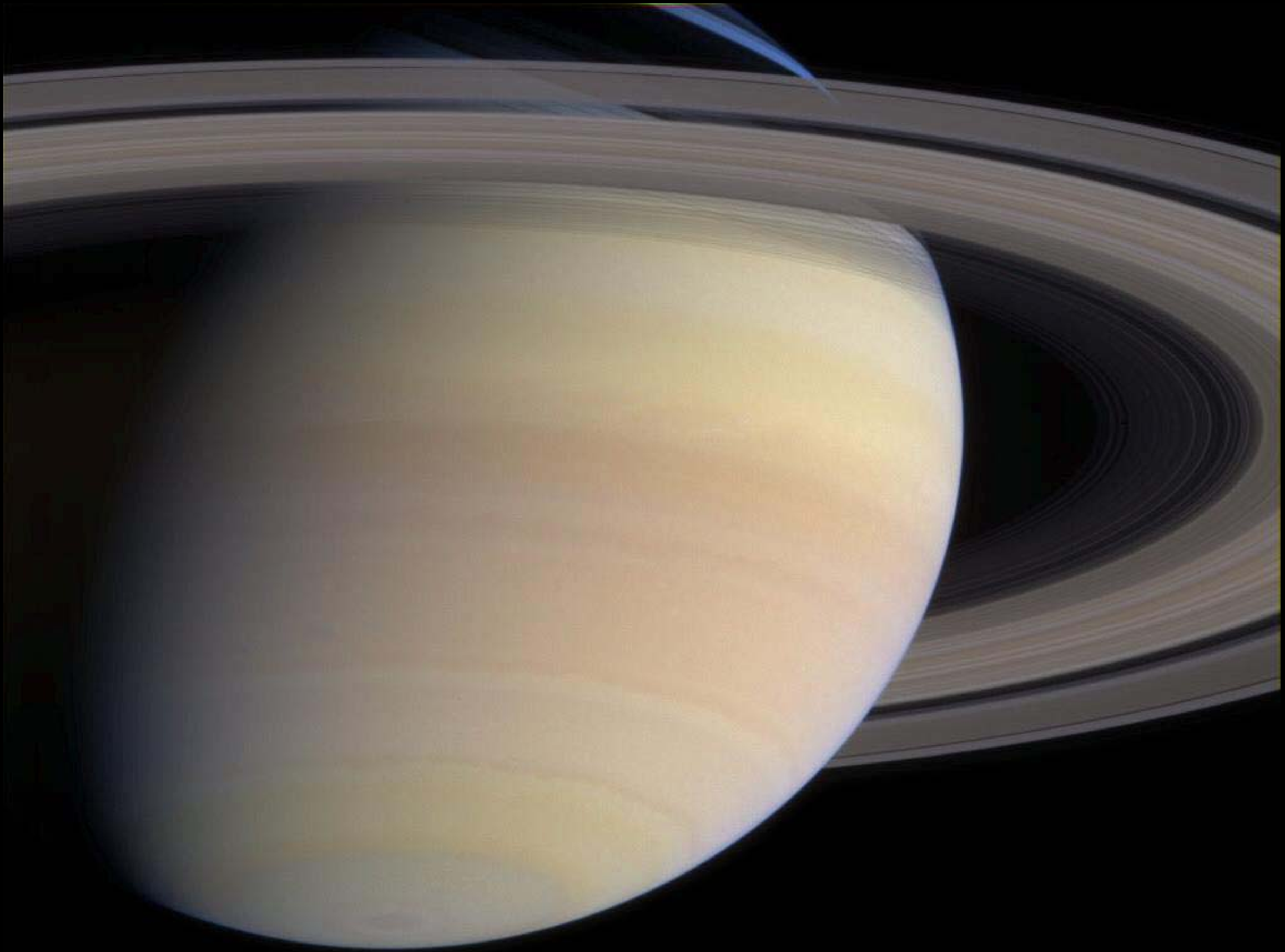
Superionic Water

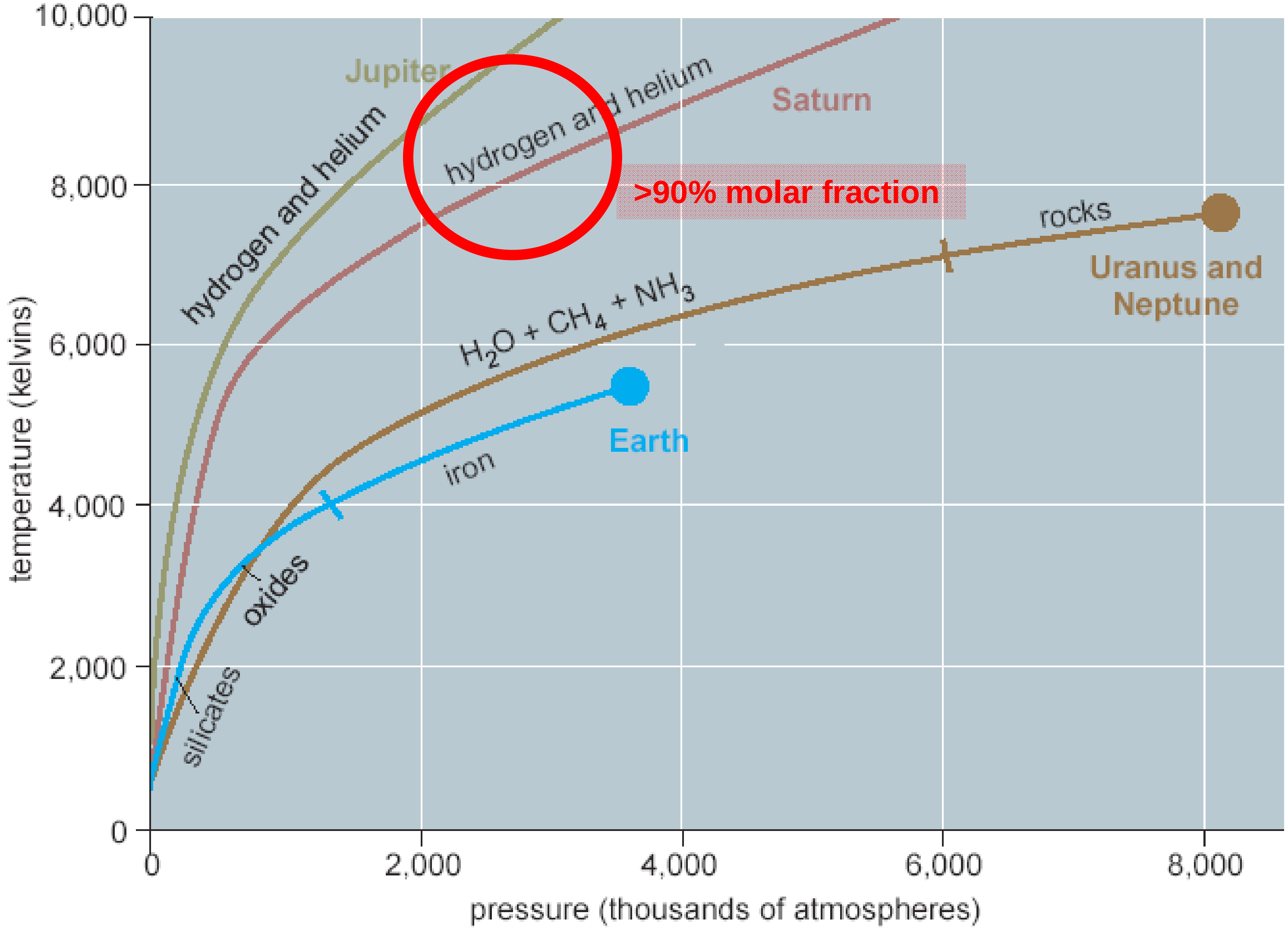
P = 150 GPa
T = 2500 K



Proton diffusion by hopping

Oxygen sublattice remains crystalline



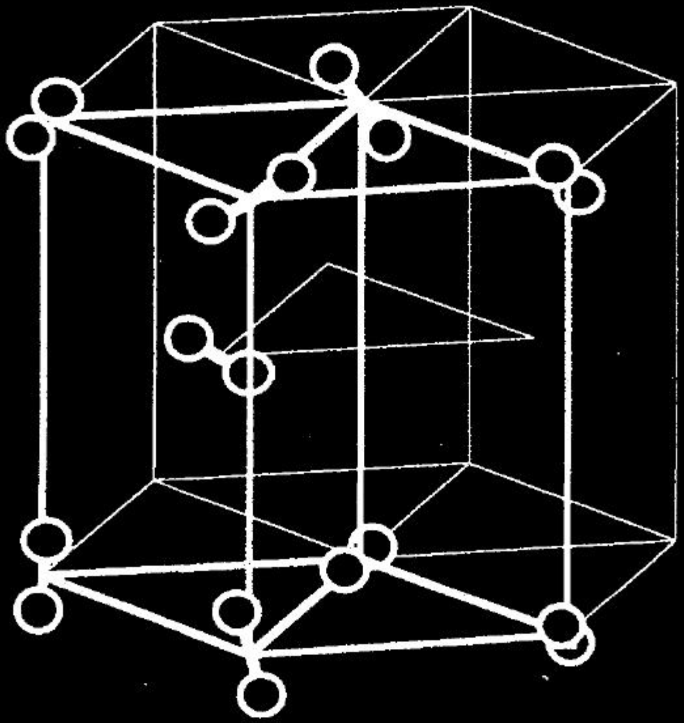


>90% molar fraction

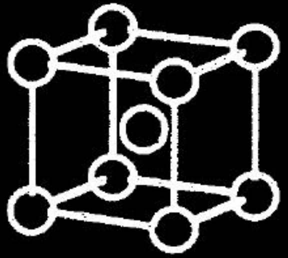
E. Wigner and H.B. Huntington

"On the possibility of a metallic modification of hydrogen"

J. Chem. Phys. 3, 764 (1935)

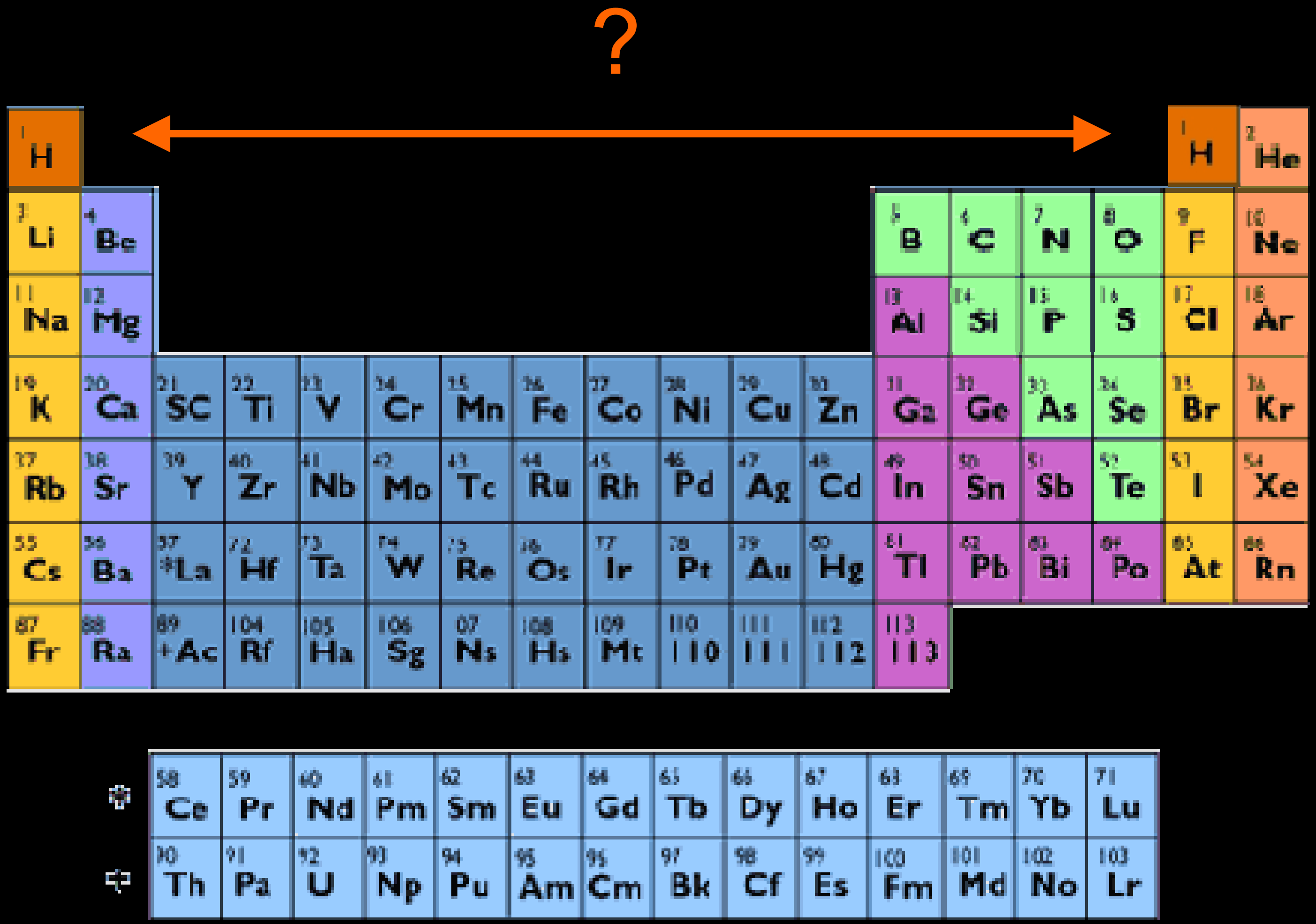


Molecular hydrogen



Monatomic hydrogen

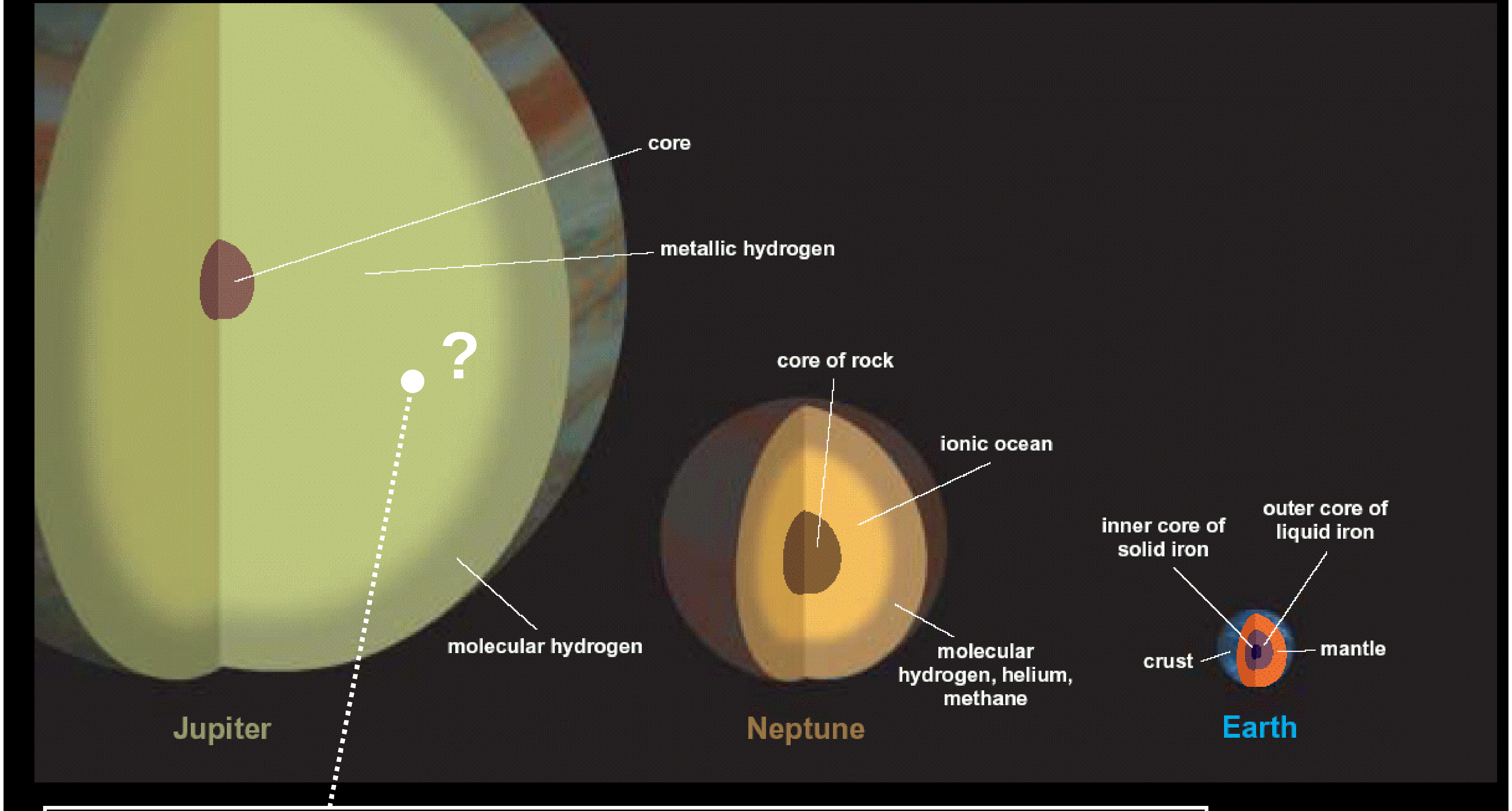
Hemley and Mao, Rev Mod Phys



?

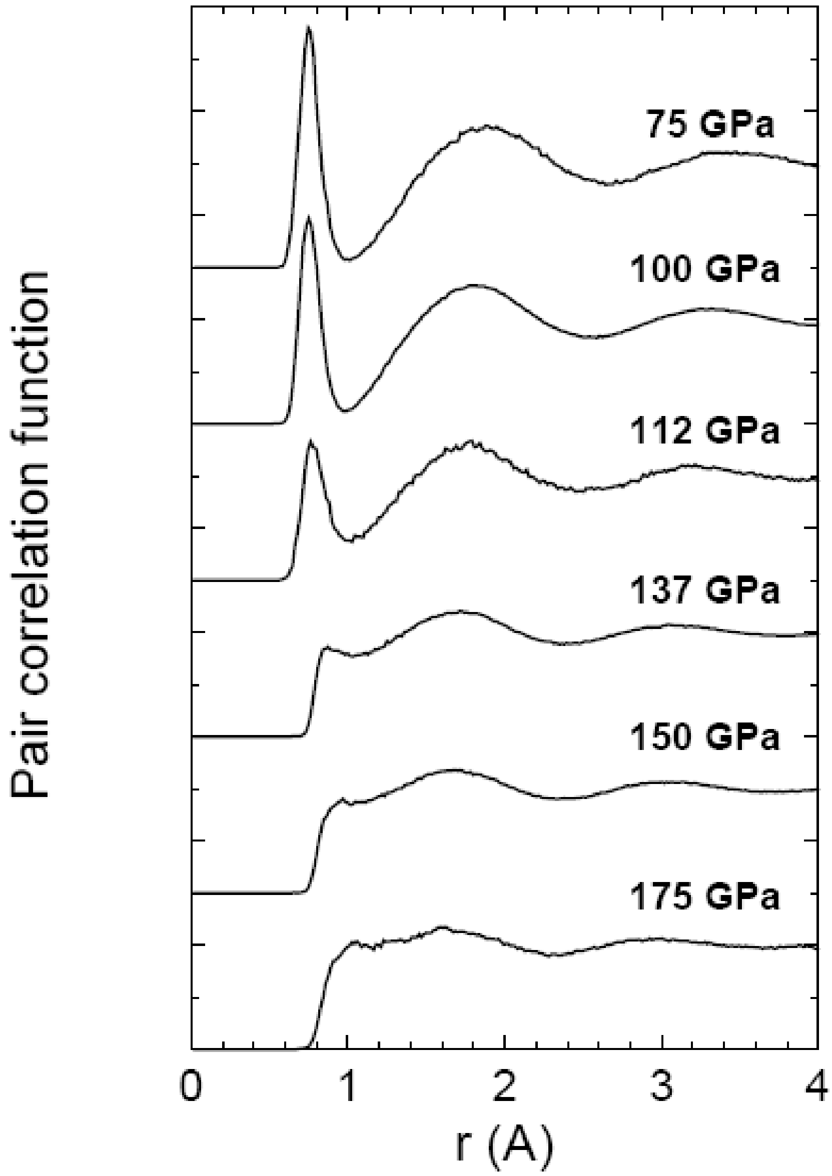
1 H																1 H	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 SC	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 *La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 +Ac	104 Rf	105 Ha	106 Sg	07 Ns	108 Hs	109 Mt	110 110	111 111	112 112	113 113					

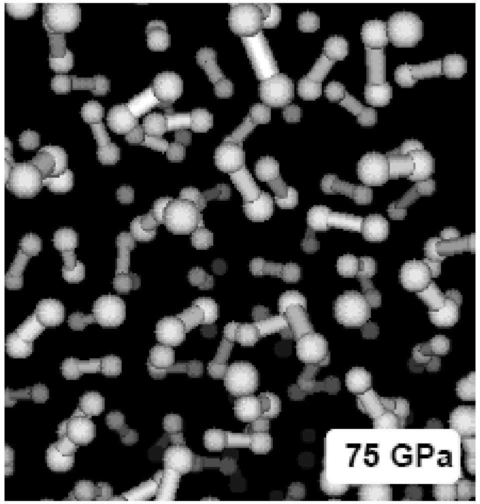
*	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
+	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

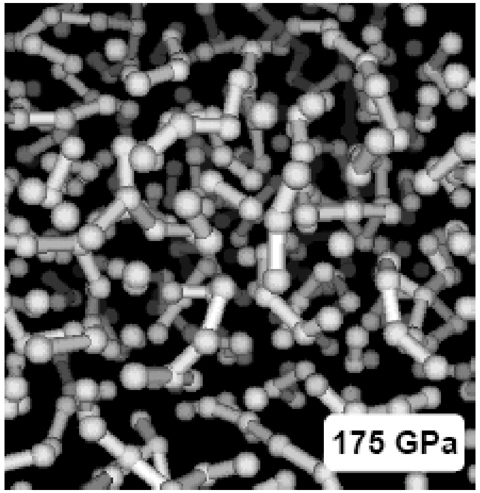


- At which depth does hydrogen become an electrical conductor?
- Is metallization accompanied by a sharp density change?

Molecular to non-molecular transition



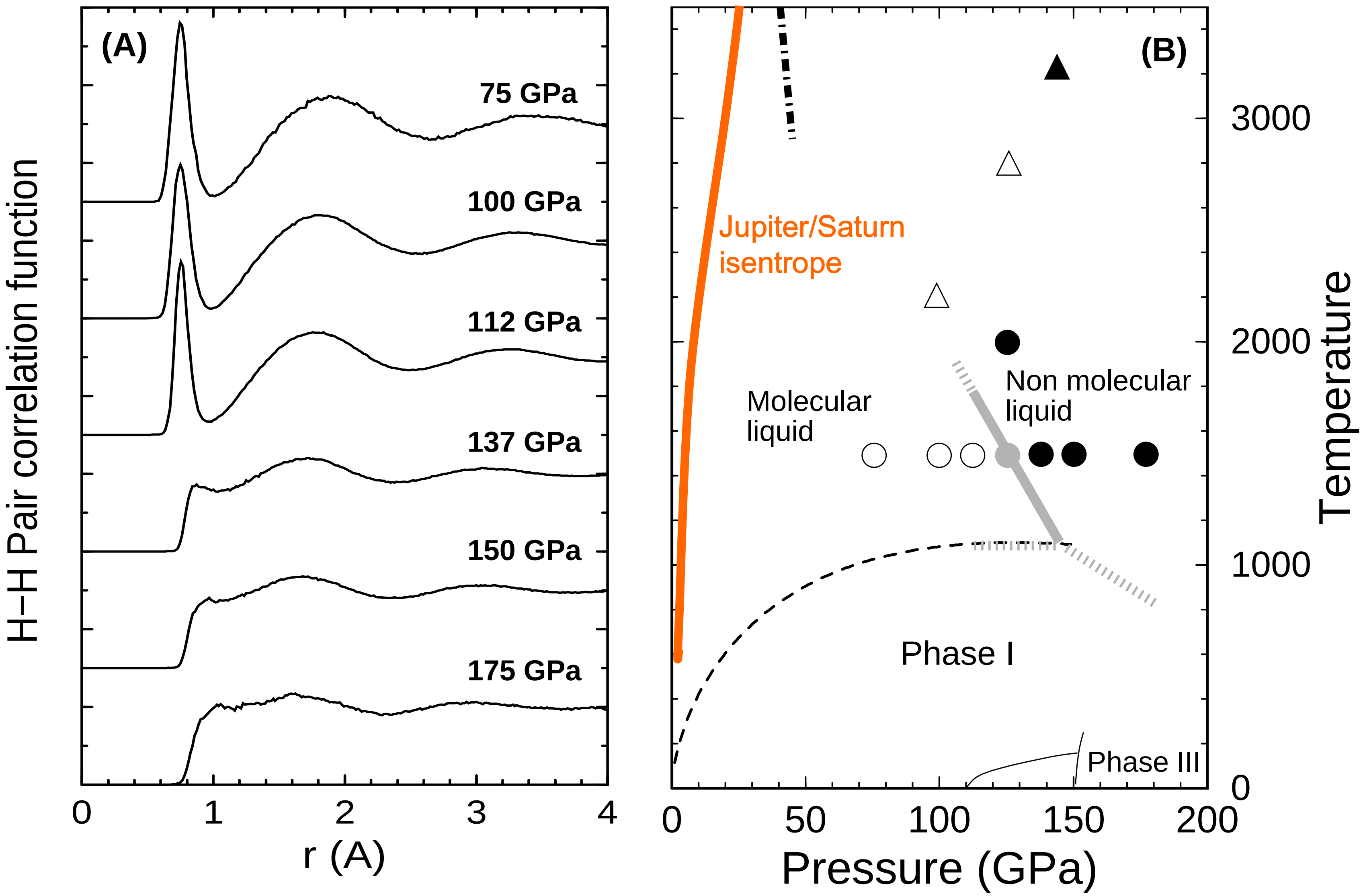




S. Scandolo, Proc. Natl. Acad. Sci. USA, 2003

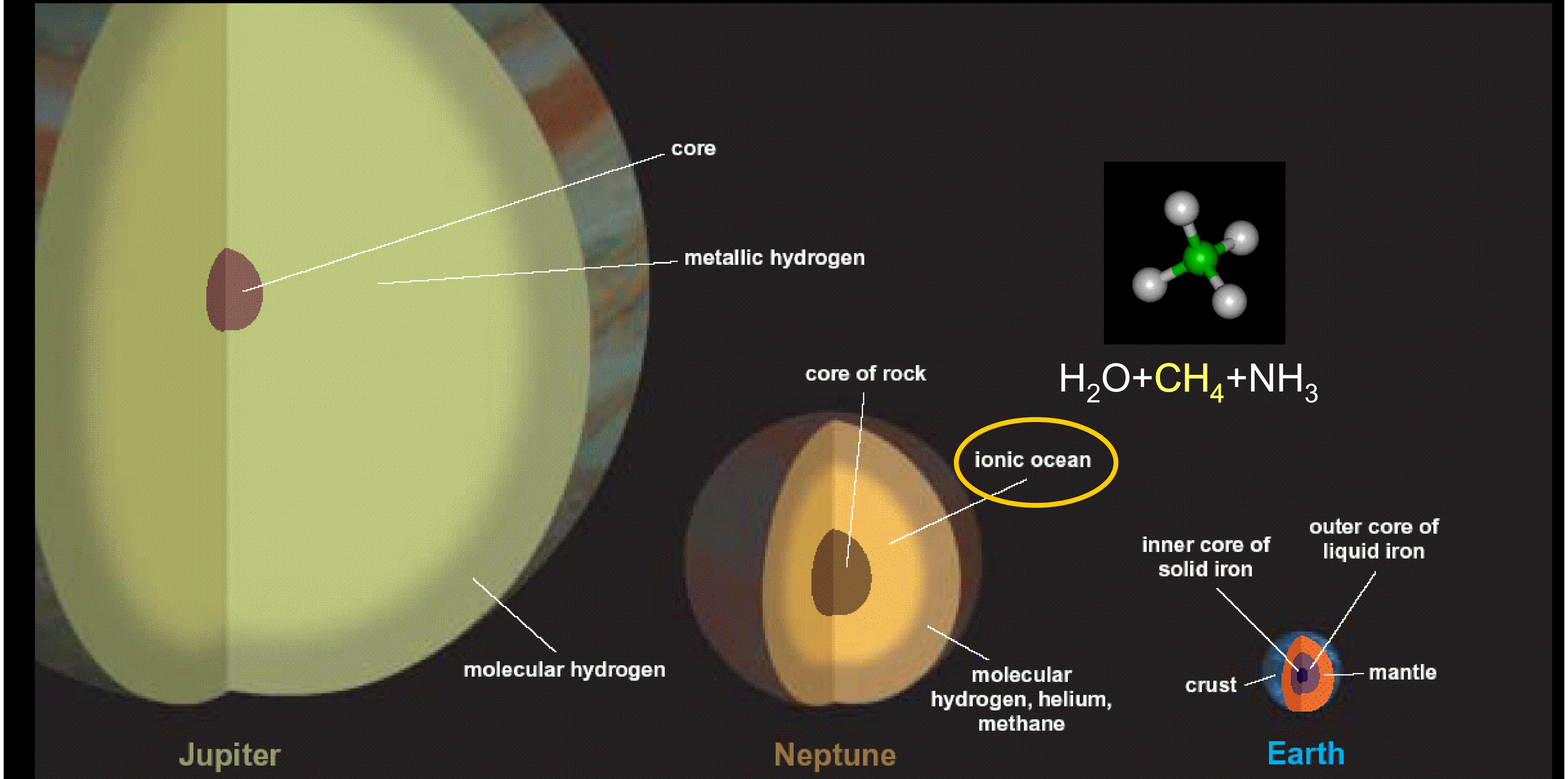
Is there a first-order phase transition inside Jupiter/Saturn?

S. Scandolo, Proc. Natl. Acad. Sci. USA, 2003



Diamonds in the sky?

Scandolo & Jeanloz, American Scientist (2003)

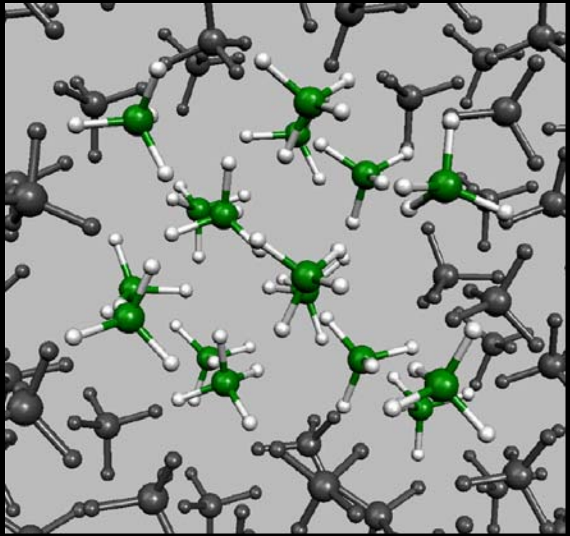


$H_2O+CH_4+NH_3$

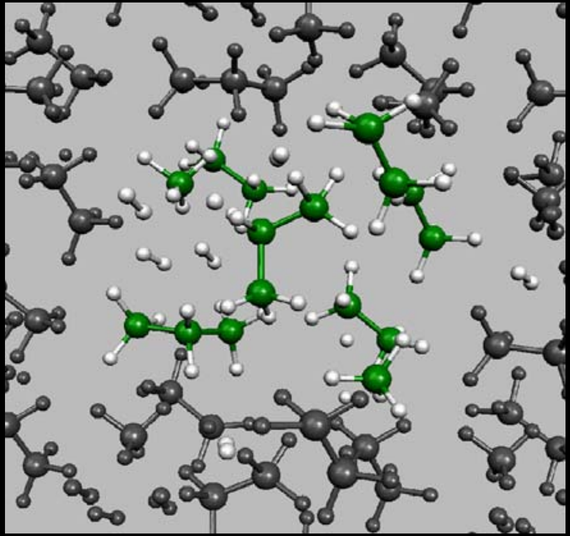
Marvin Ross, "Diamonds in the sky"
Nature (1981)

Methane was found to
dissociate under a shock wave

Dissociation of methane at extreme (planetary) conditions

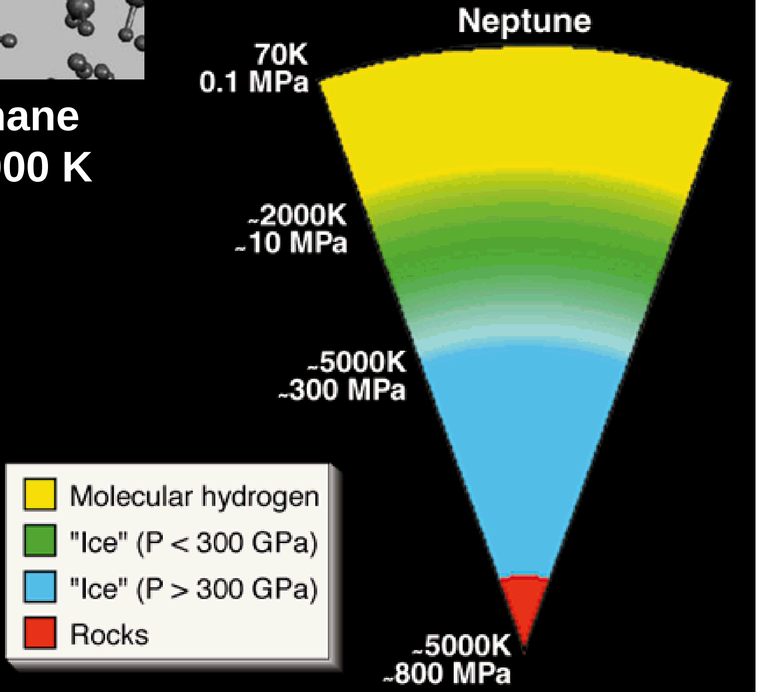


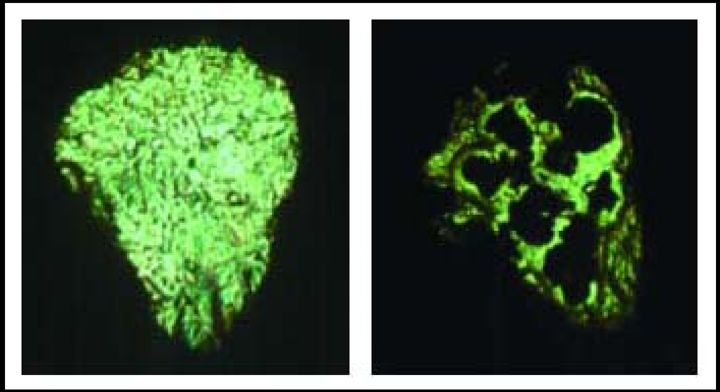
Compressed methane



Compressed methane after heating to 4000 K

F. Ancilotto et al., Science 275, 1288 (1997)

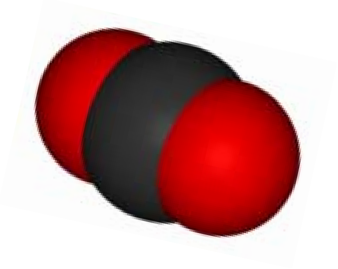




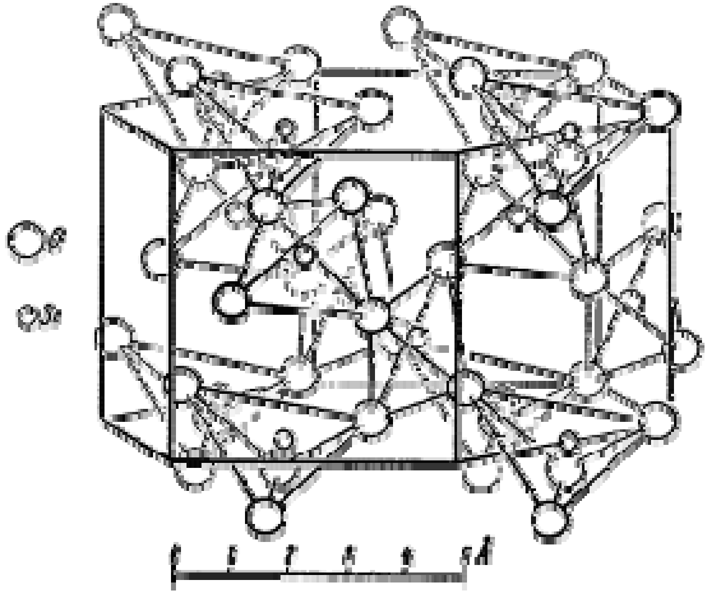
L.R. Benedetti et al., Science 283, 100 (1999)

“Polymeric” CO_2

CO_2

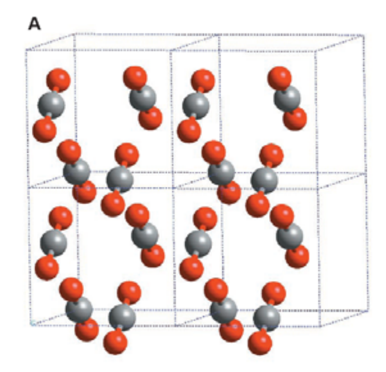


SiO_2



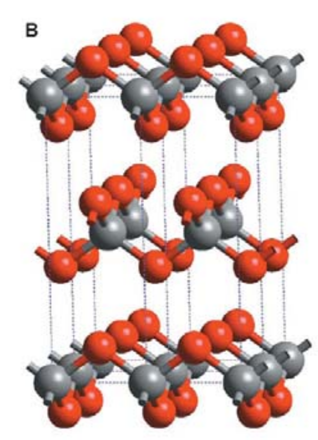
Silica-like CO_2 : the crystal phases

Serra, Cavazzoni, Chiarotti, Scandolo, Tosatti, Science 284, 788 (1999)



Molecular CO_2
(phase III)

1000 K
100 GPa



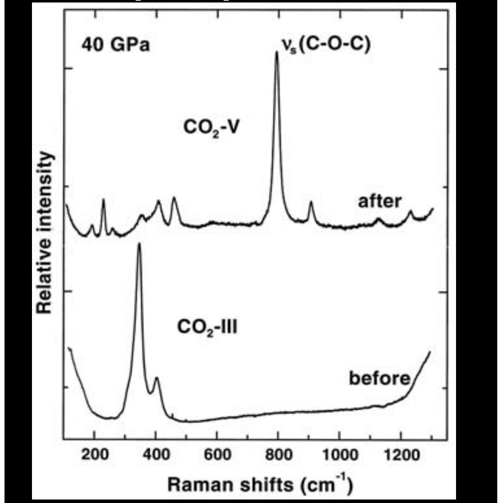
Layered tetrahedral CO_2

+ Molecular CO_2 predicted to tranform into a silica-like crystal at high pressure

+ Silica-like phases of CO_2 predicted to be ultrahard

Experimental confirmation of silica-like CO_2

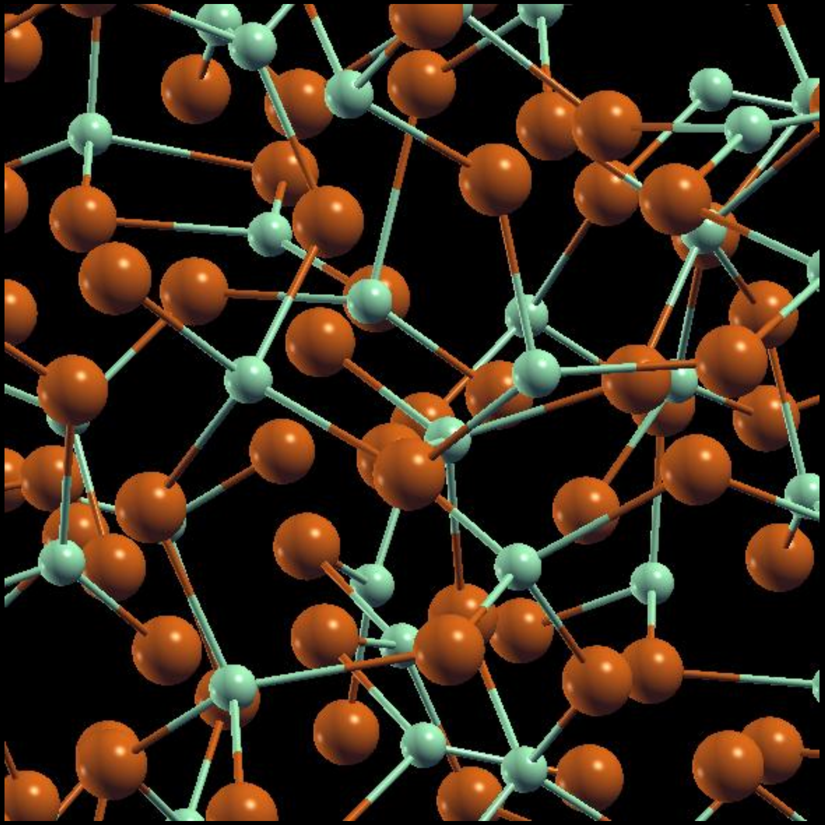
Yoo et al, Science 283, 1510 (1999)



Crystal structure of silica-like CO_2 not yet determined

Is there a glass analog?

Silica-like CO_2 : an amorphous phase?



Compression by ab-initio molecular dynamics gives:

At 1000 K and 100 GPa: a crystalline (layered) phase

At 2000 K and 80 GPa: an amorphous phase

Serra, Cavazzoni, Chiarotti, Scandolo, Tosatti, Science 284, 788 (1999)

NATURE|Vol 441|15 June 2006

SOLID-STATE CHEMISTRY

A glass of carbon dioxide

Paul F. McMillan

Carbon is unusual in its family of elements because it has gaseous oxides. But under high pressure, carbon dioxide forms crystalline solids and can become a glass — so revealing the chemical family resemblance.

Last Updated: Thursday, 15 June 2006, 11:16 GMT 12:16 UK

Dry ice creates toughened glass

A form of solid carbon dioxide that could be used to make ultra-hard glass or coatings for microelectronic devices has been discovered.

The material, named amorphous carbonia, was created by an Italian led team.

The scientists told the journal Nature that the material was always thought to be possible but, until now, had never been created in the lab.

It was made by squeezing

Silicon is easily converted into

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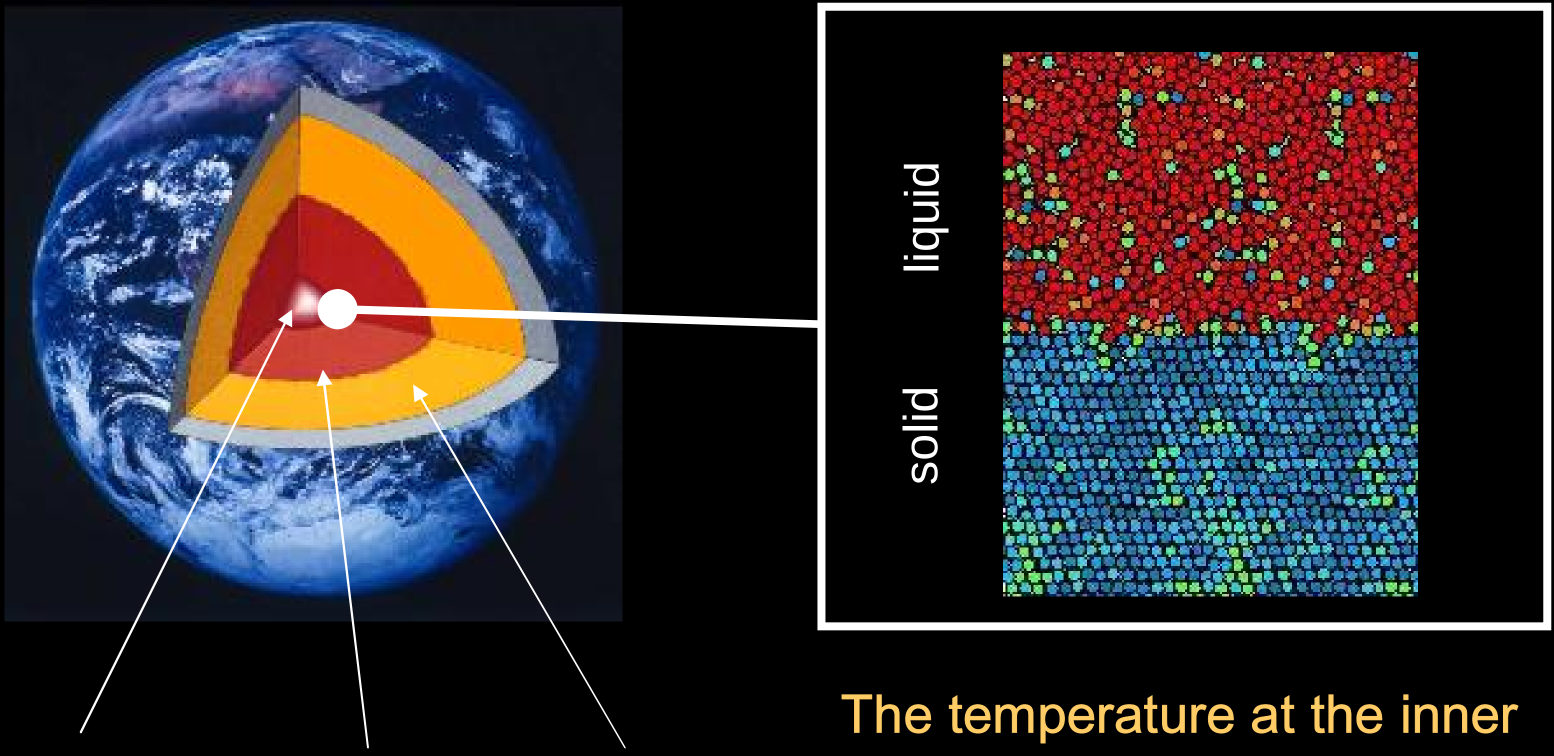
Down to Earth…

How hot is the centre of the Earth?



Inner core
(solid Fe)

Outer core
(liquid Fe)

Mantle

The temperature at the inner core boundary coincides with the melting temperature of Fe at 330 GPa

A number of mineral physics phenomena are difficult to address or even beyond reach for first-principles simulations, because of time scale and size limitations.

Examples include

thermal conductivity

highly viscous silicate melts

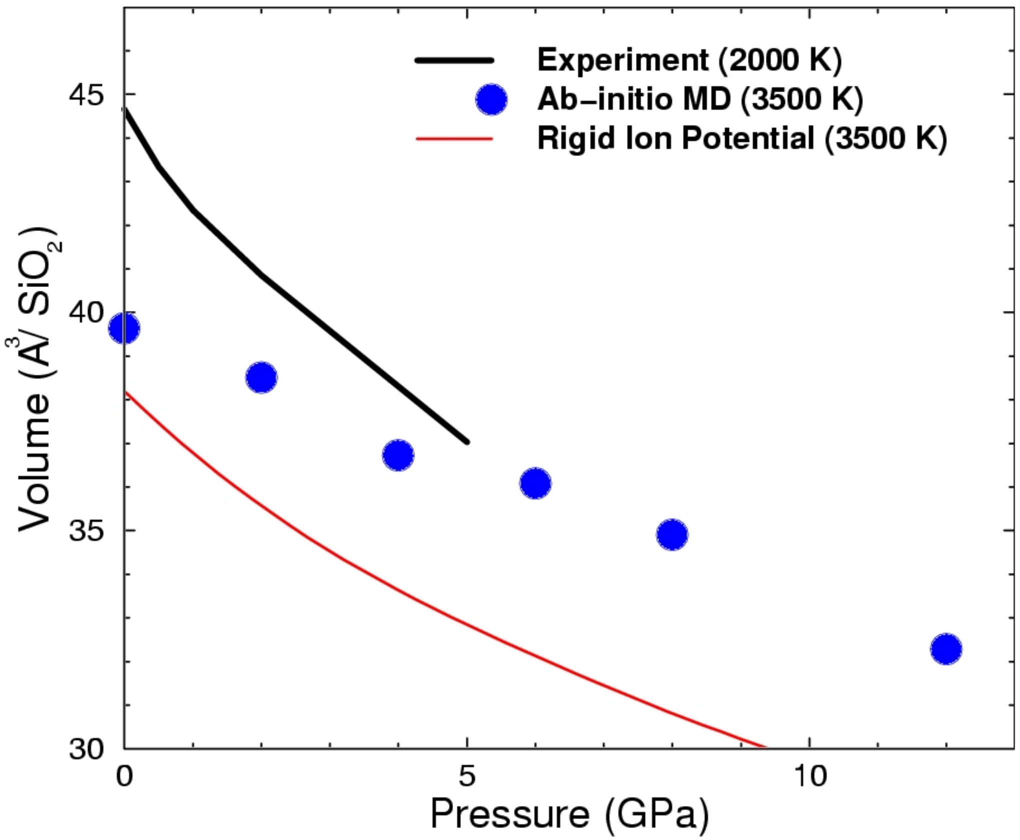
melting temperatures (some aspects of)

rheological properties at high T

etc…

Volume –vs– Pressure in Liquid Silica

T = 3500 K

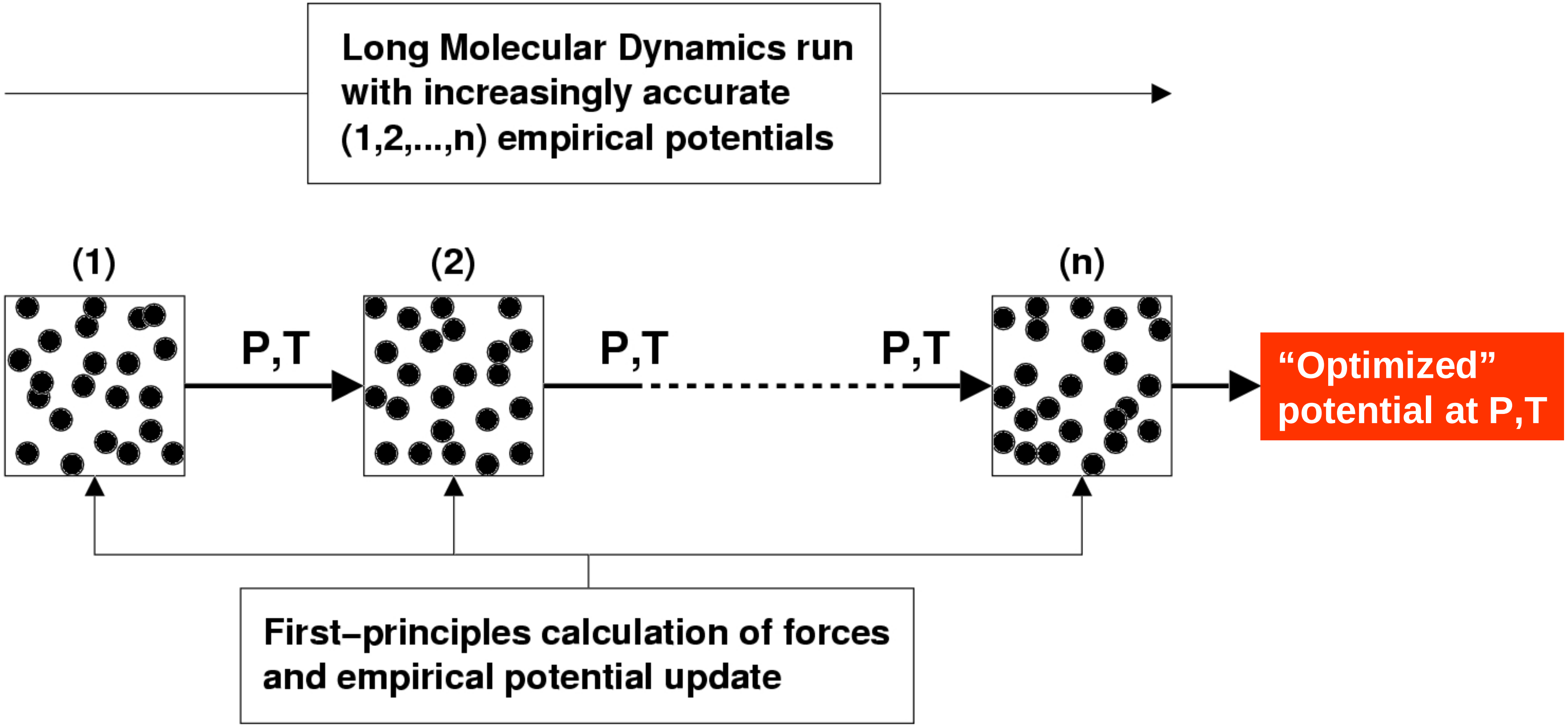


Experiment: Gaetani et al. (1998)

Ab–initio MD: A. Trave et al. Phys. Rev. Lett (2002)

Rigid ion: van Beest, Kramer, van Santen (1990)

The “optimized” potential method



Long Molecular Dynamics run with increasingly accurate (1,2,...,n) empirical potentials

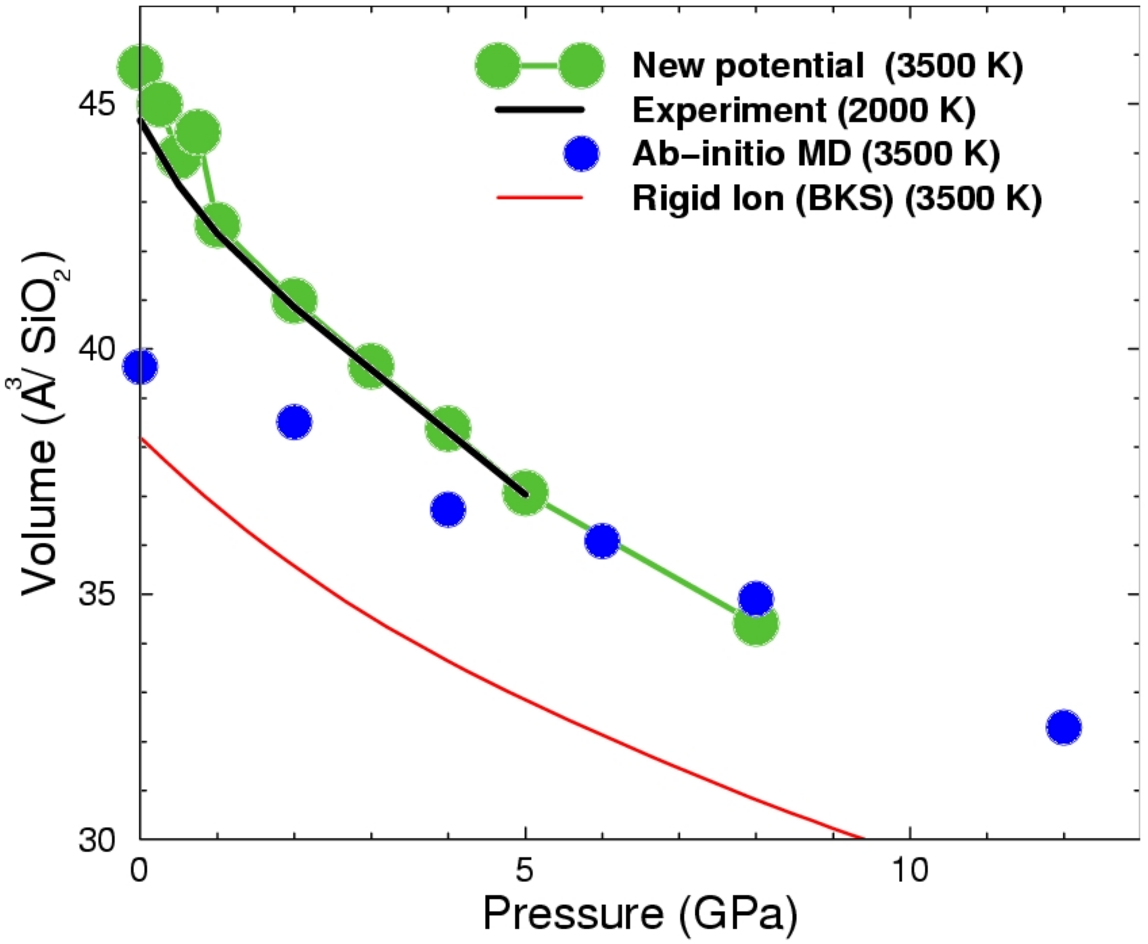
“Optimized” potential at P,T

First–principles calculation of forces and empirical potential update

A. Laio et al, Science 287, 1027 (2000)

Volume –vs– Pressure in Liquid Silica

T = 3500 K



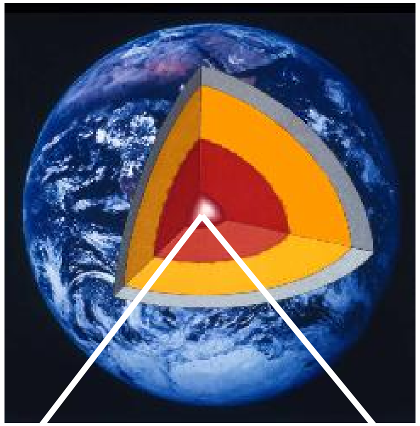
P. Tangney and S. Scandolo
JCP 117, 8898 (2002)

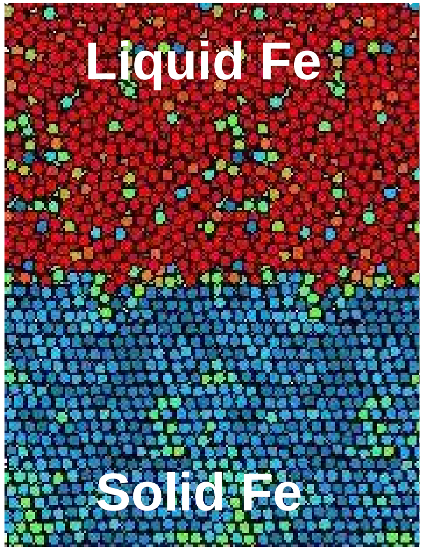
Experiment: Gaetani et al. (1998)

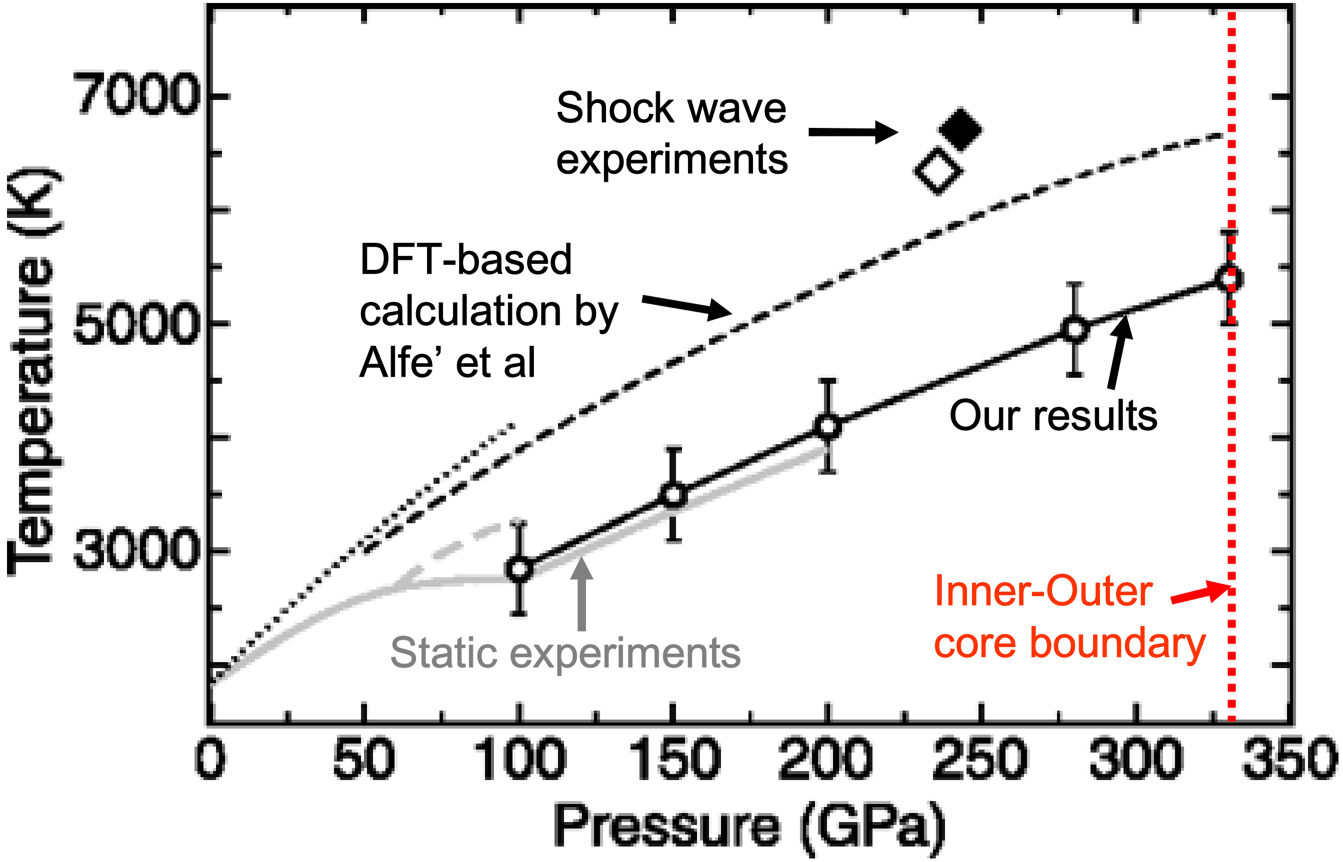
Ab–initio MD: A. Trave et al. Phys. Rev. Lett (2002)

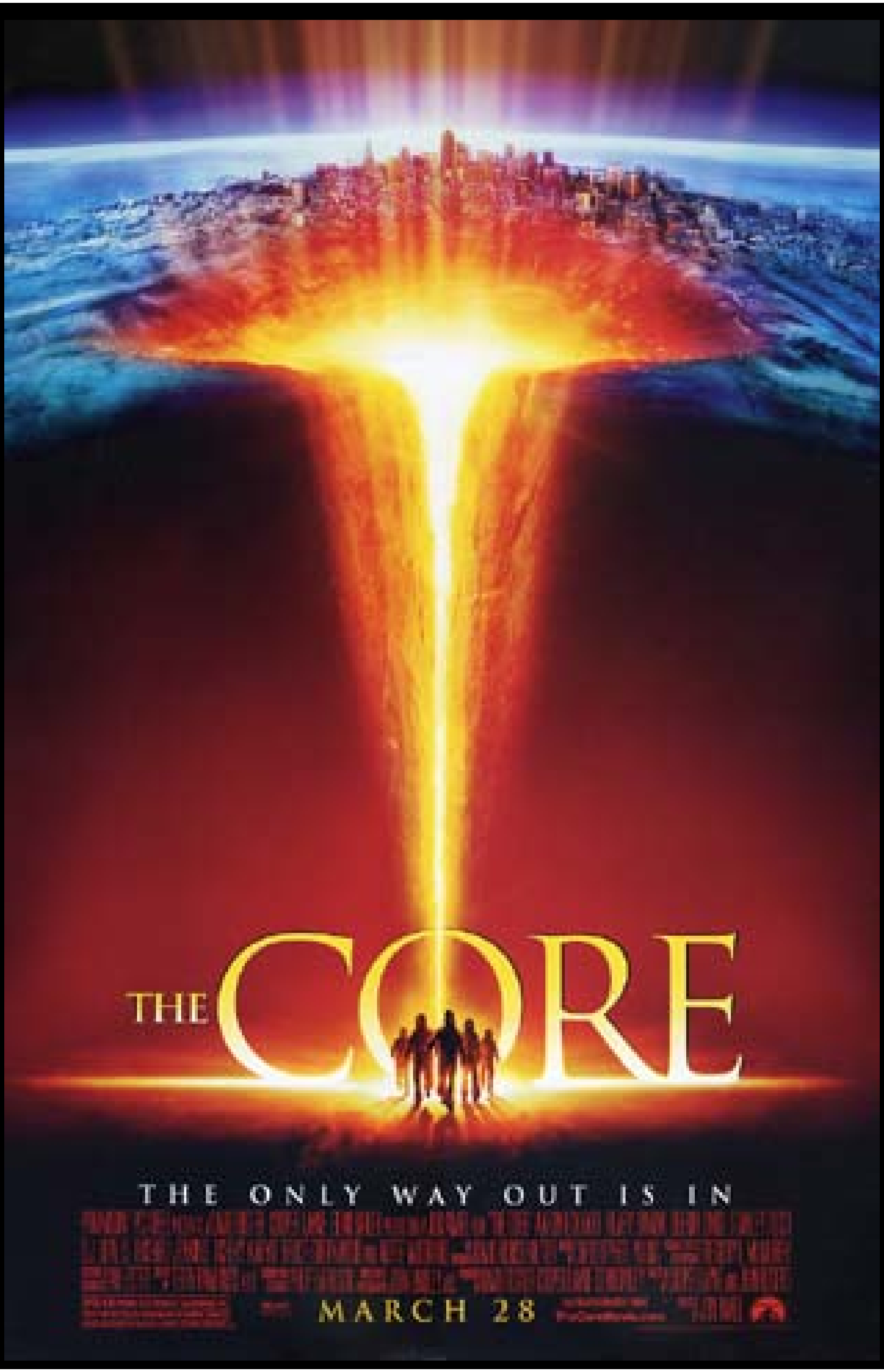
Rigid ion: van Beest, Kramer, van Santen (1990)

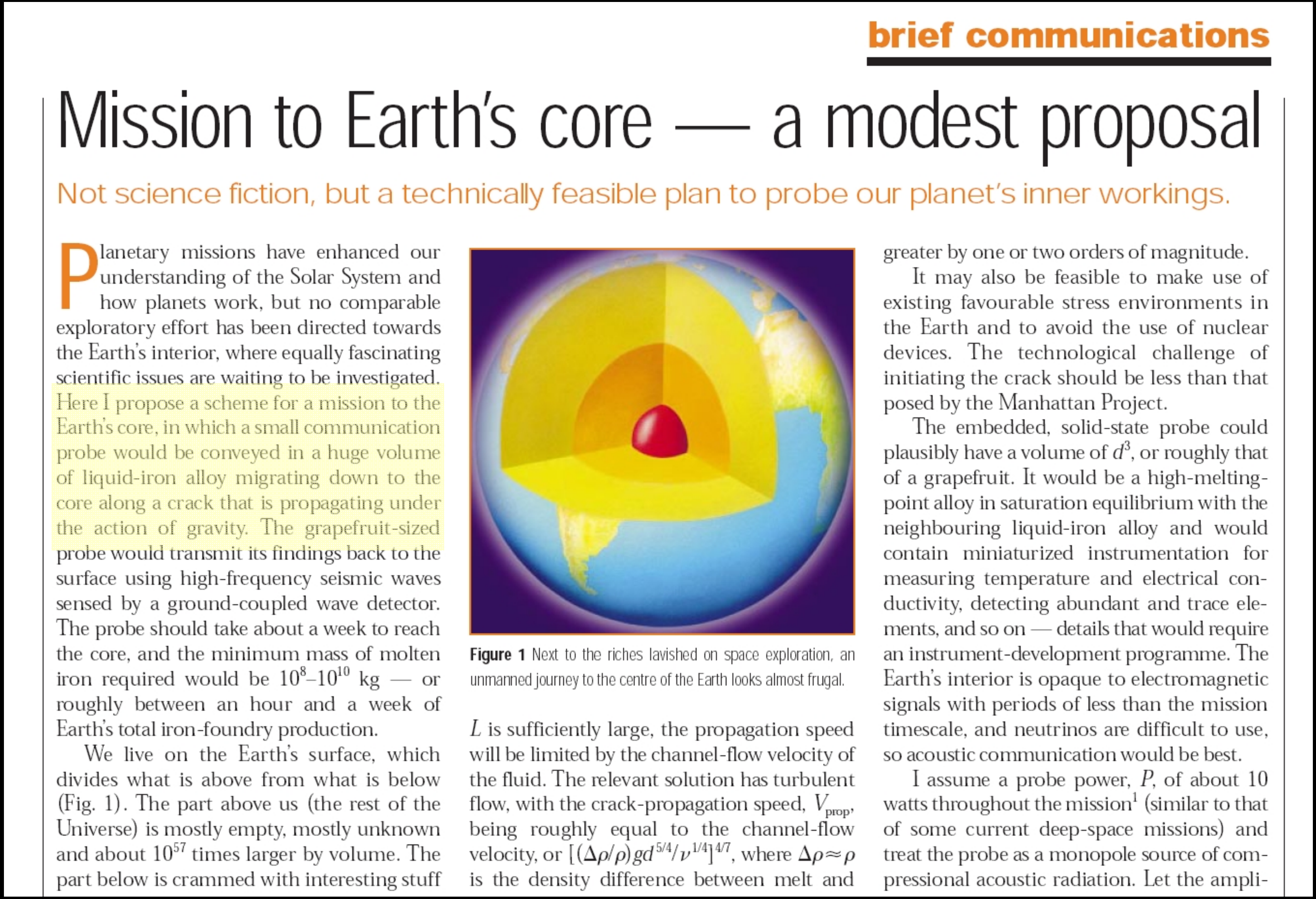
How hot is the Earth’s core?






A. Laio et al, Science 287, 1027 (2000)


THE CORE
THE ONLY WAY OUT IS IN
MARCH 28



brief communications

Mission to Earth's core — a modest proposal

Not science fiction, but a technically feasible plan to probe our planet's inner workings.

Planetary missions have enhanced our understanding of the Solar System and how planets work, but no comparable exploratory effort has been directed towards the Earth's interior, where equally fascinating scientific issues are waiting to be investigated. Here I propose a scheme for a mission to the Earth's core, in which a small communication probe would be conveyed in a huge volume of liquid-iron alloy migrating down to the core along a crack that is propagating under the action of gravity. The grapefruit-sized probe would transmit its findings back to the surface using high-frequency seismic waves sensed by a ground-coupled wave detector. The probe should take about a week to reach the core, and the minimum mass of molten iron required would be 10^8–10^{10} kg — or roughly between an hour and a week of Earth's total iron-foundry production.

We live on the Earth's surface, which divides what is above from what is below (Fig. 1). The part above us (the rest of the Universe) is mostly empty, mostly unknown and about 10^{57} times larger by volume. The part below is crammed with interesting stuff

Figure 1 Next to the riches lavished on space exploration, an unmanned journey to the centre of the Earth looks almost frugal.

L is sufficiently large, the propagation speed will be limited by the channel-flow velocity of the fluid. The relevant solution has turbulent flow, with the crack-propagation speed, V_{prop}, being roughly equal to the channel-flow velocity, or $[(\Delta\rho/\rho)gd^{5/4}/\nu^{1/4}]^{4/7}$, where $\Delta\rho\approx\rho$ is the density difference between melt and

greater by one or two orders of magnitude.

It may also be feasible to make use of existing favourable stress environments in the Earth and to avoid the use of nuclear devices. The technological challenge of initiating the crack should be less than that posed by the Manhattan Project.

The embedded, solid-state probe could plausibly have a volume of d^3, or roughly that of a grapefruit. It would be a high-melting-point alloy in saturation equilibrium with the neighbouring liquid-iron alloy and would contain miniaturized instrumentation for measuring temperature and electrical conductivity, detecting abundant and trace elements, and so on — details that would require an instrument-development programme. The Earth's interior is opaque to electromagnetic signals with periods of less than the mission timescale, and neutrinos are difficult to use, so acoustic communication would be best.

I assume a probe power, P, of about 10 watts throughout the mission[1] (similar to that of some current deep-space missions) and treat the probe as a monopole source of compressional acoustic radiation. Let the ampli-

D. Stevenson, Nature 423, 239 (2003)

Thanks to:

M.-S. Lee
M. Fontana
L. Giacomazzi
J. Christie
Y. Liang **ICTP**
A. Young
A. Hernandez Nieves
J. Montoya
R. Rousseau
C. Miranda
P. Tangney

A. Laio
S. Serra
E. Tosatti **SISSA**
F. Tassone

G. Profeta **L’Aquila**

R. Car
X. Wang **Princeton**

...and a countless number of experimentalists...