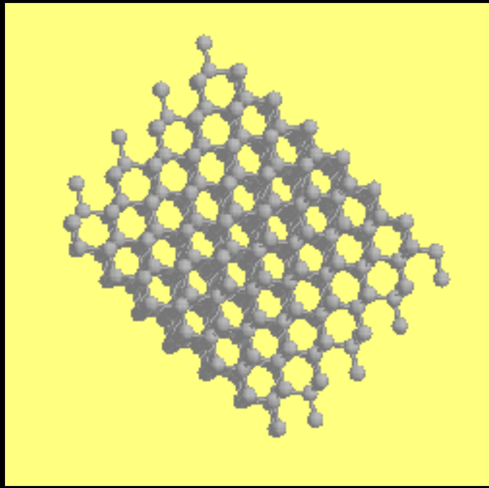
A solid-state physicist's journey to the centers of planets

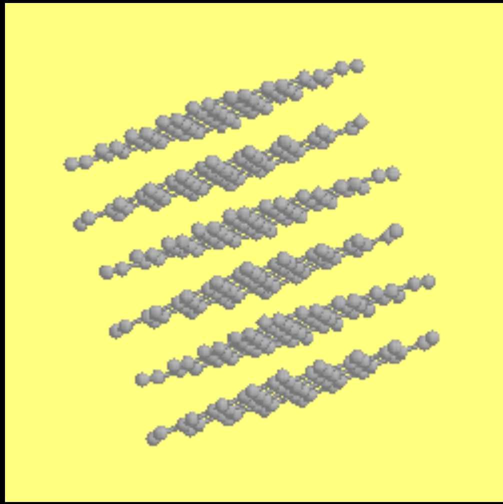
Sandro Scandolo
(ICTP, Trieste, Italy)

Physics Colloquium @ Univ. Pavia, April 2020

Diamond

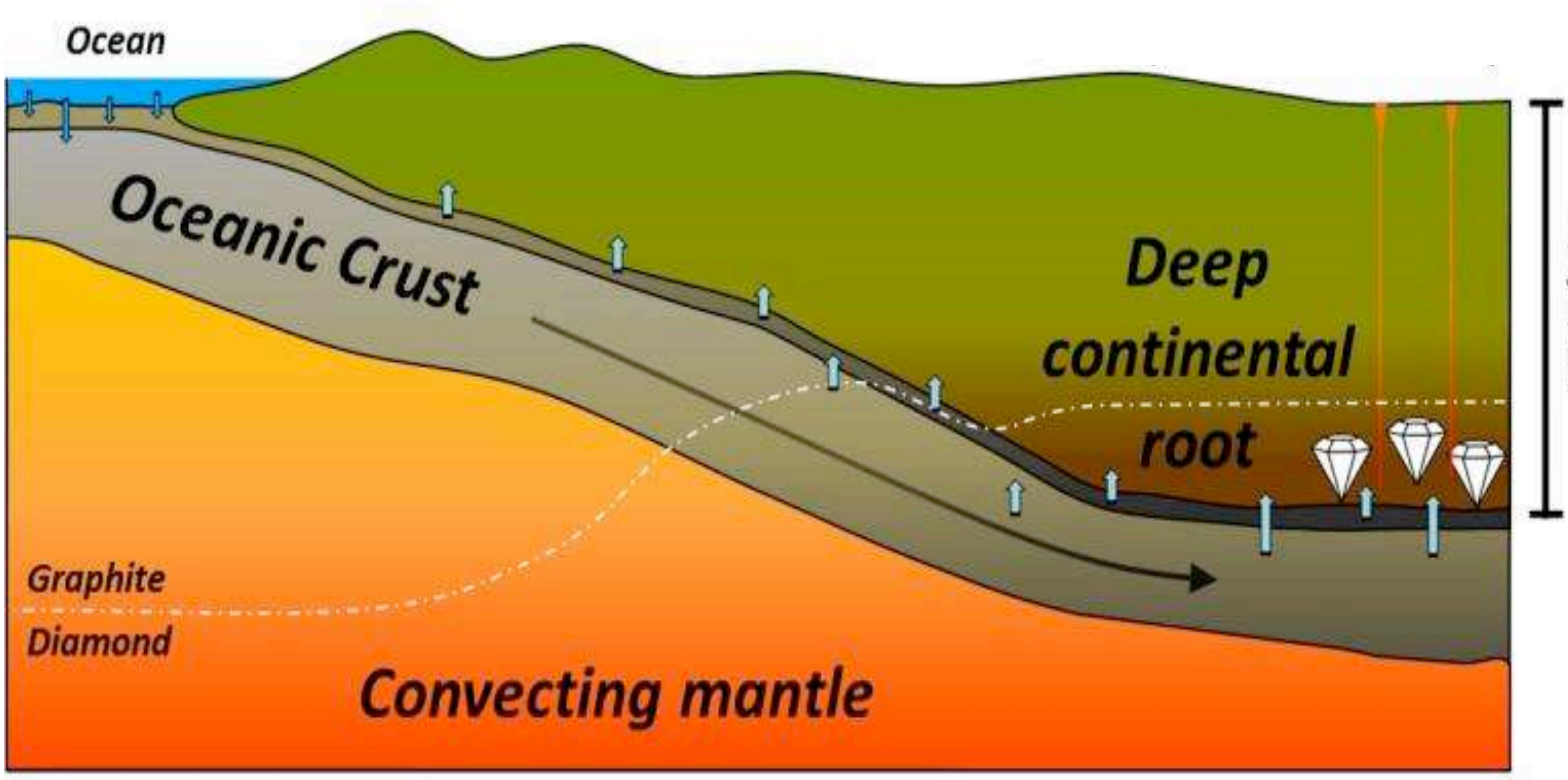


Graphite

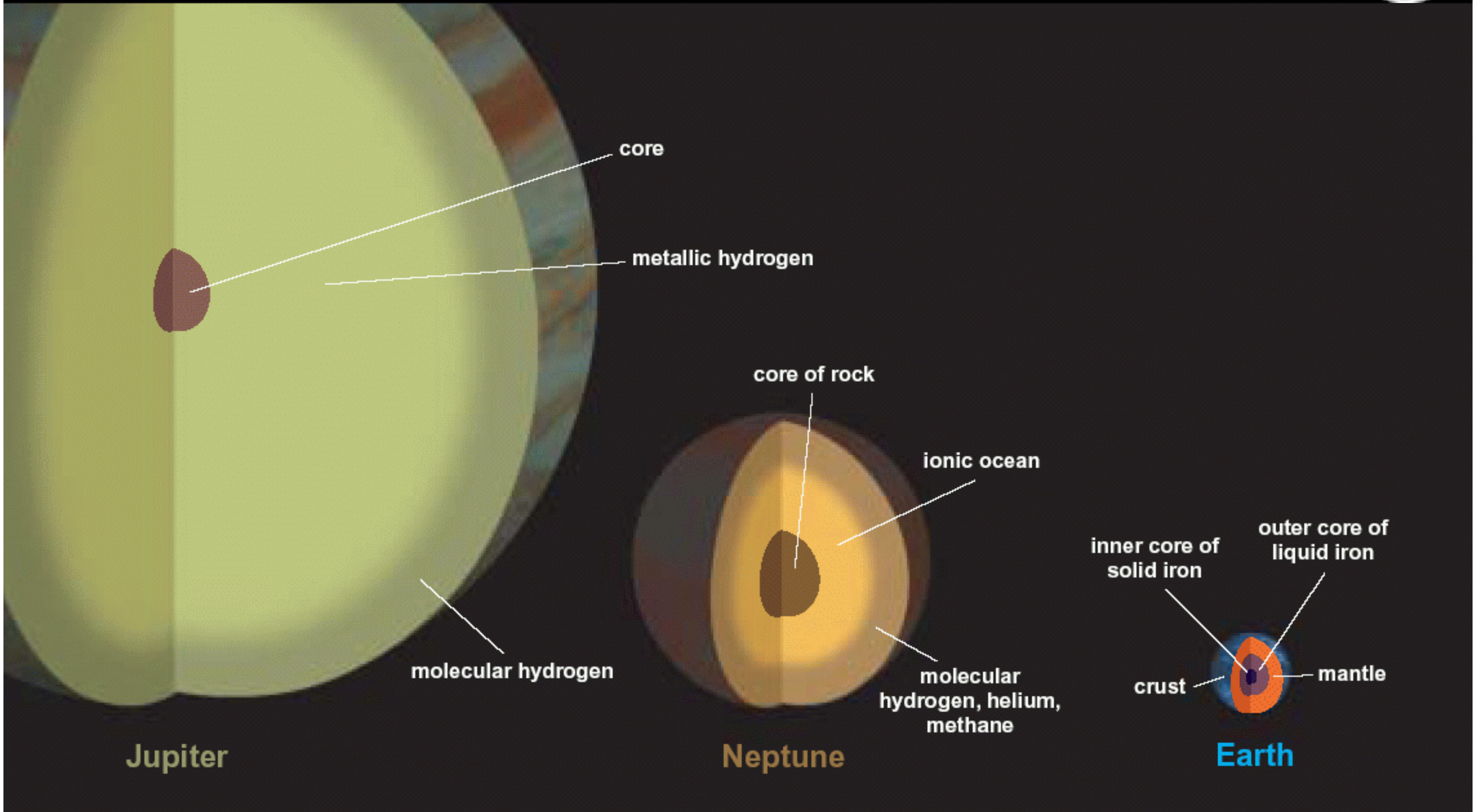


P ~ 14 GPa (room T)
P ~ 6 GPa (2000 K)

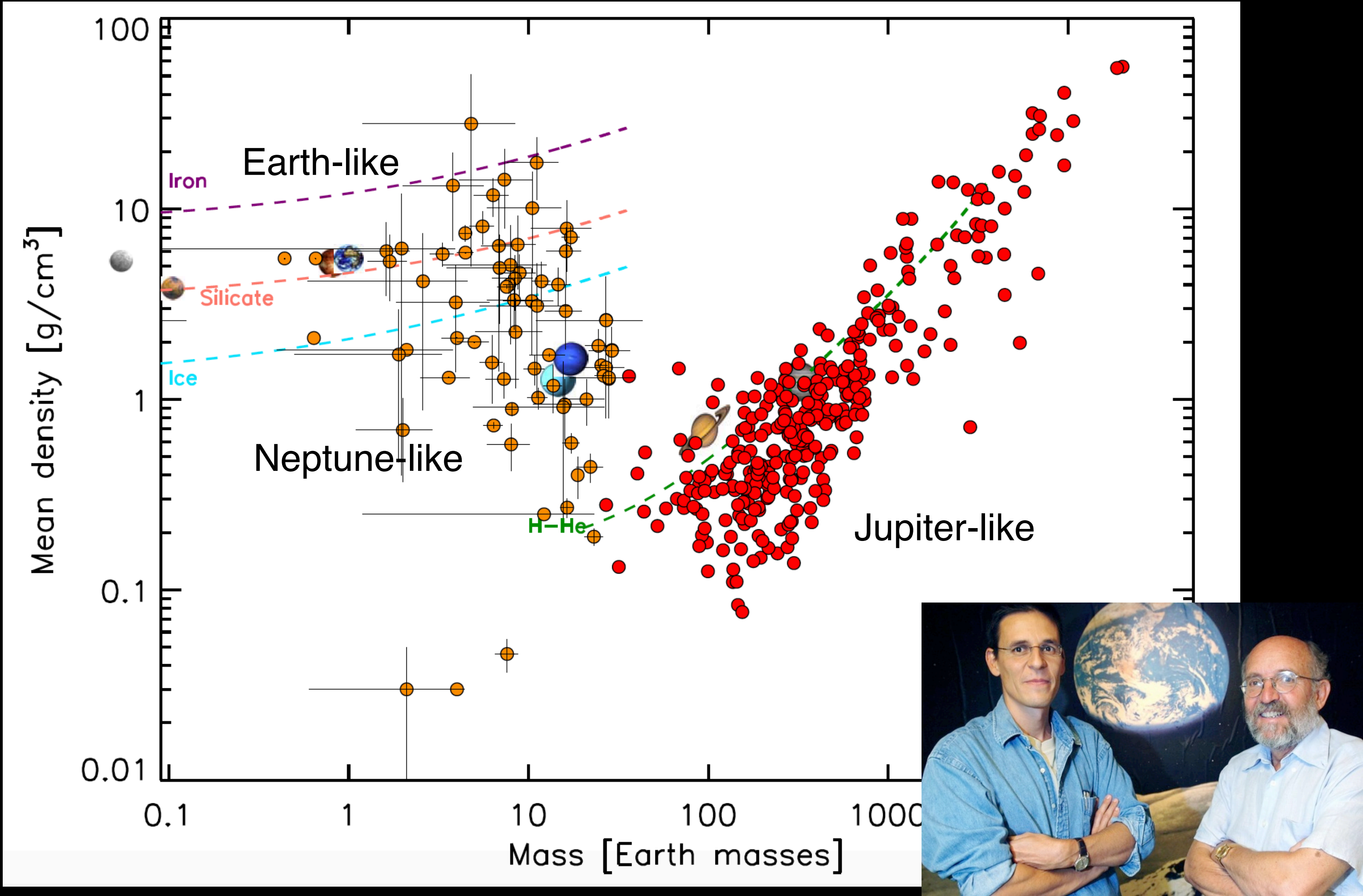
How do diamonds form?



Scandolo & Jeanloz, American Scientist (2003)



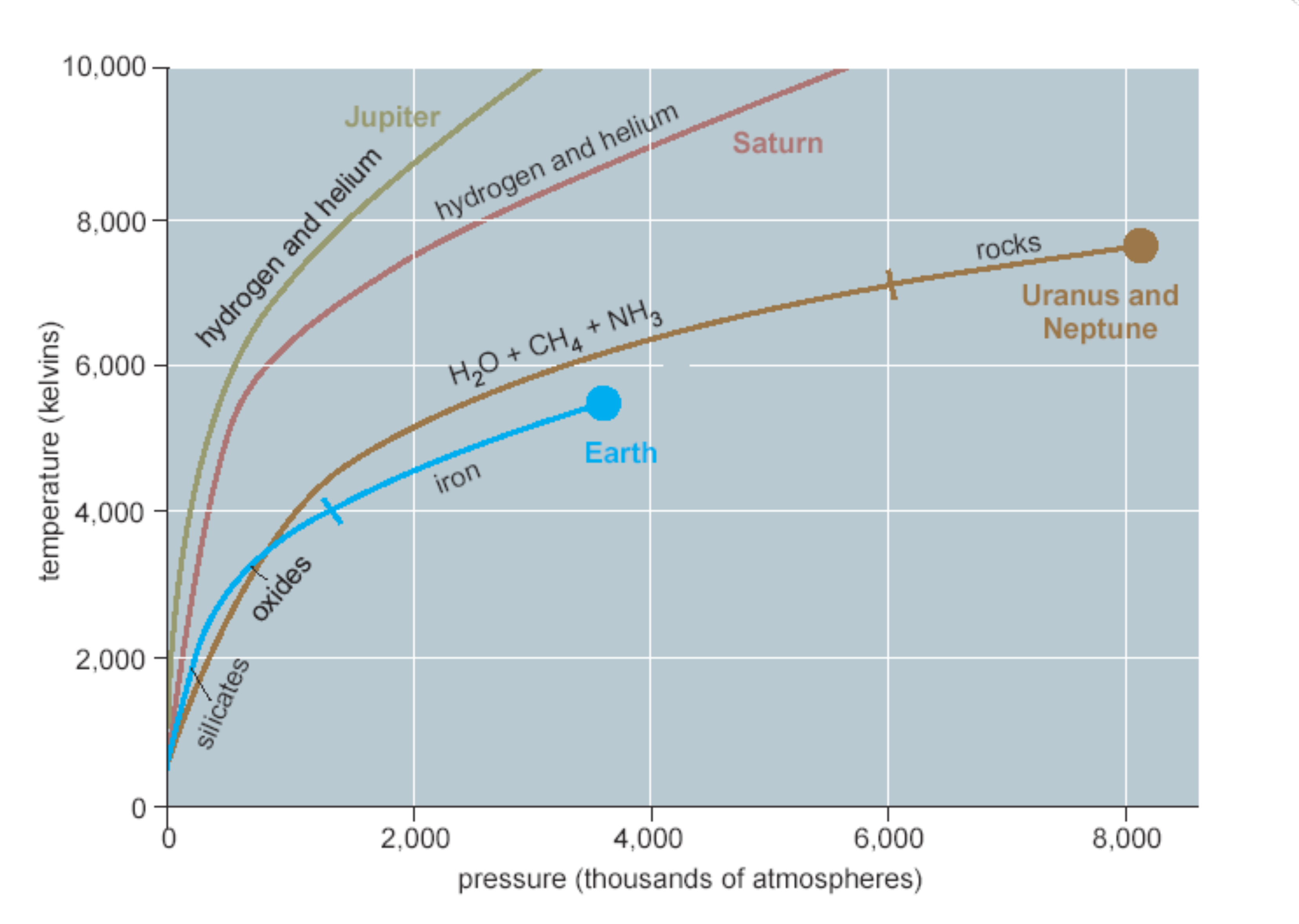
Exoplanets



H. Rauer (TU Berlin)

Queloz & Mayor, Nobel Physics 2019

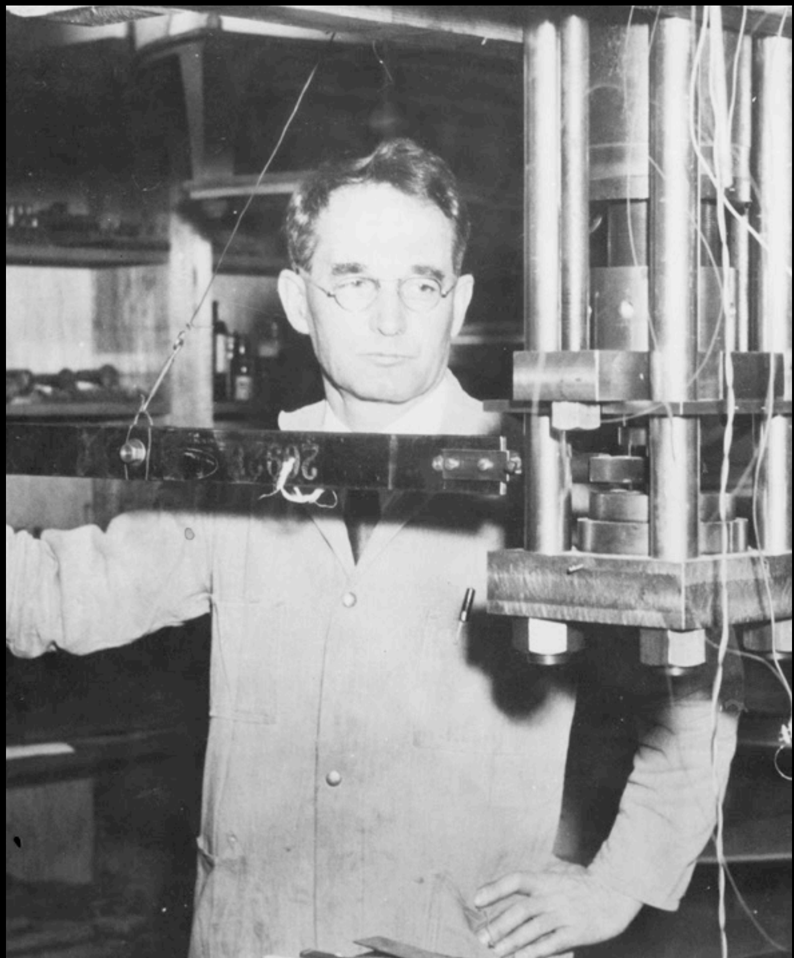
Scandolo & Jeanloz, American Scientist (2003)



High pressure: the early days

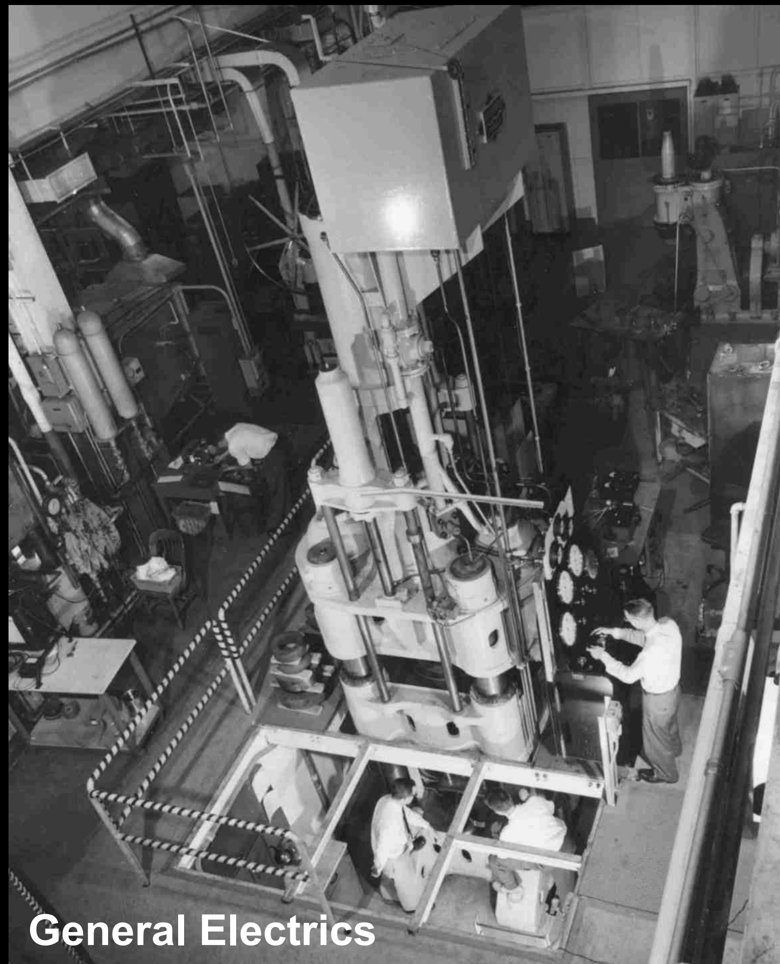
1946:

Nobel to Percy Bridgman

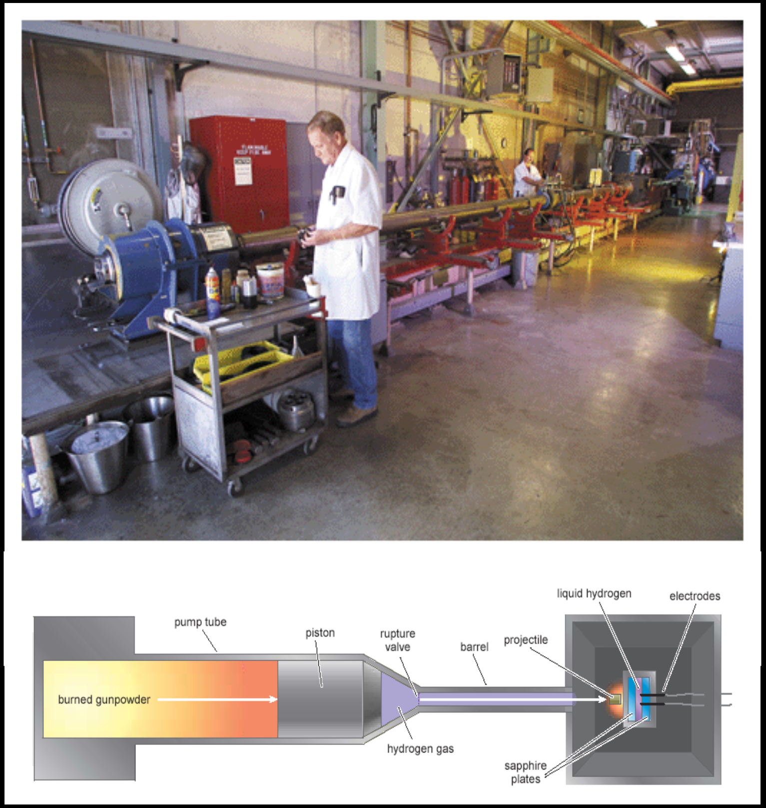


1955:

The first man-made diamonds

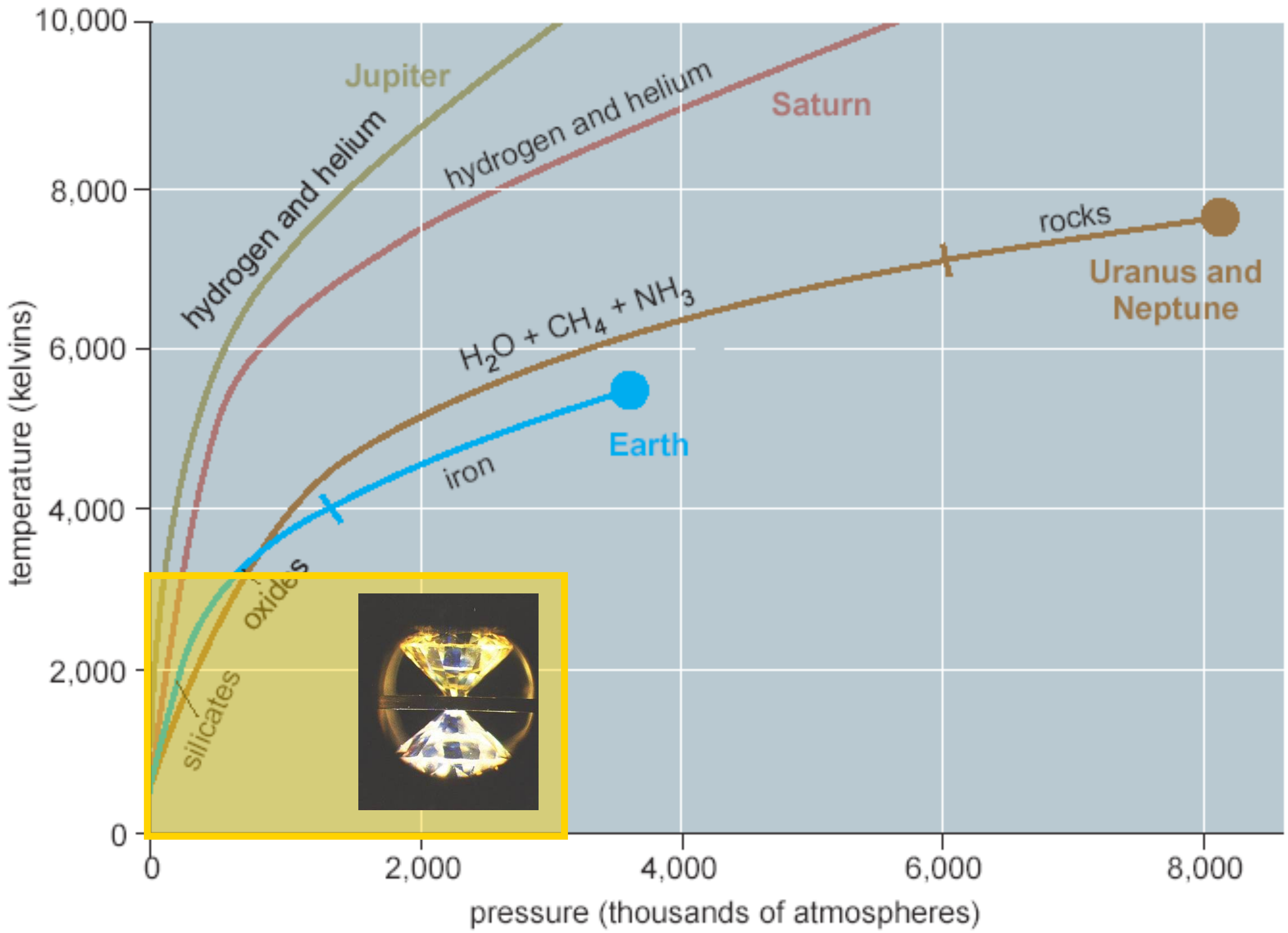

General Electrics

High pressure: today



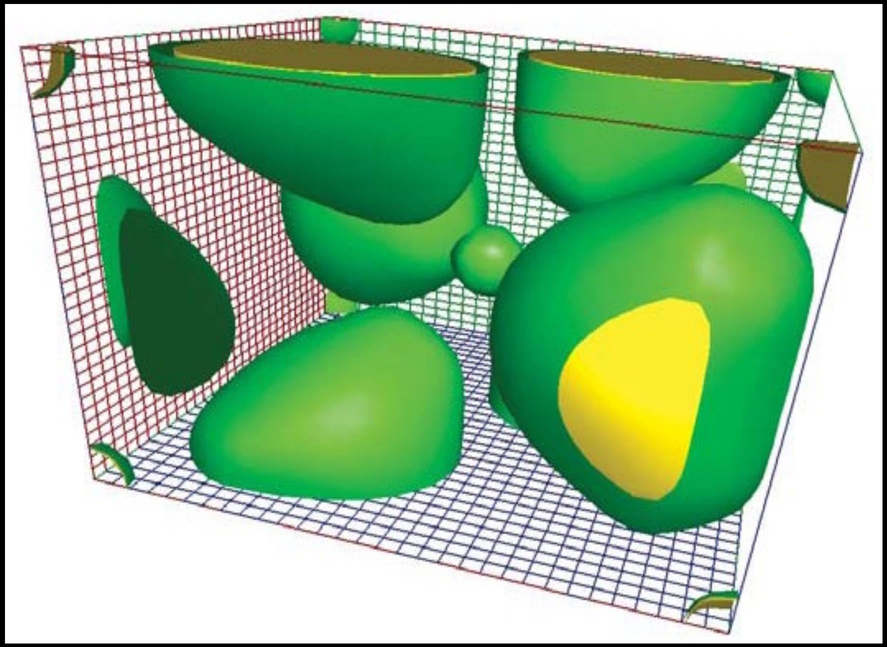
Shock waves

Diamond anvil cell



10,000
8,000
6,000
4,000
2,000
0
temperature (kelvins)
Jupiter
hydrogen and helium
hydrogen and helium
Saturn
rocks
Uranus and
Neptune
H2O + CH4 + NH3
Earth
iron
oxides
silicates
0
2,000
4,000
6,000
8,000
pressure (thousands of atmospheres)

Quantum simulations: The "standard model"



Electron charge density in SiO_2 stishovite

"Molecular dynamics" for atoms

$$Ma = F = -dE/dR$$

Schroedinger equation for electrons

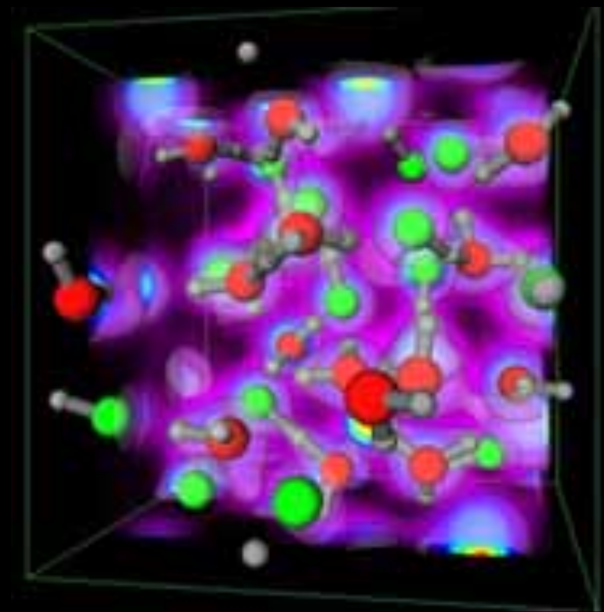
$$H\psi = E\psi$$

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

Walter Kohn (1923-2016)

Nobel prize in Chemistry 1998
(for work done in the 60's)

Density-functional theory



The energy $E[\rho(x)]$ of a collection of electrons is a unique functional of the electron density $\rho(x)$

Ab-initio molecular dynamics

http://www.quantum-espresso.org

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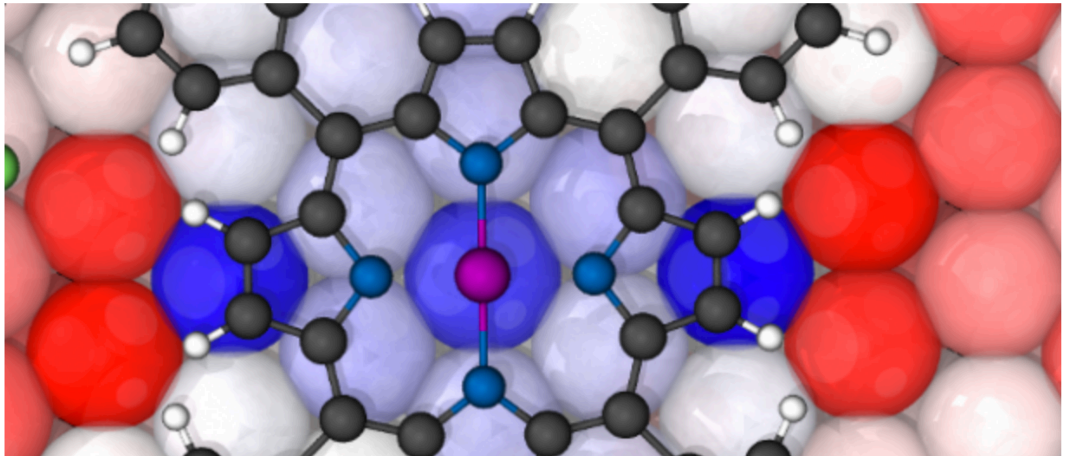
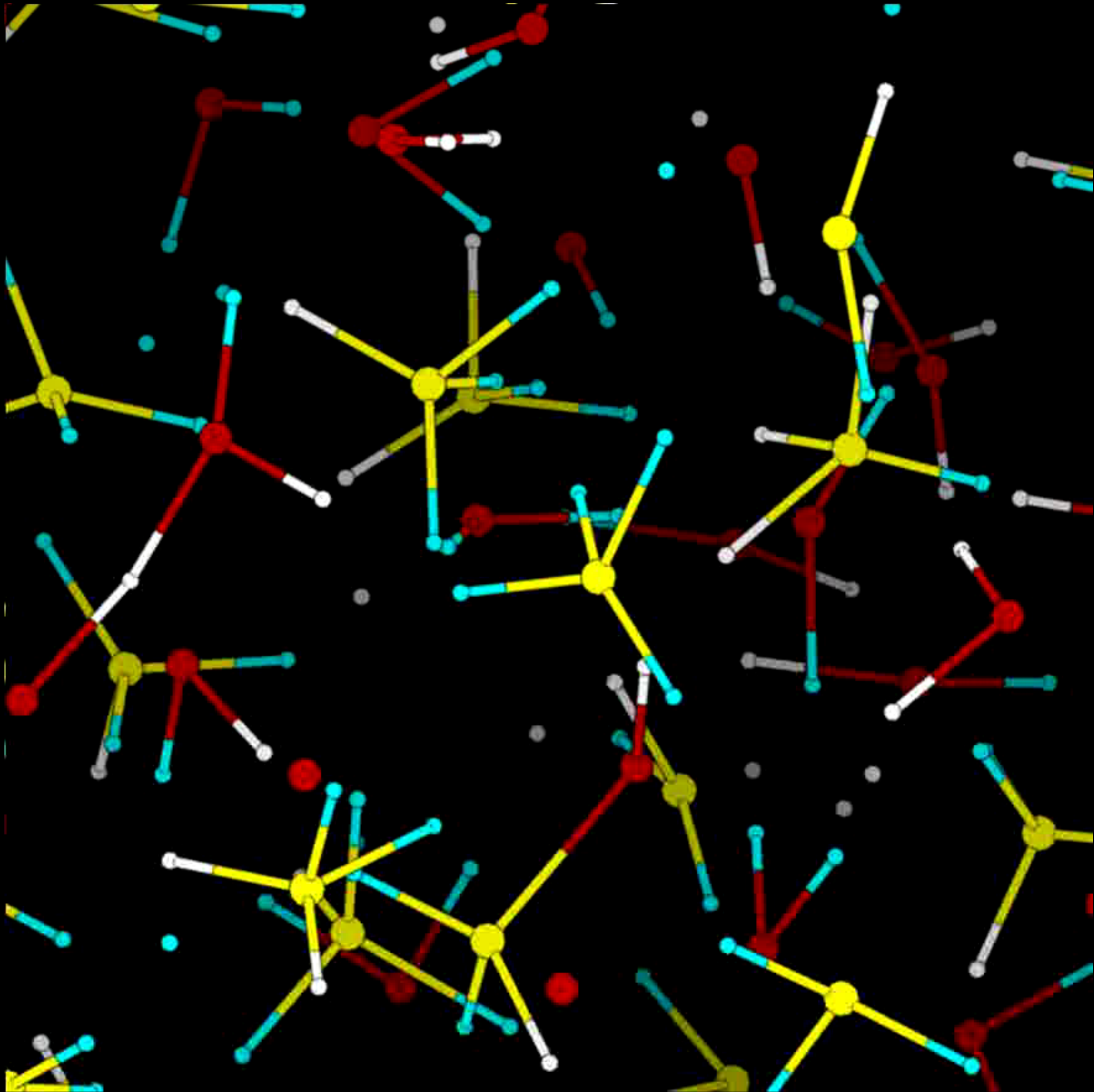
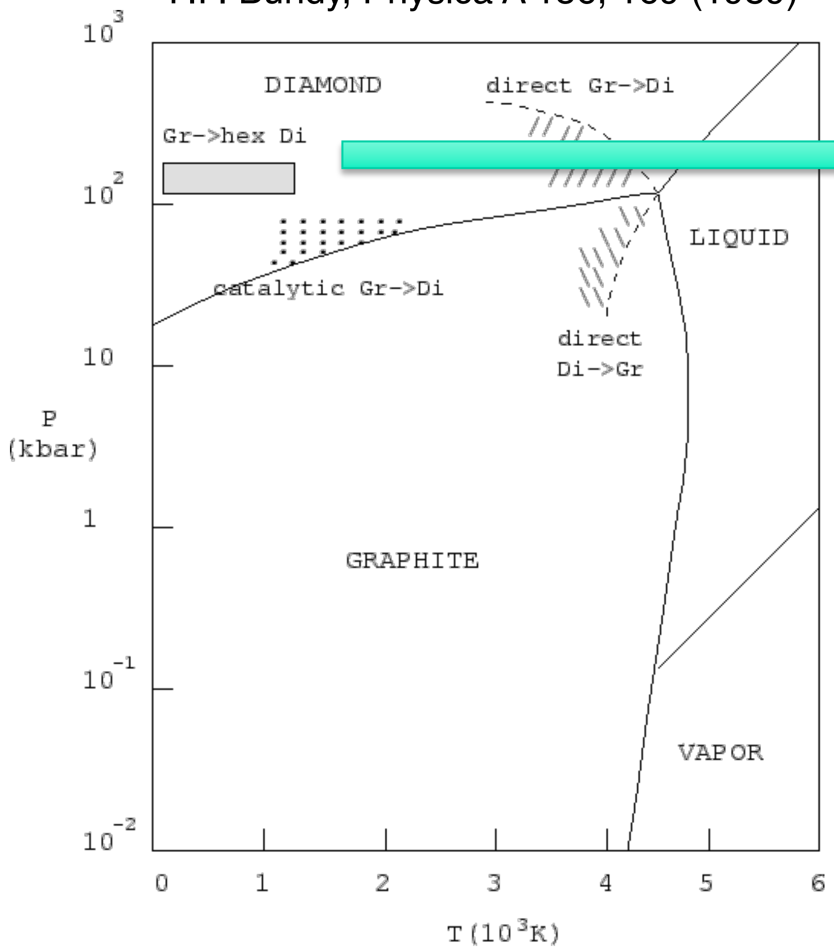


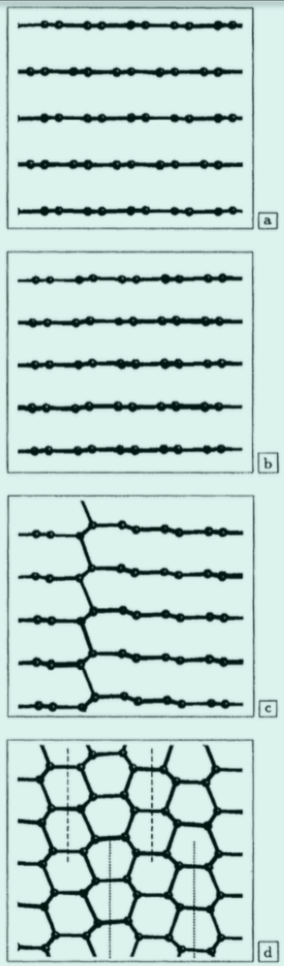
Spatially Extended Kondo State in Magnetic Molecules Induced by Interfacial Charge Transfer. Phys. Rev. Lett. 105 106601 (2010). Courtesy of H. Kulik.



Graphite-Diamond transition

F.P. Bundy, Physica A 156, 169 (1989)





Transformation path from graphite to hex diamond uncovered by ab-initio molecular dynamics

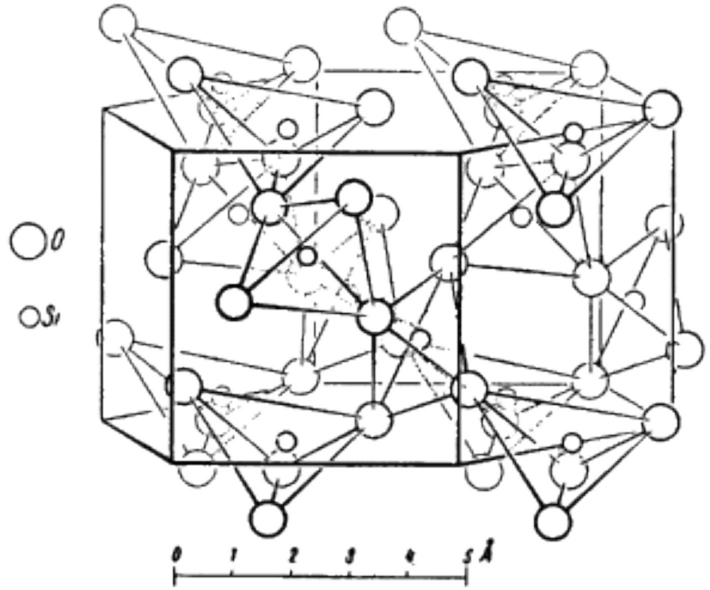
Scandolo et al,
Phys. Rev. Lett. 1995

ICTP
The Abdus Salam
International Centre
for Theoretical Physics
IAEA

Non-molecular CO_2

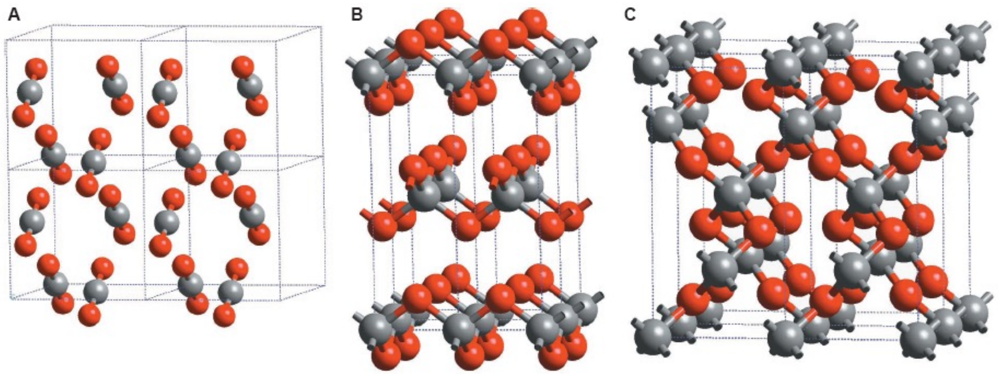
CO_2

SiO_2



Non-molecular CO_2

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

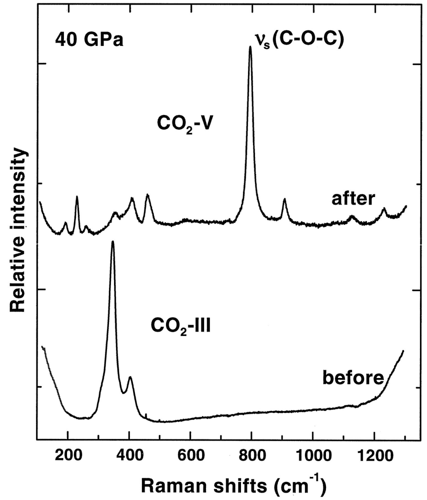


Molecular CO_2

Candidate theoretical structures for silica-like CO_2

Experimental confirmation of silica-like CO_2

Yoo et al, Science 283, 1510 (1999)



Disappearance of molecular peaks

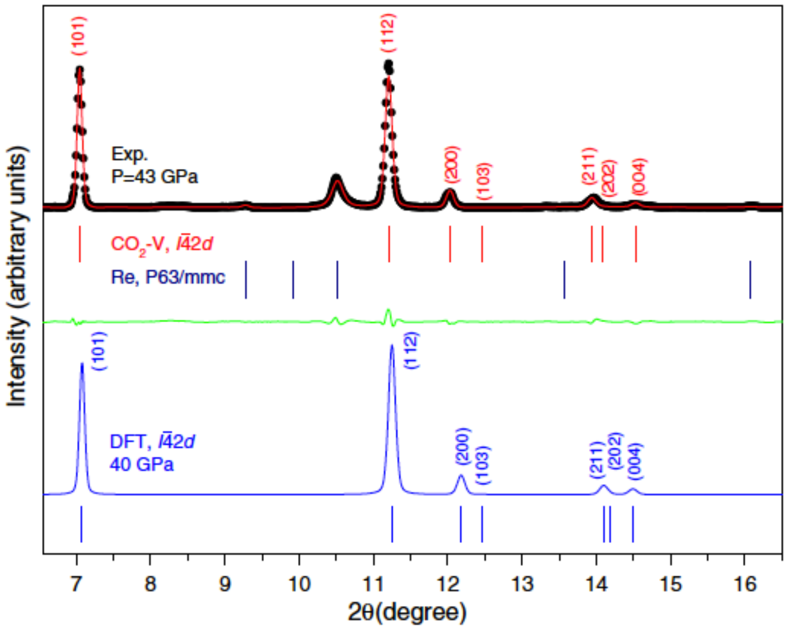
Formation of C-O-C bonds

+ Molecular CO_2 tranforms into a silica-like crystal at about 50 GPa

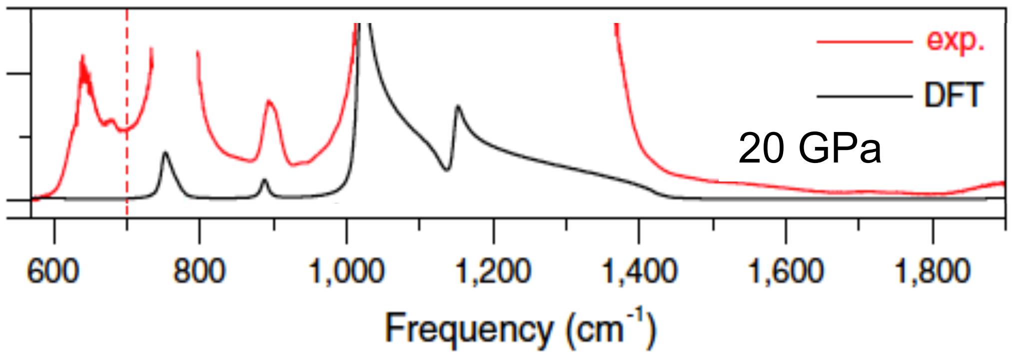
+ Silica-like phases of CO_2 predicted to be ultrahard

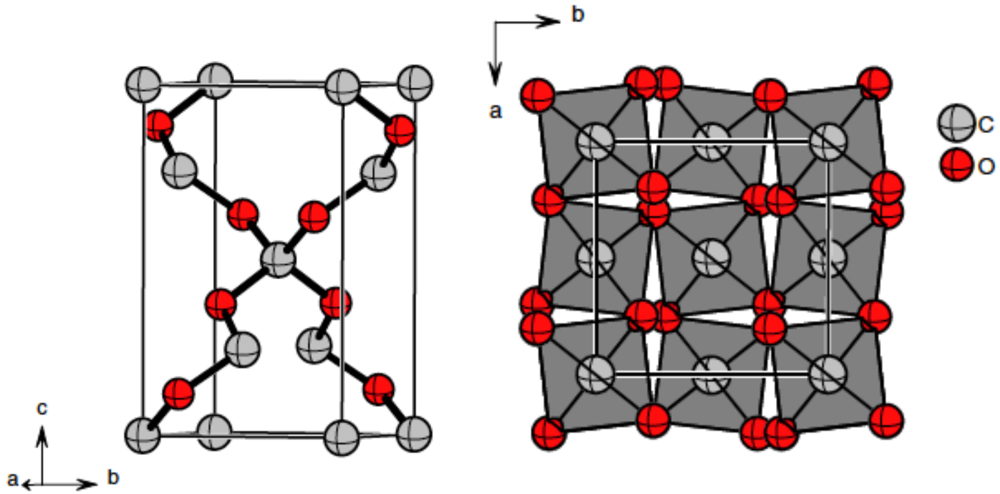
Non-molecular CO_2:
β-cristobalite confirmed

X-ray diffraction



IR spectroscopy

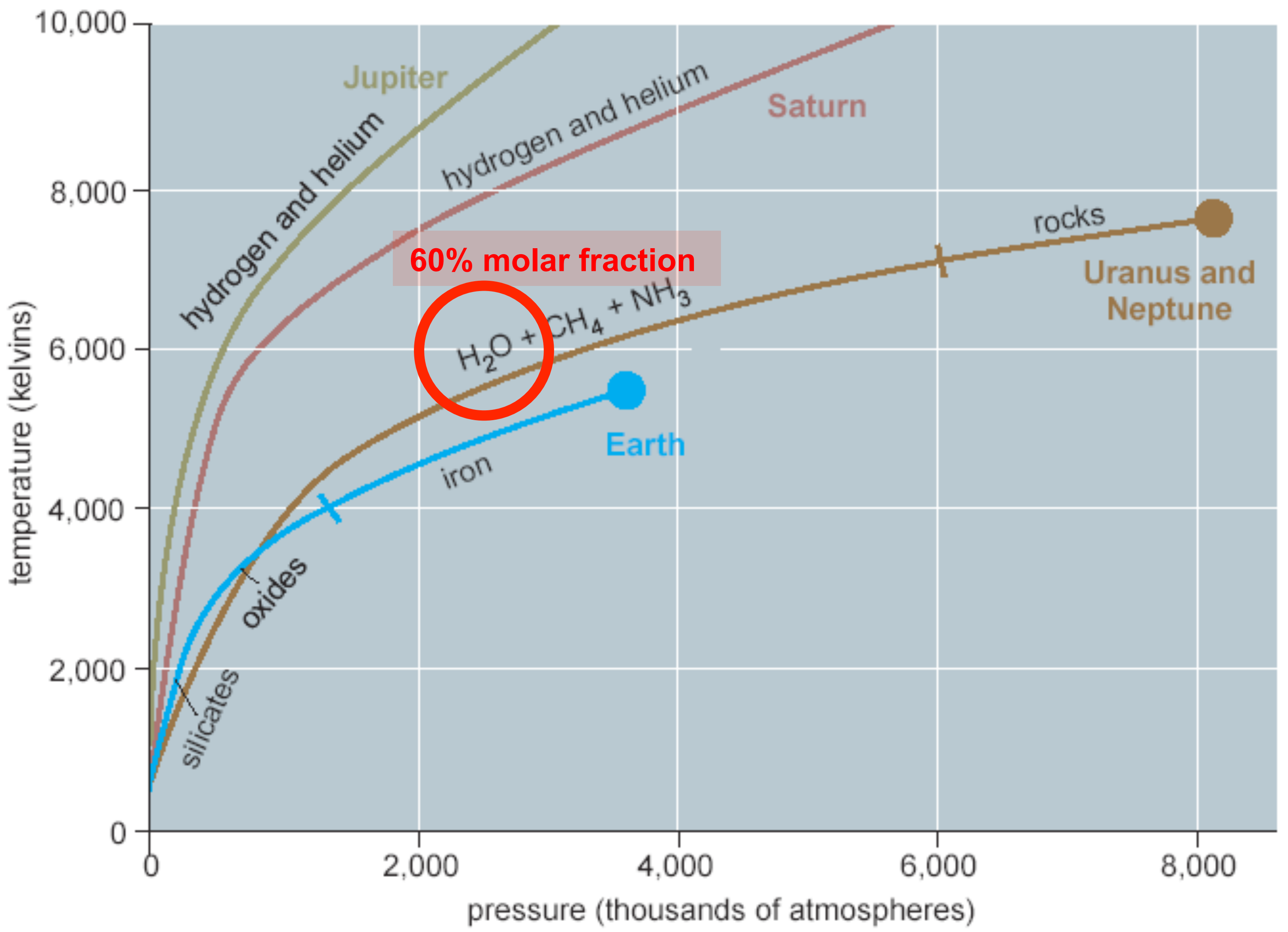




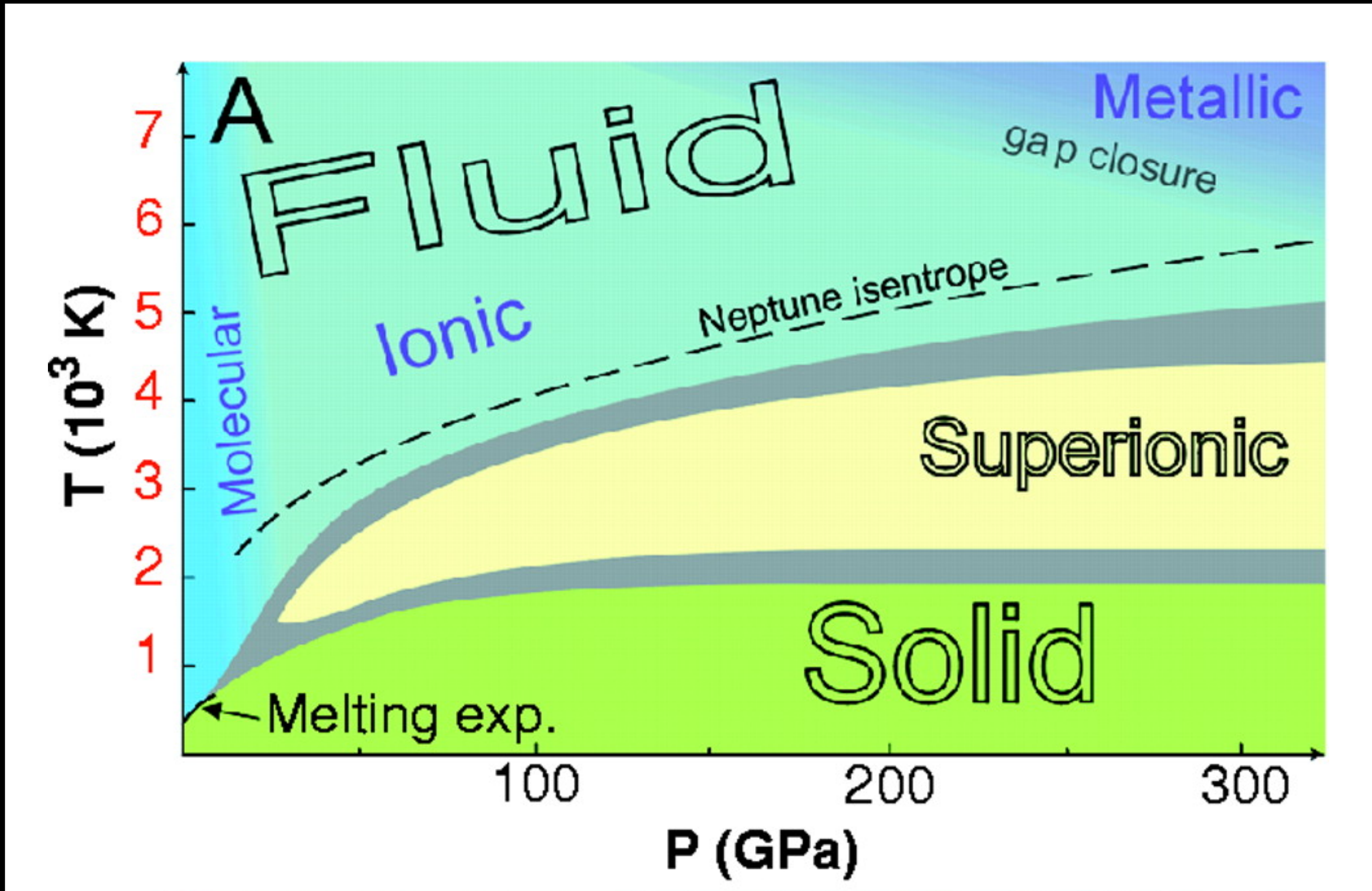
Sample laser-heated with CO_2 laser

Santoro, Gorelli, Bini, Haines, Cambon, Levelut, Montoya, Scandolo, PNAS 2012

Water and methane at planetary conditions


10,000
8,000
6,000
4,000
2,000
0
temperature (kelvins)
0
2,000
4,000
6,000
8,000
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

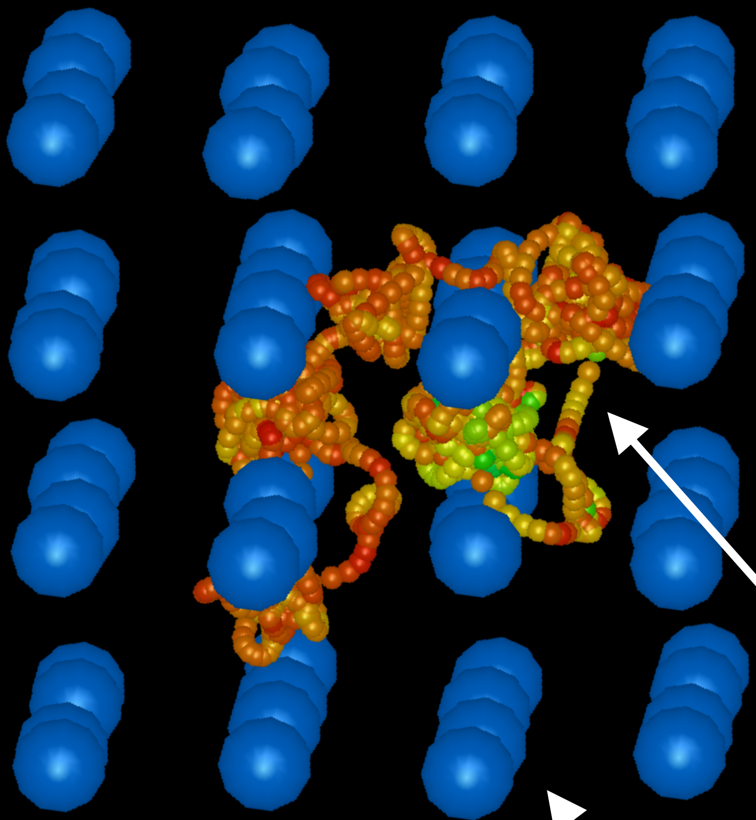
phase diagram of water from first principles



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)



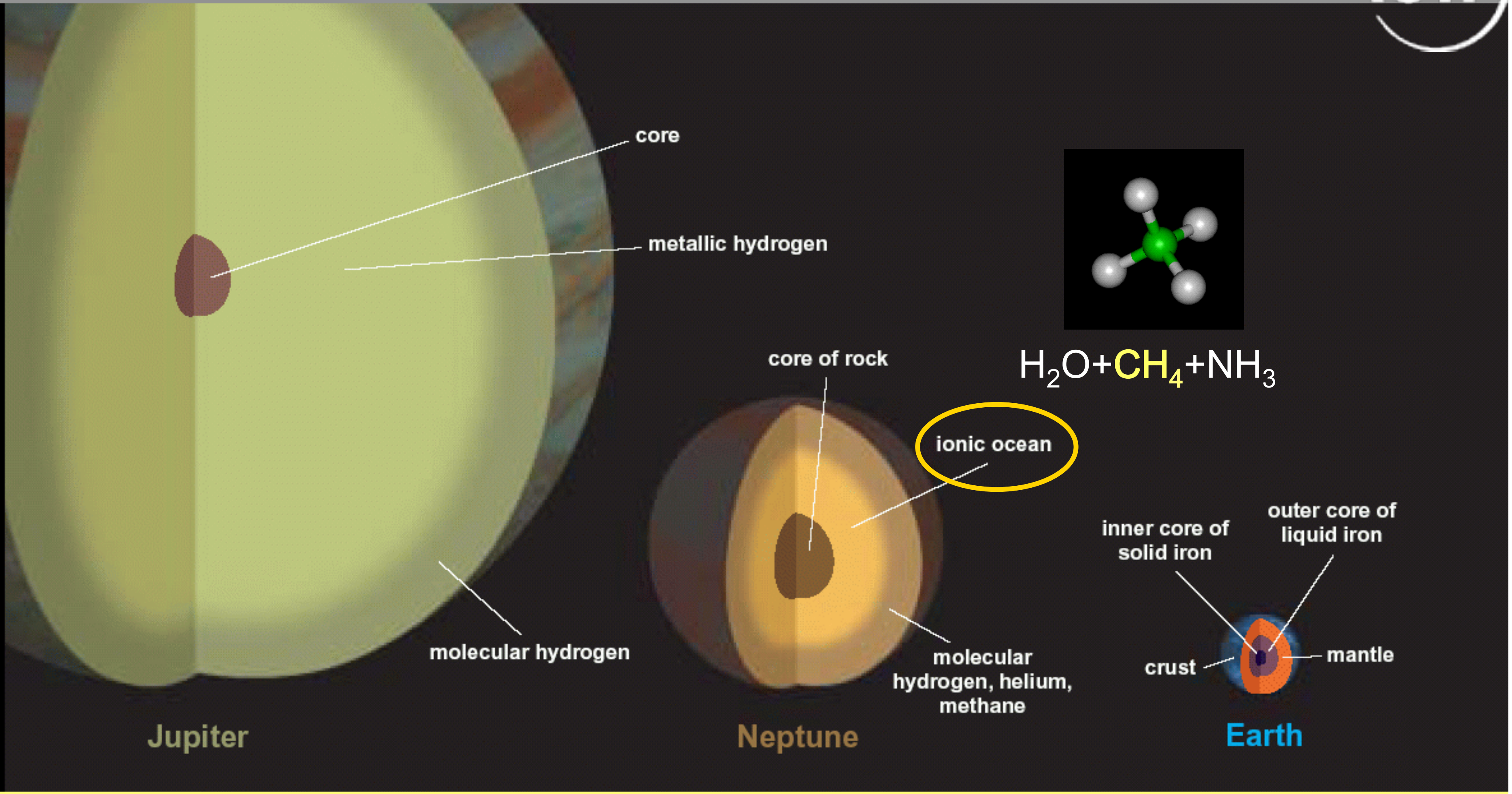
Superionic Water

P = 150 GPa
T = 2500 K

Proton diffusion by hopping

Oxygen sublattice remains crystalline

Scandolo & Jeanloz, American Scientist (2003)

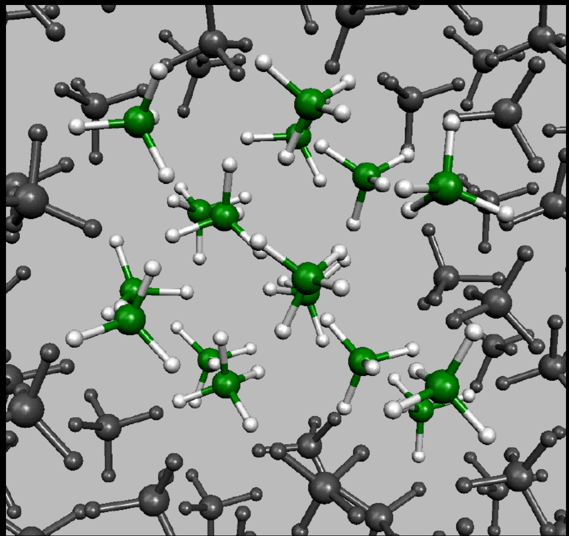


$H_2O+CH_4+NH_3$

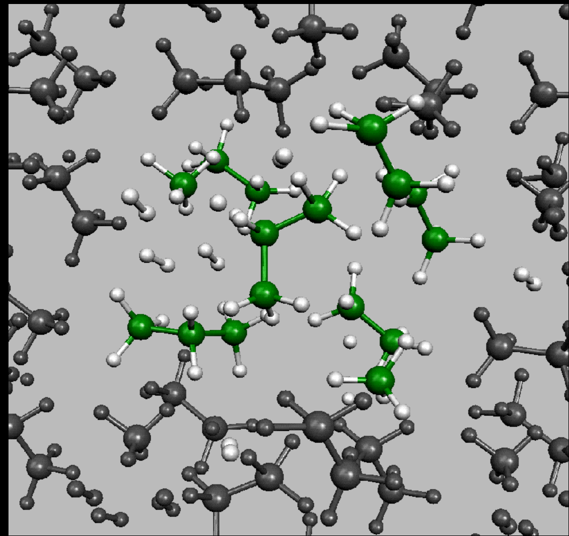
Marvin Ross, “Diamonds in the sky”
Nature (1981)

Methane was found to dissociate under a shock wave

Dissociation of methane at extreme (planetary) conditions

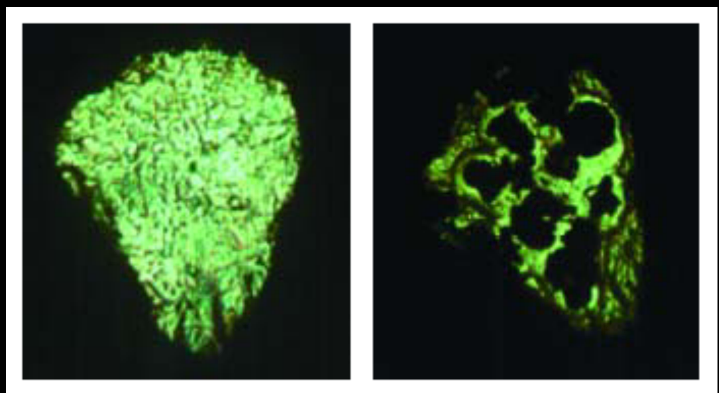


Compressed methane

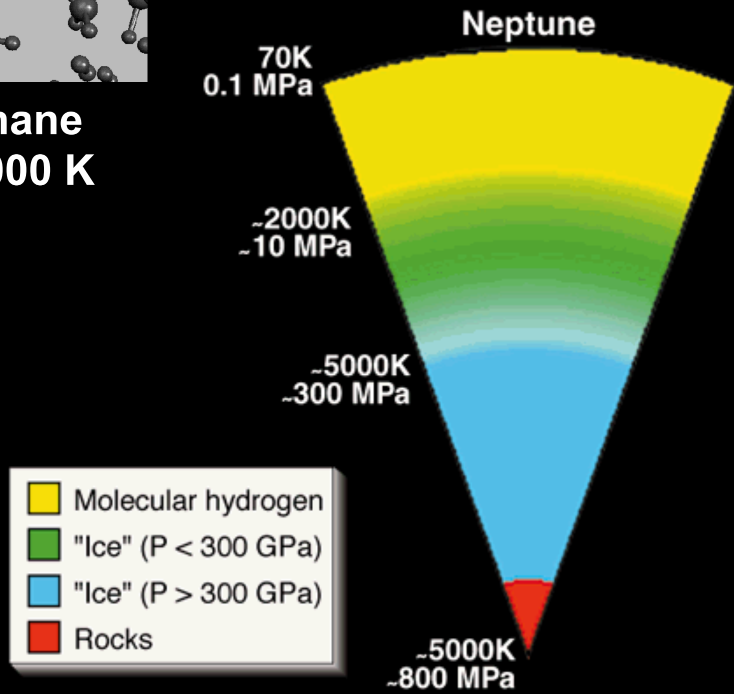


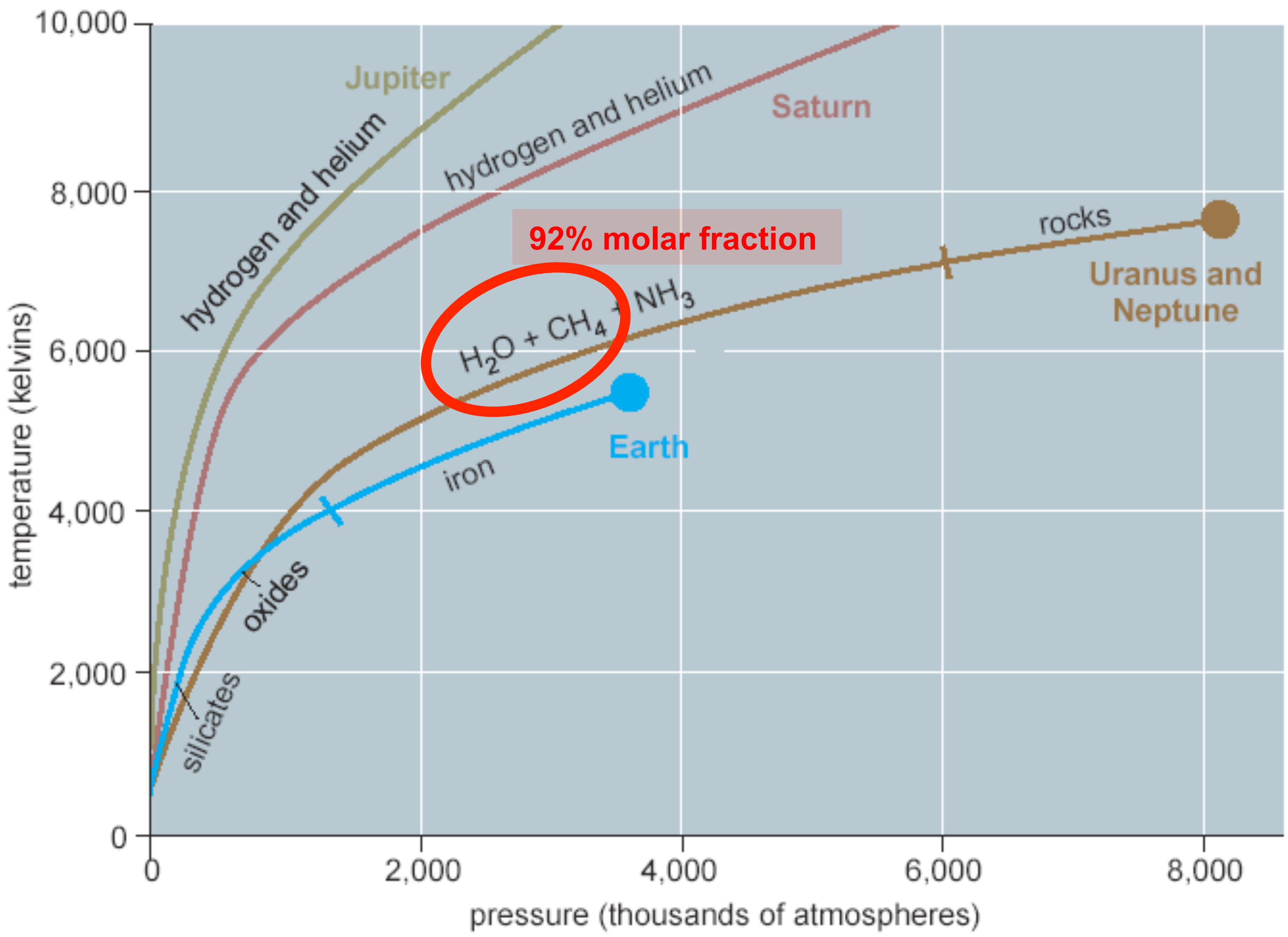
Compressed methane
after heating to 4000 K

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



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




92% molar fraction
Jupiter
hydrogen and helium
hydrogen and helium
Saturn
$H_2O + CH_4 + NH_3$
rocks
Uranus and
Neptune
Earth
iron
oxides
silicates
temperature (kelvins)
10,000
8,000
6,000
4,000
2,000
0
2,000
4,000
6,000
8,000
pressure (thousands of atmospheres)

CH_4 / H_2O mixtures at extreme conditions

92% of the Uranus and Neptune ice layer

Fluid inclusions, abiogenic formation of methane

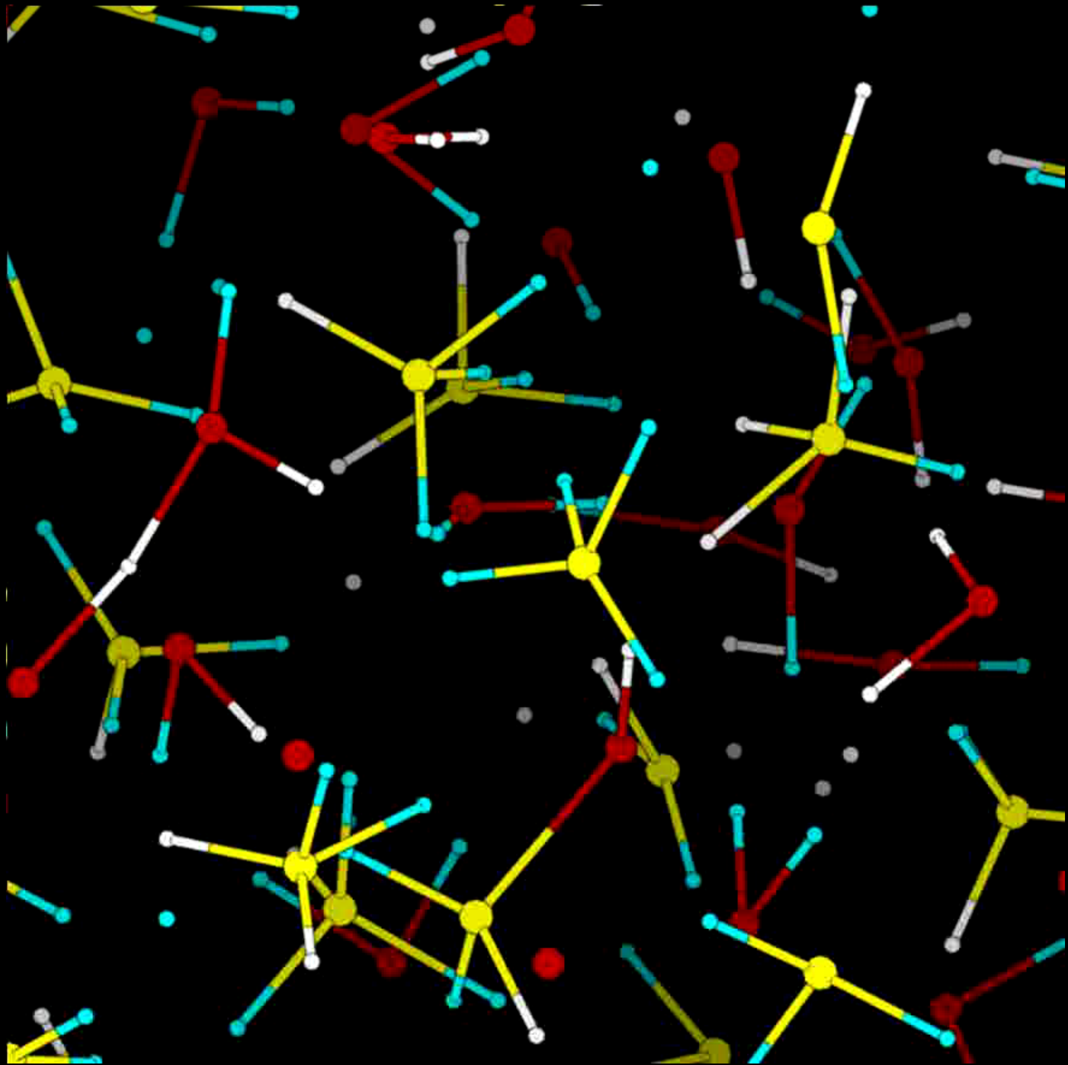
Prototype of hydrophobic interactions

How corrosive is ionized water?

Methane hydrate clathrates

SIMULATIONS: 26 CH_4 + 38 H_2O at 4 different P-T

Methane / water mixture at 50 GPa



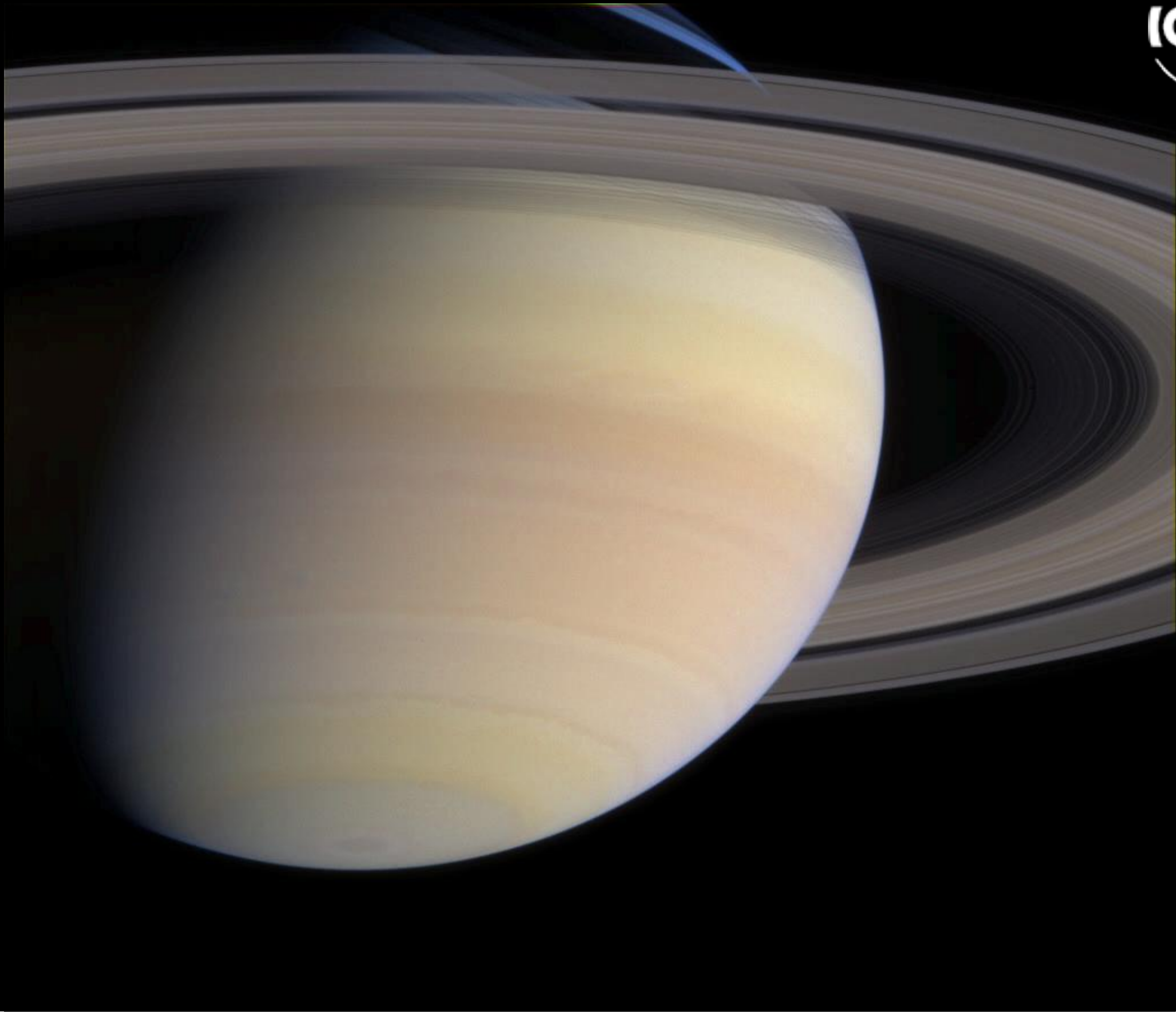
Fast proton diffusion by proton hopping between adjacent molecules

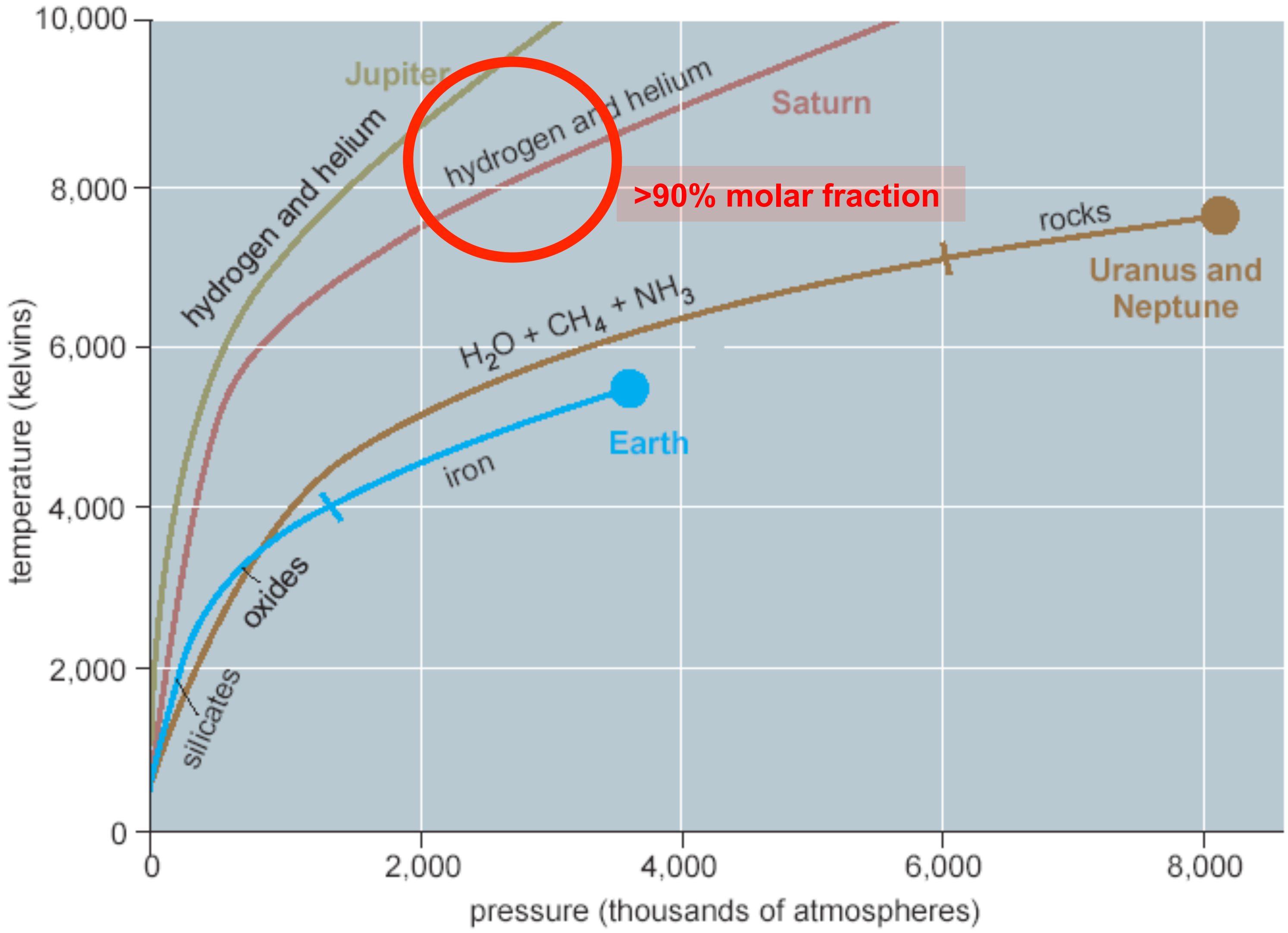
Methane "attacked" by ionized water

Occasional formation of C-O bonds

No formation of longer hydrocarbons (C-C bonds)

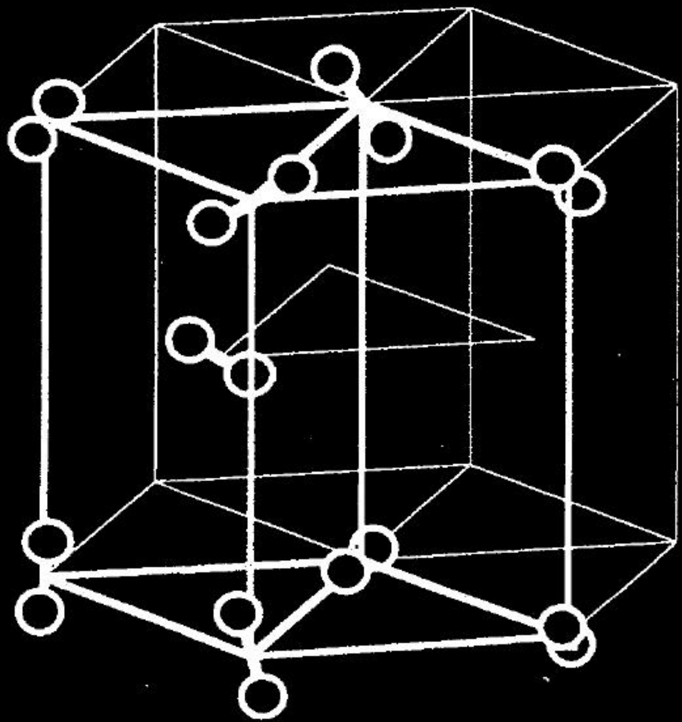
M.-S. Lee and S. Scandolo, Nature Comm. 2011



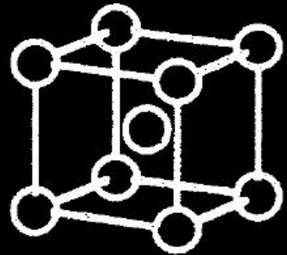


10,000
8,000
6,000
4,000
2,000
0
temperature (kelvins)
Jupiter
hydrogen and helium
hydrogen and helium
Saturn
>90% molar fraction
rocks
Uranus and
Neptune
H2O + CH4 + NH3
Earth
iron
oxides
silicates
0
2,000
4,000
6,000
8,000
pressure (thousands of atmospheres)

E. Wigner and H.B. Huntington
"On the possibility of a metallic modification of hydrogen"
J. Chem. Phys. 3, 764 (1935)

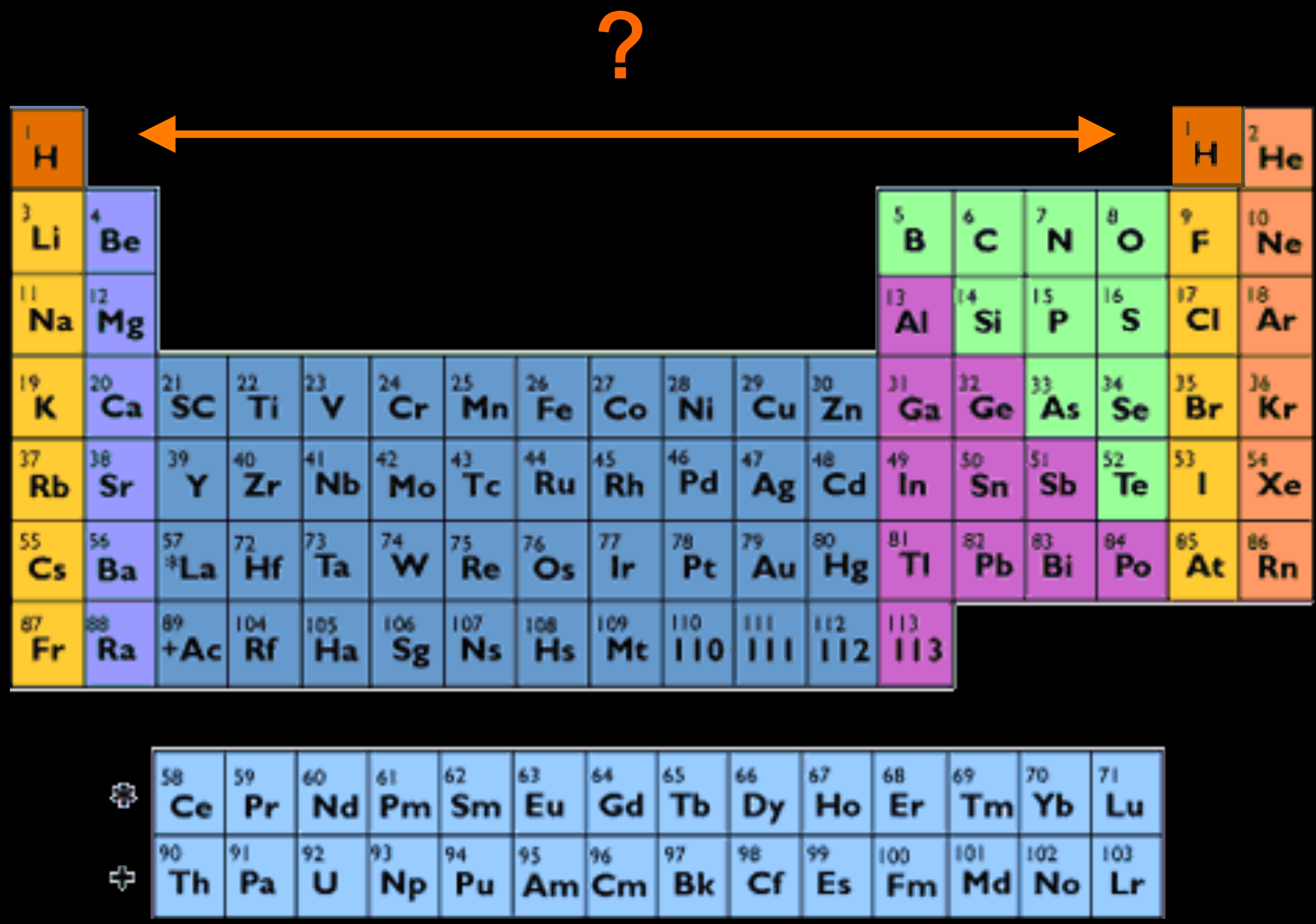


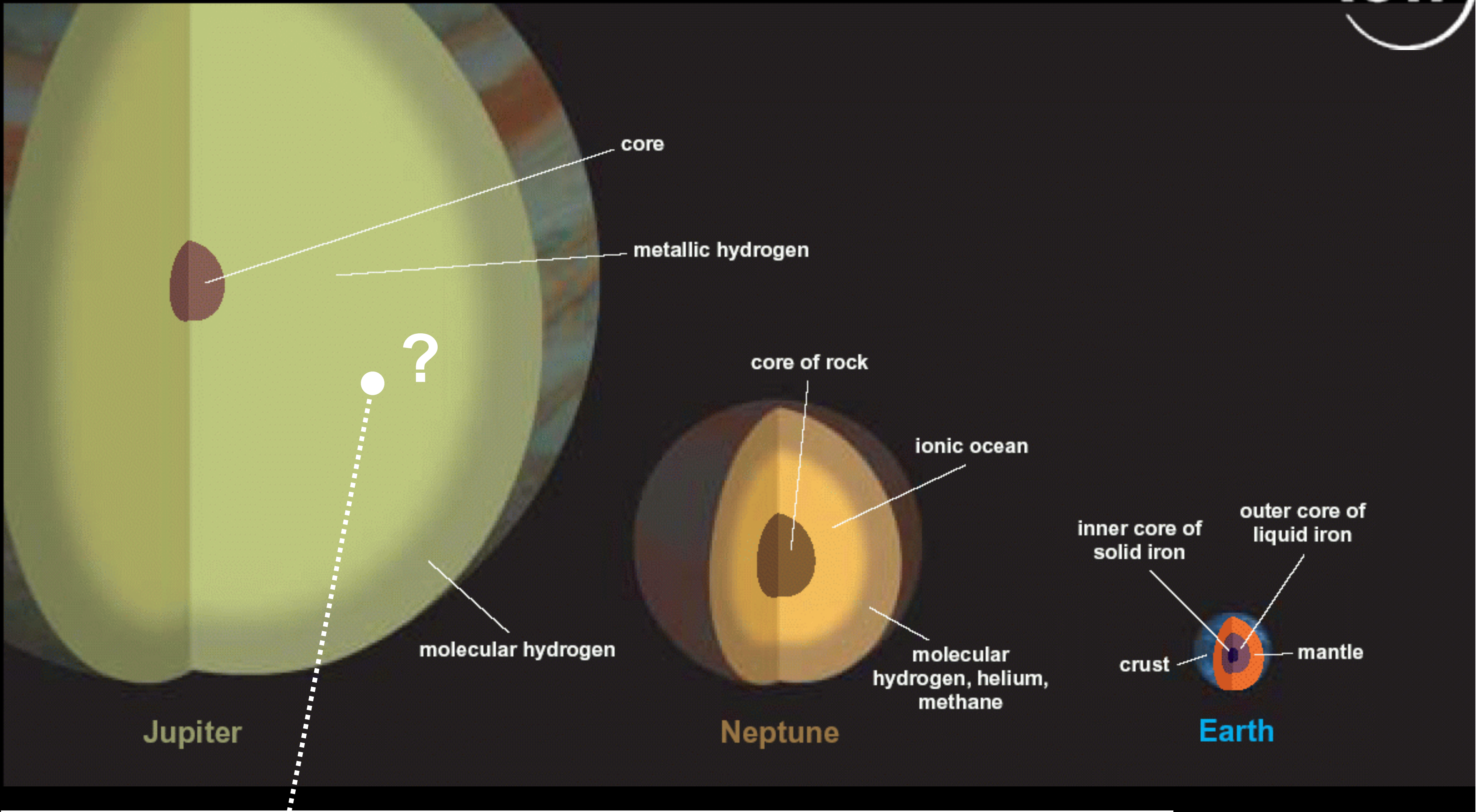
Molecular hydrogen



Monatomic hydrogen

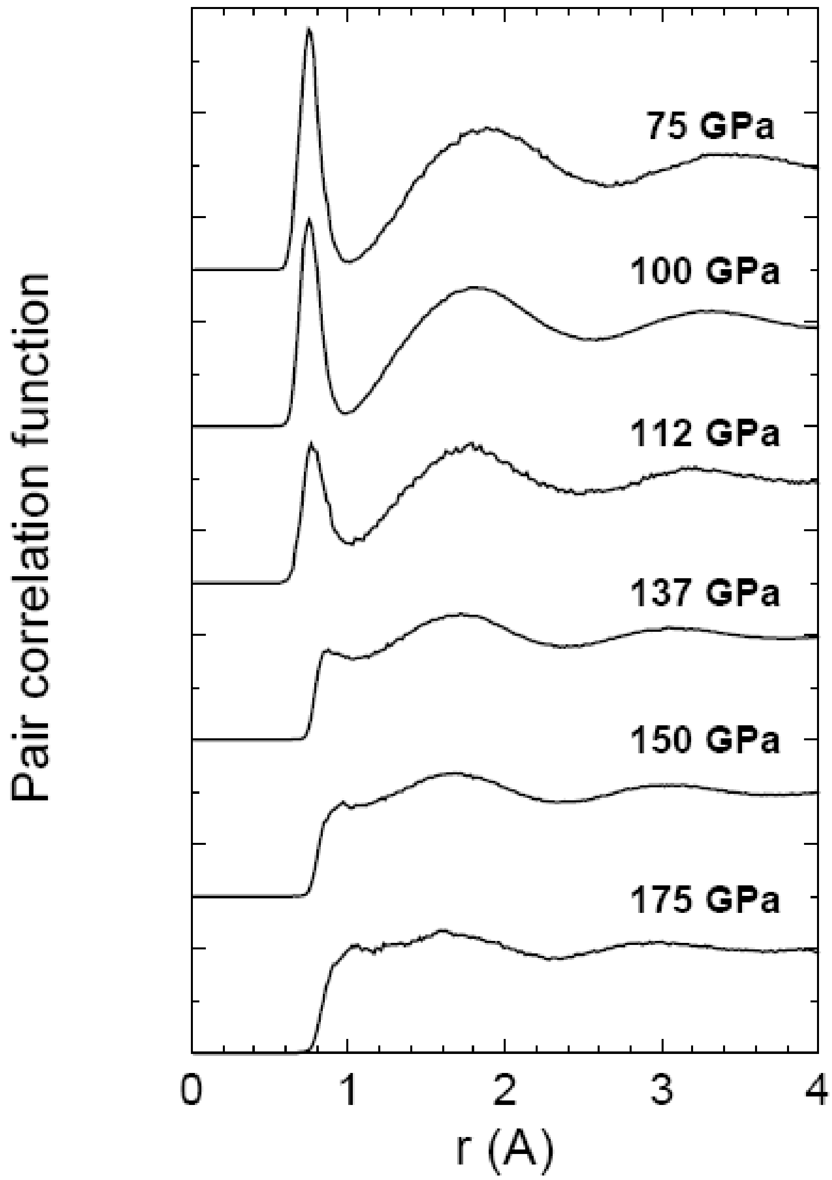
Hemley and Mao, Rev Mod Phys

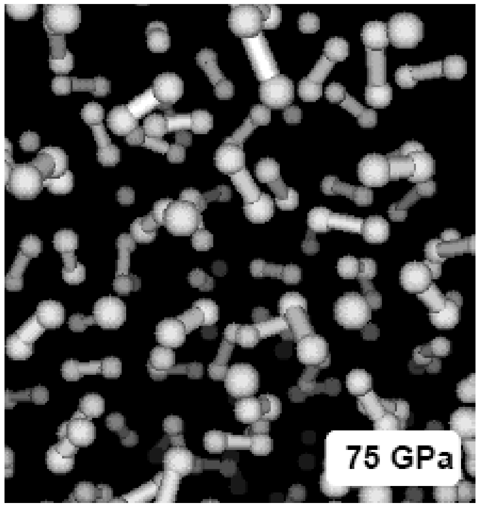

?
1 H
1 H
2 He
3 Li
4 Be
5 B
6 C
7 N
8 O
9 F
10 Ne
11 Na
12 Mg
13 Al
14 Si
15 P
16 S
17 Cl
18 Ar
19 K
20 Ca
21 SC
22 Ti
23 V
24 Cr
25 Mn
26 Fe
27 Co
28 Ni
29 Cu
30 Zn
31 Ga
32 Ge
33 As
34 Se
35 Br
36 Kr
37 Rb
38 Sr
39 Y
40 Zr
41 Nb
42 Mo
43 Tc
44 Ru
45 Rh
46 Pd
47 Ag
48 Cd
49 In
50 Sn
51 Sb
52 Te
53 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
107 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

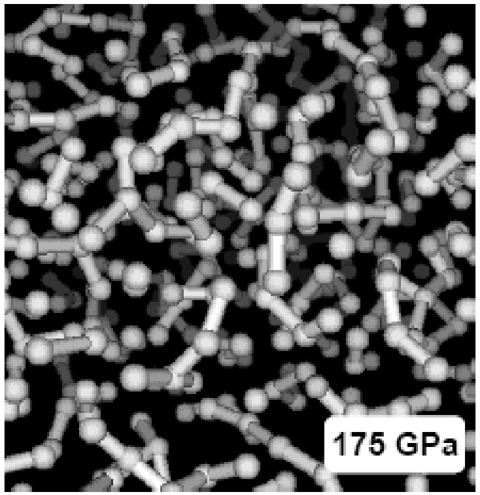


- At which depth does hydrogen become an electrical conductor?
- Is metallization accompanied by a sharp density change?

Molecular to non-molecular transition



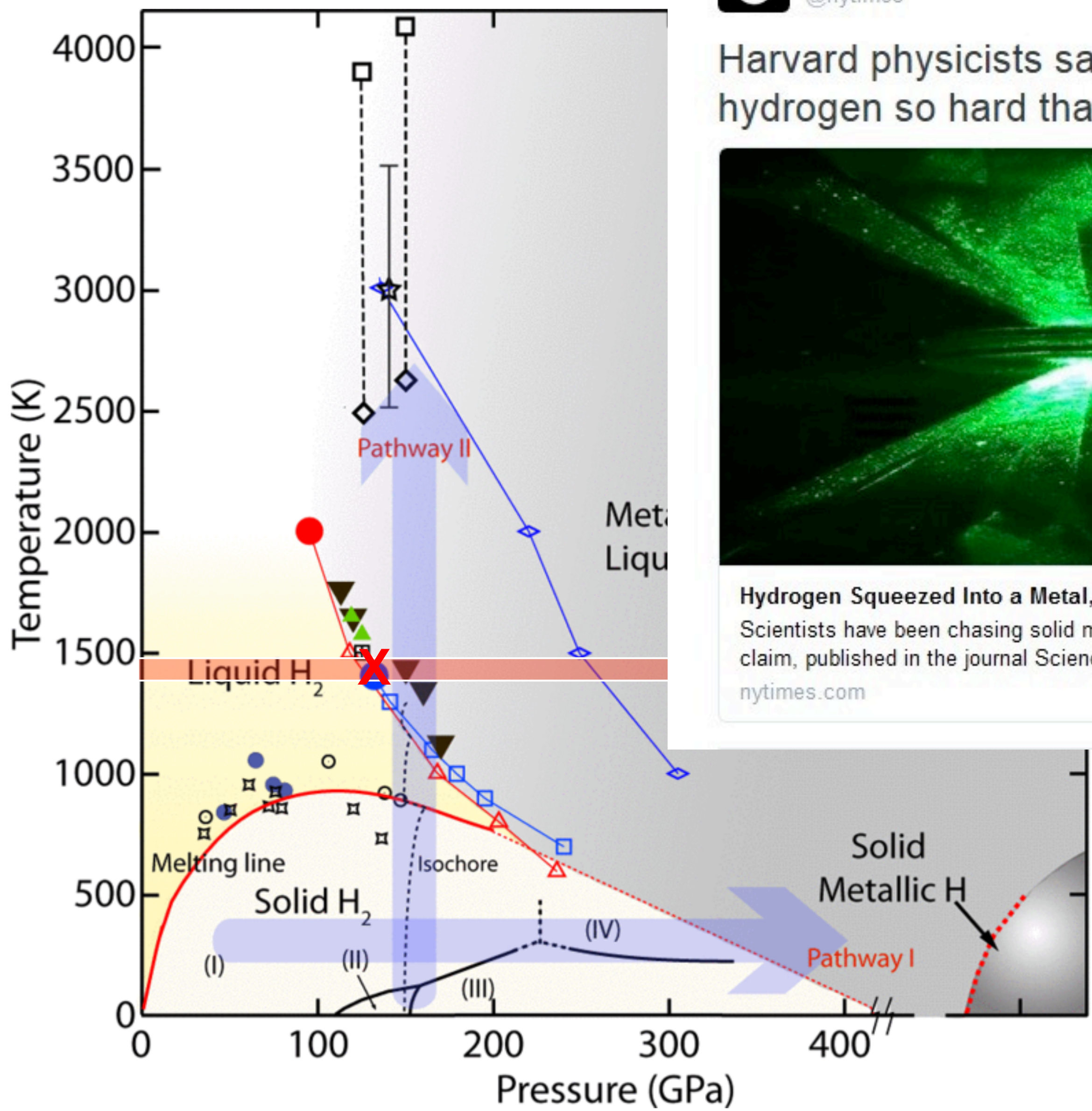




S. Scandolo, Proc. Natl. Acad. Sci. USA, 2003

Metallic hydrogen

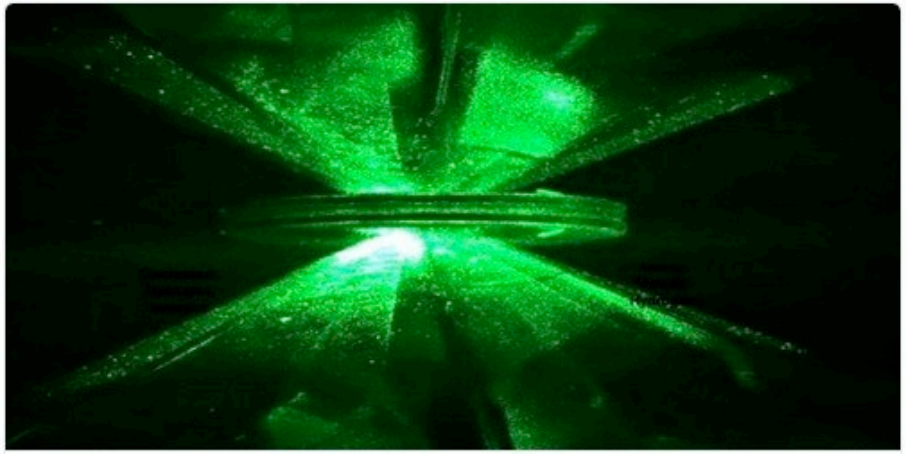
January 2017



The New York Times @nytimes

Follow

Harvard physicists say they've squeezed hydrogen so hard that it turned into a metal



Hydrogen Squeezed Into a Metal, Possibly Solid, Harvard Physicists Say

Scientists have been chasing solid metallic hydrogen for decades. The latest claim, published in the journal Science, draws debate.

nytimes.com

Take-home message

"Ab-initio Molecular Dynamics" is the most powerful theoretical tool to study atomic dynamics

Atomic diffusion, vibrations, phase transitions, chemical reactions, structural determination, thermal transport, etc…

Advantages:

- ✔ **any chemical species, with chemical accuracy**
- ✔ **availability of open source codes**

Limitations:

- ✖ **a few hundred atoms, up to 100 picoseconds**
- ✖ **large computational resources**

The Abdus Salam
International Centre
for Theoretical Physics

Thanks!

@sandro.scandolo