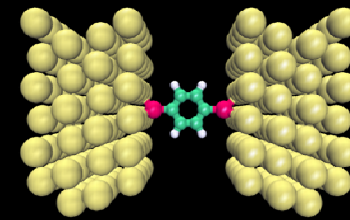
Condensed Matter Physics at ICTP



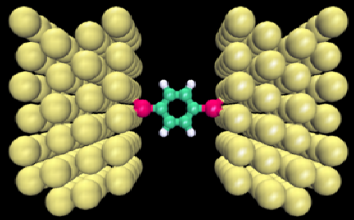
Sandro Scandolo

The Abdus Salam International Center for Theoretical Physics

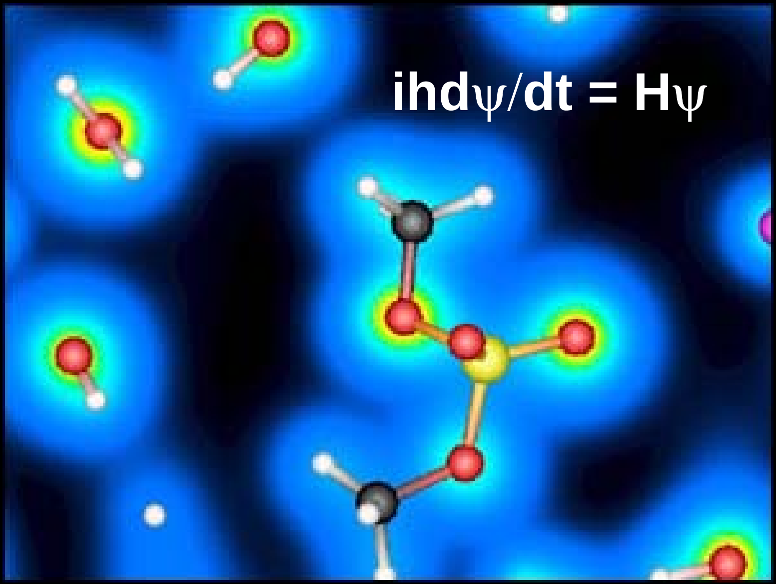
The Condensed Matter and Statistical Physics Group

(left to right)
M. Kiselev
R. Gebauer
N. Binggeli
S. Scandolo
M. Poropat
E. Tosatti
V. Kravtsov
M. Marsili
R. Zecchina
S. Franz

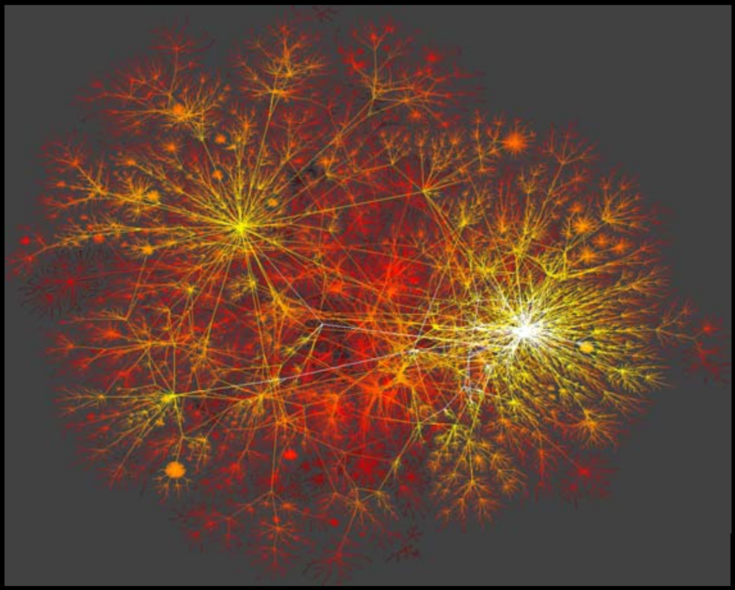
The Condensed Matter and Statistical Physics Group



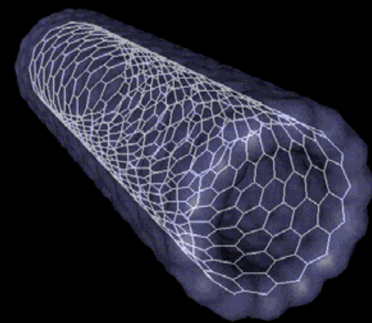
Nanoscience:
quantum simulations to design new nanomaterials

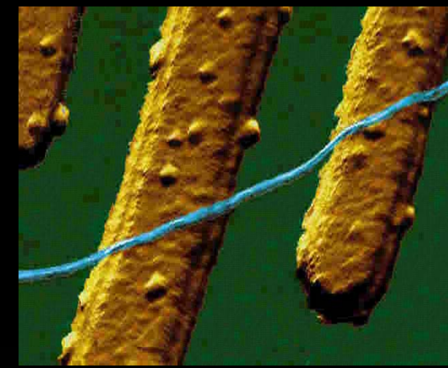


Complex systems and networks:
Internet, financial markets, social networks

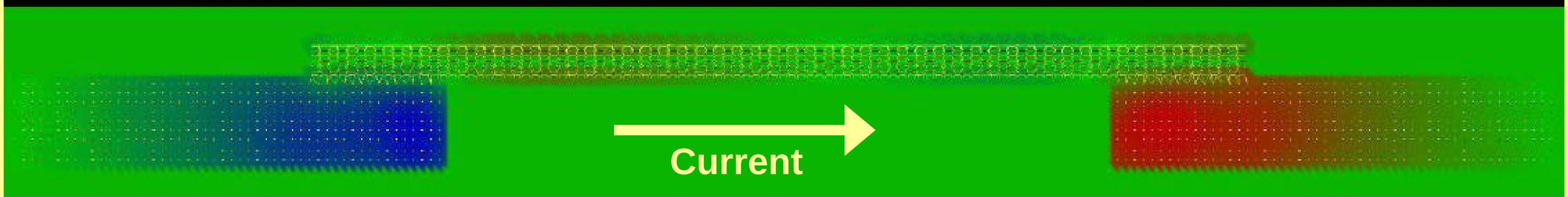


Electronic nanodevices: the resistance of carbon nanotubes

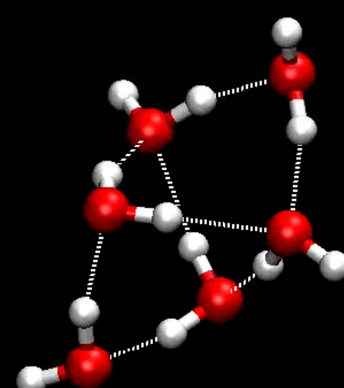




R. Gebauer et al, Phys Rev Lett, 2005



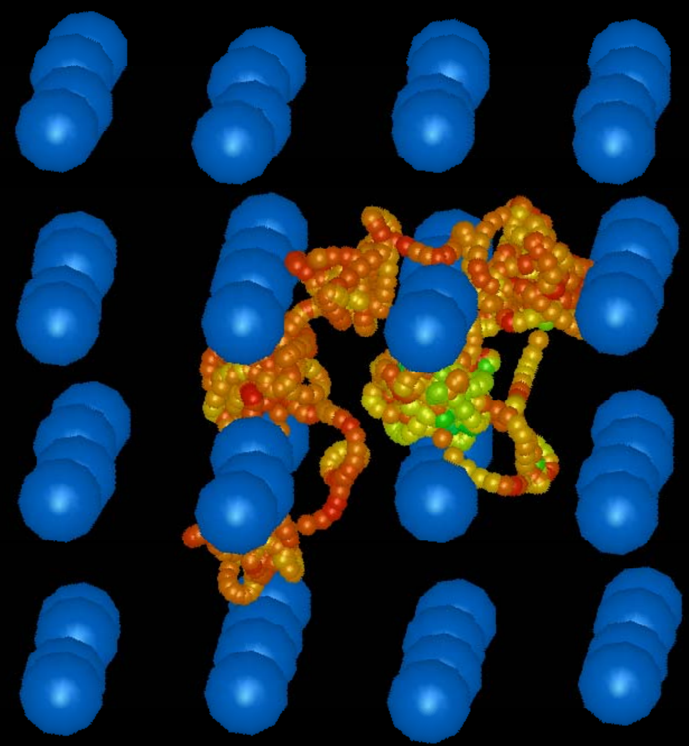
Water nanodrops: an important contributor to the greenhouse effect



S. Scandolo et al, J. Chem. Phys 2008

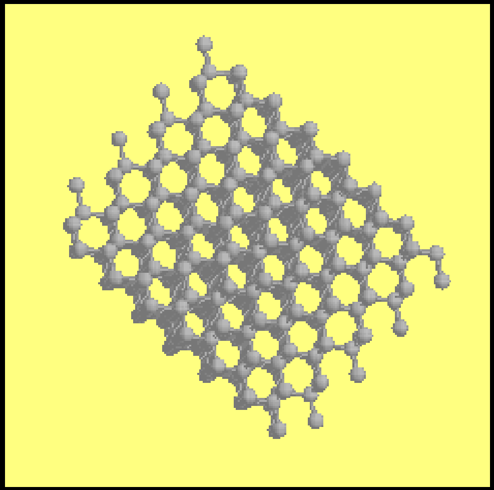
Simulating matter at extreme conditions

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

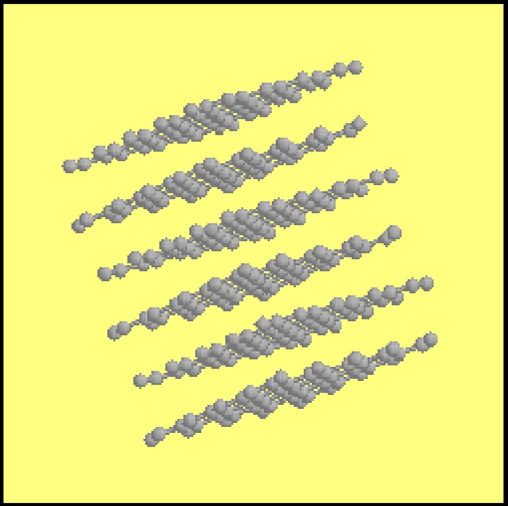


ICTP-IEAE Workshop
April 2009

Diamond



Graphite

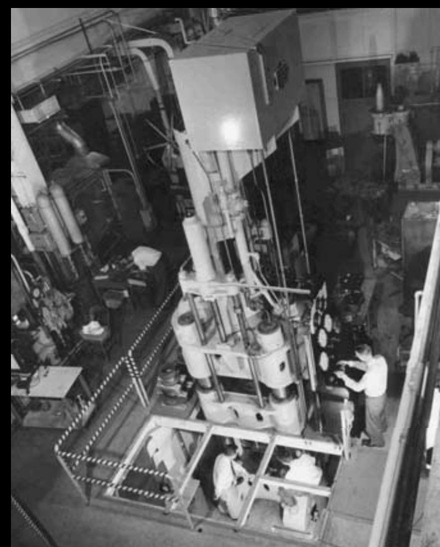


High pressure in

Physics

1935: prediction of metallic hydrogen

Materials Science

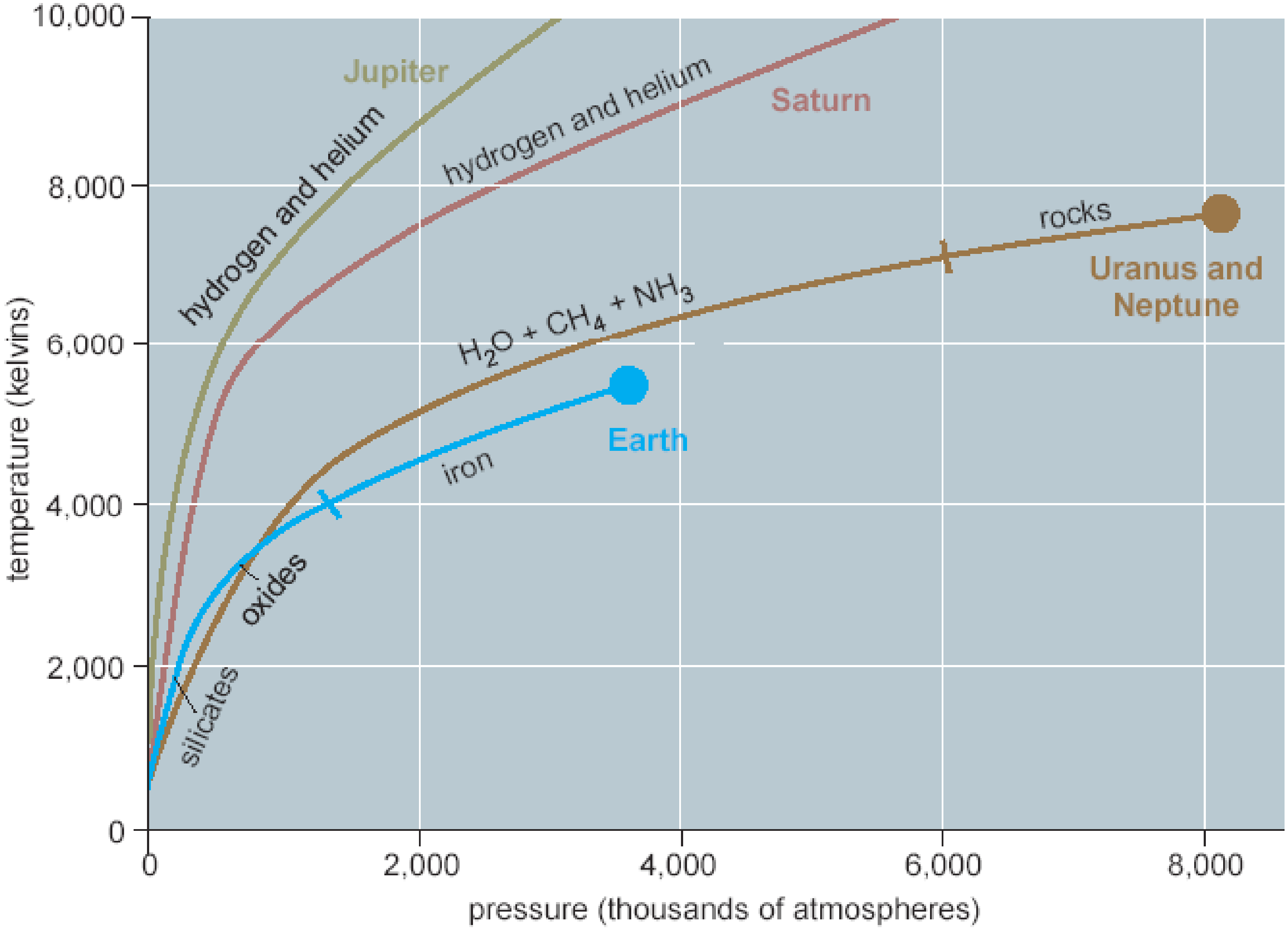


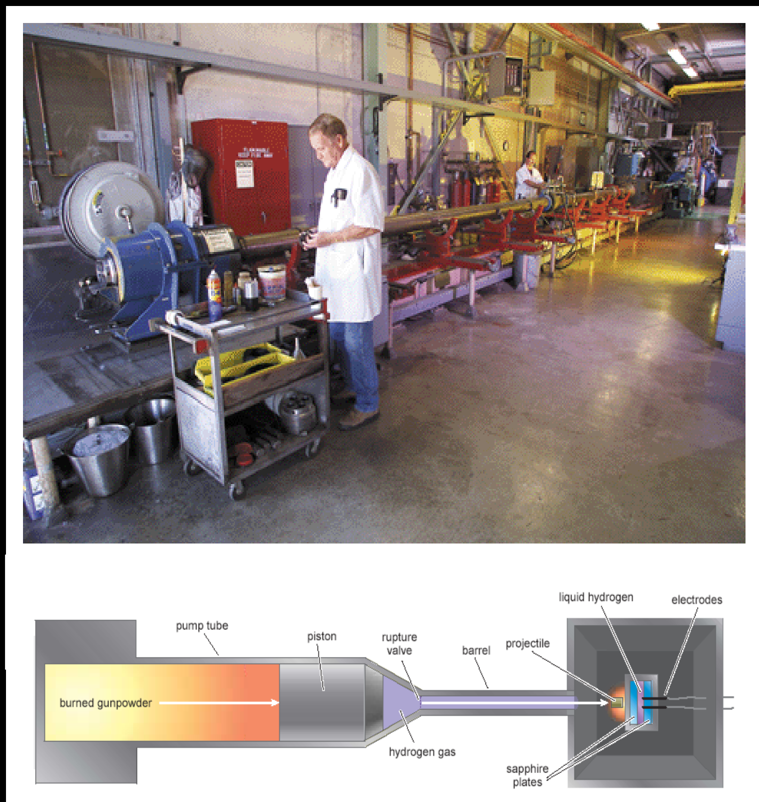
1951: the first man-made diamonds

Planetary Science

1991: Earth's core conditions reproduced in the laboratory

Scandolo & Jeanloz, American Scientist (2003)

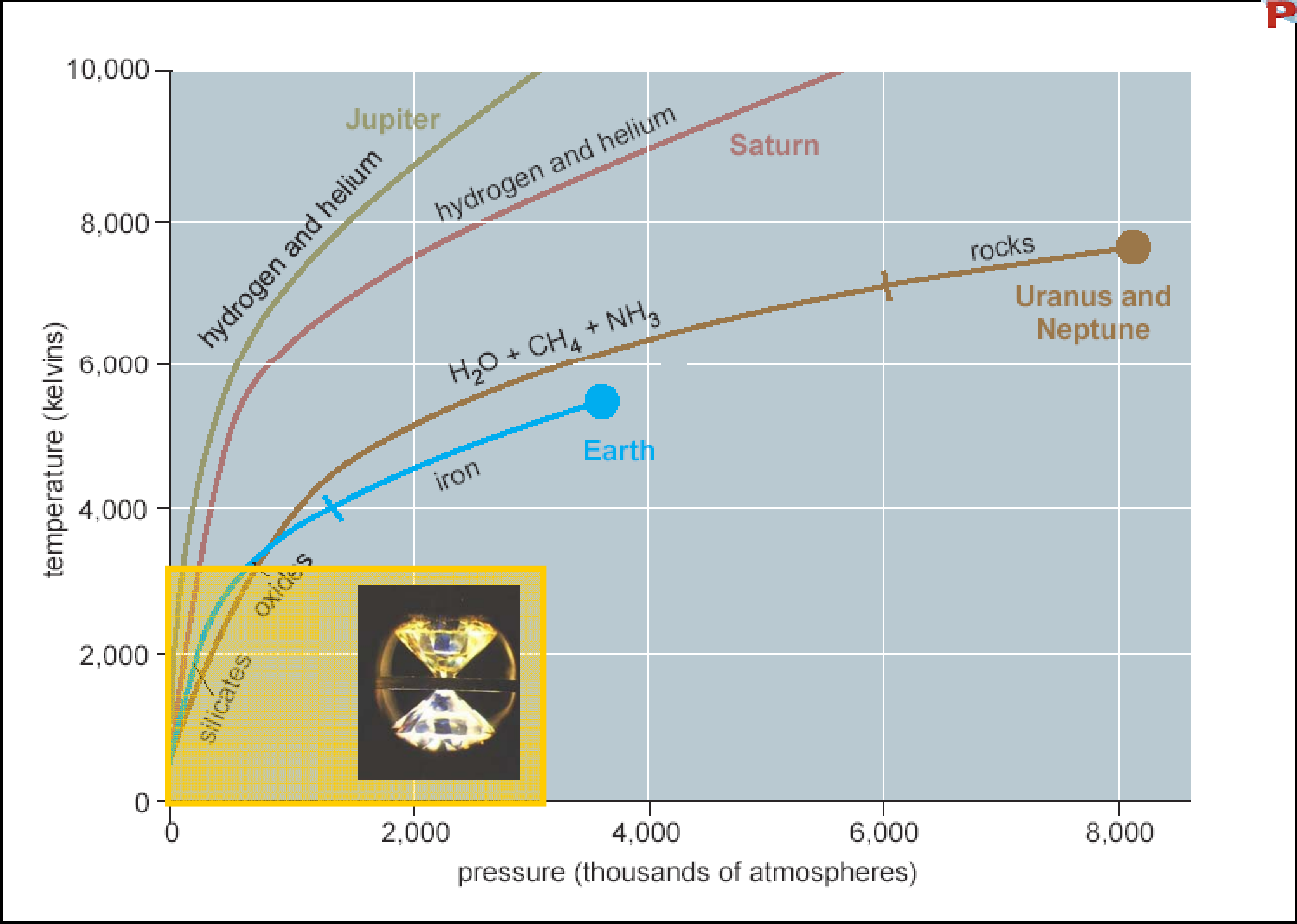




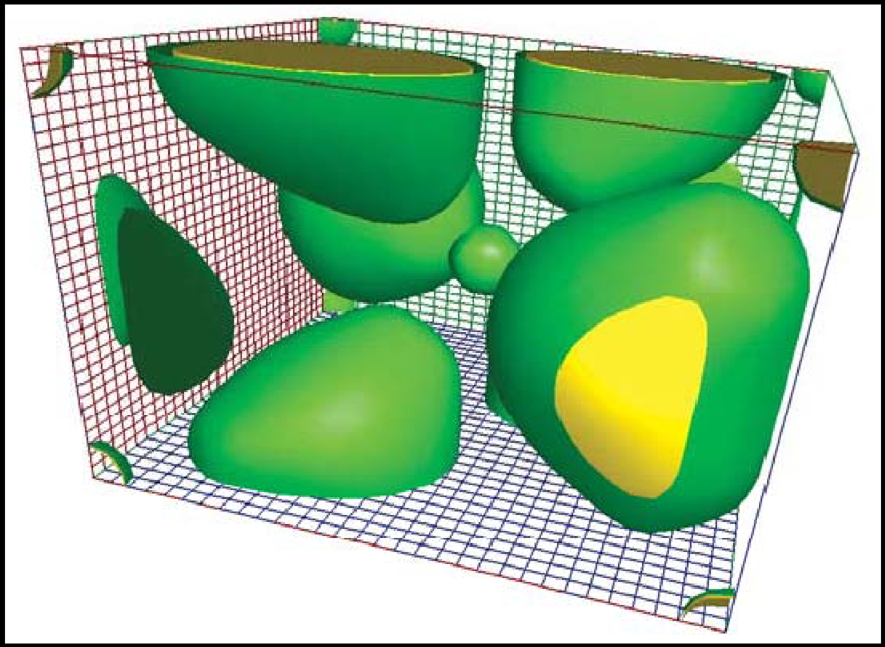
Shock waves

Diamond anvil cell

Scandolo & Jeanloz, American Scientist (2003)



Quantum simulations: The "standard model"



Electron charge density in SiO_2 stishovite

"Molecular dynamics" for atoms

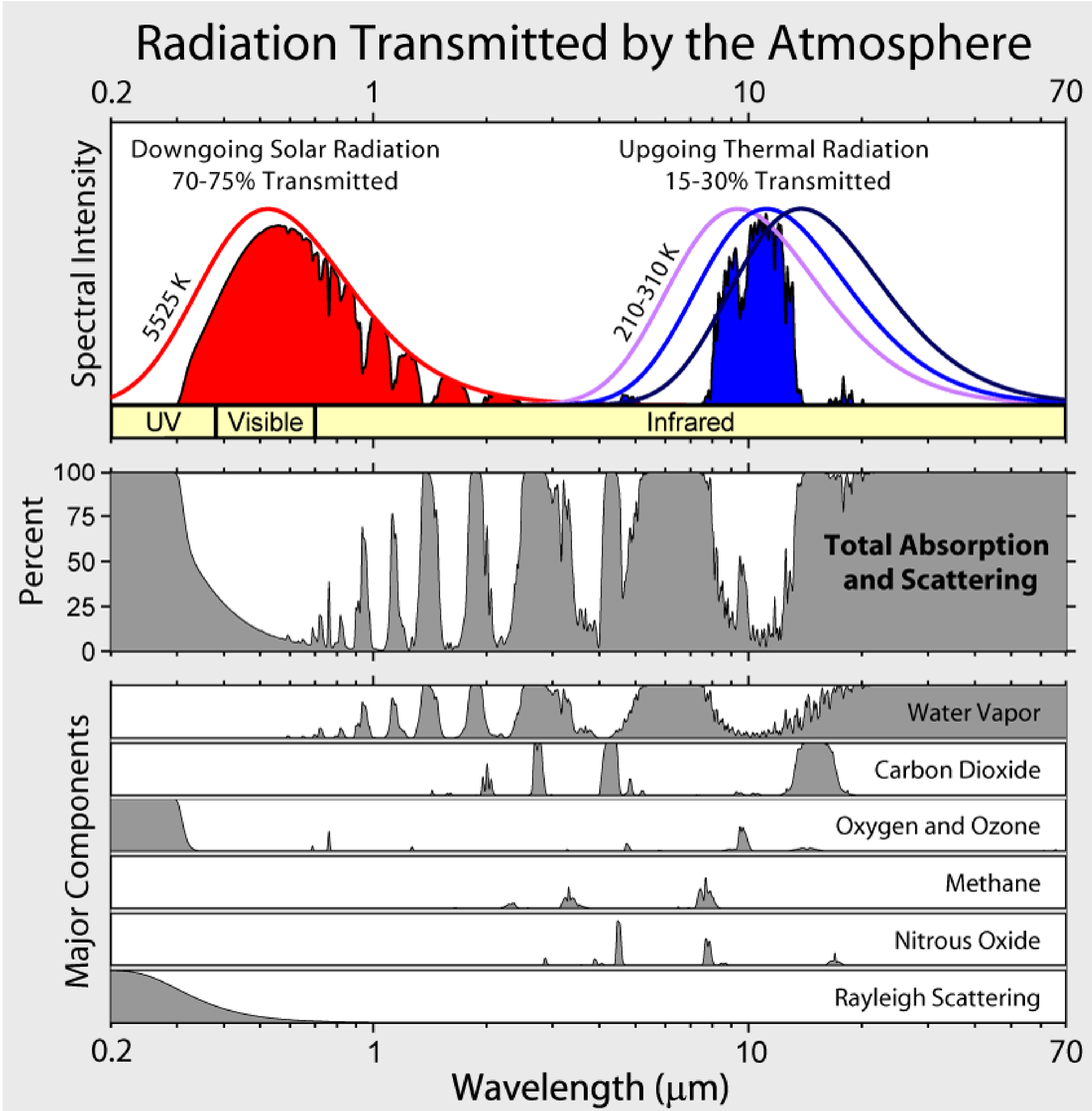
$Ma = F = -dE/dR$

Schroedinger equation for electrons

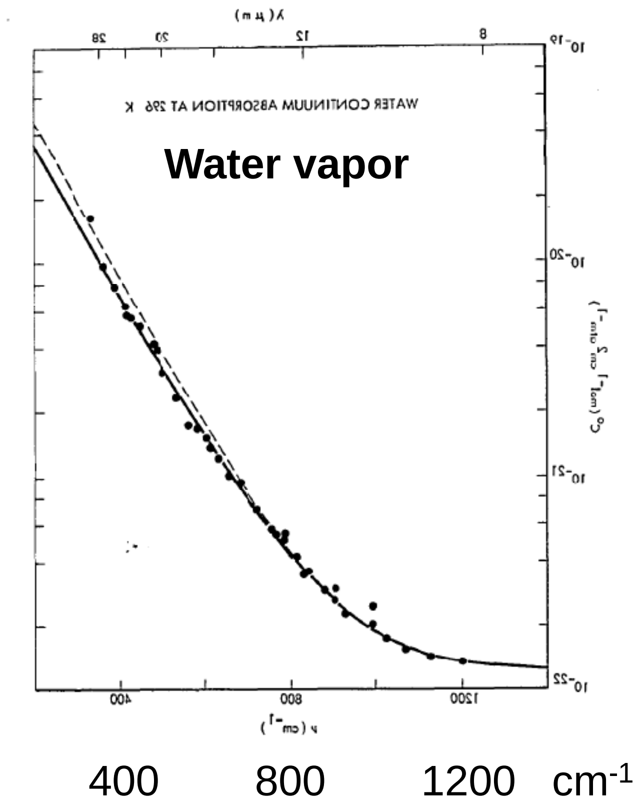
$H\psi = E\psi$

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


Radiation Transmitted by the Atmosphere
0.2
1
10
70
Spectral Intensity
Downgoing Solar Radiation
70-75% Transmitted
Upgoing Thermal Radiation
15-30% Transmitted
5525 K
210-310 K
UV
Visible
Infrared
100
75
50
25
0
Percent
Total Absorption and Scattering
Major Components
Water Vapor
Carbon Dioxide
Oxygen and Ozone
Methane
Nitrous Oxide
Rayleigh Scattering
0.2
1
10
70
Wavelength (µm)

Far-IR water vapor absorption



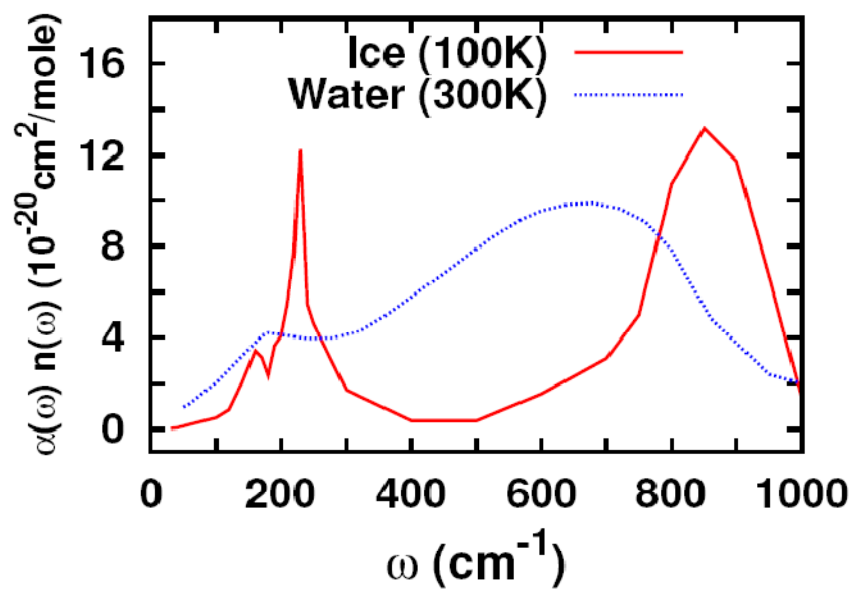
NB: Isolated water molecule does not absorb in the far-IR

Vapor absorption must be due to

1) **collisional broadening or**
2) **water nanodroplets (mostly dimers)**

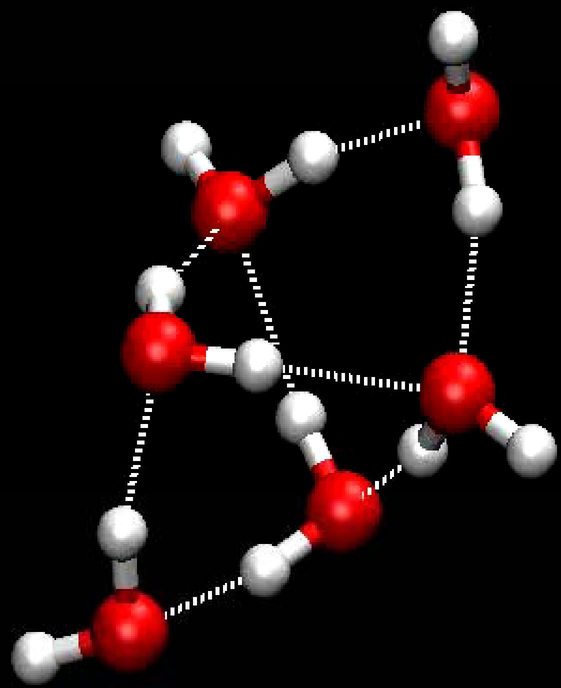
Collisional broadening does not have the correct temperature dependence

Absorption shape of water nanodroplets would have to be different than bulk forms



Water vapor absorption is different from ice and liquid water

Ab-initio molecular dynamics at 200 K



"Fluid" dynamics even at 200 K

Jumps between different locally stable conformations (ring, book, cage)

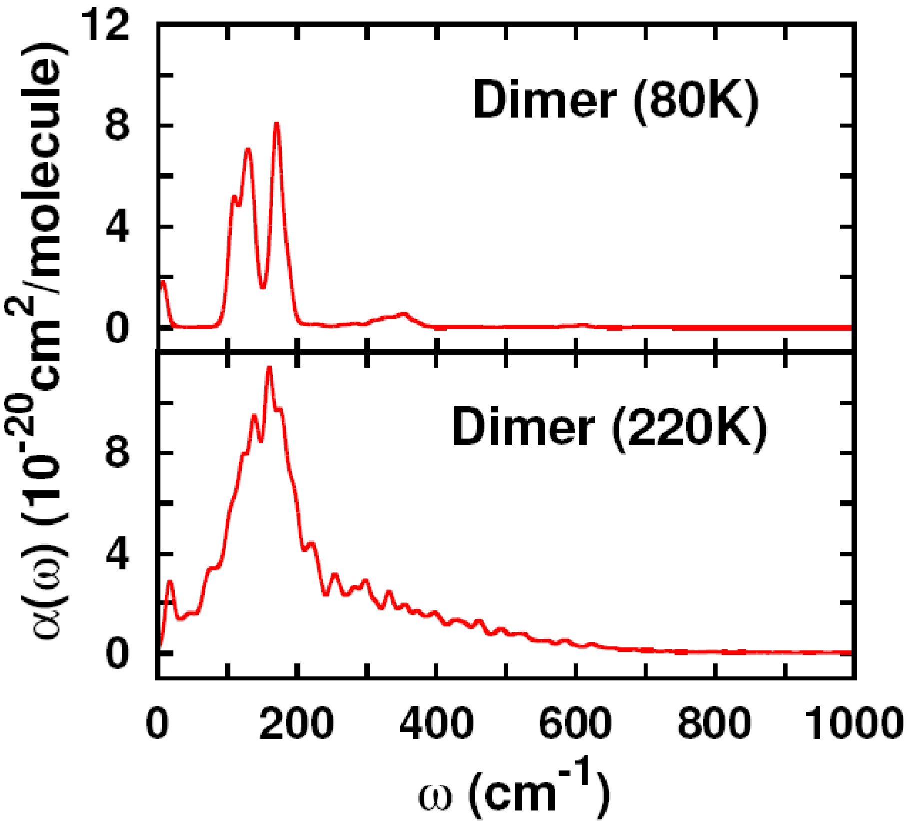
Ring conformation predominant due to entropic effects

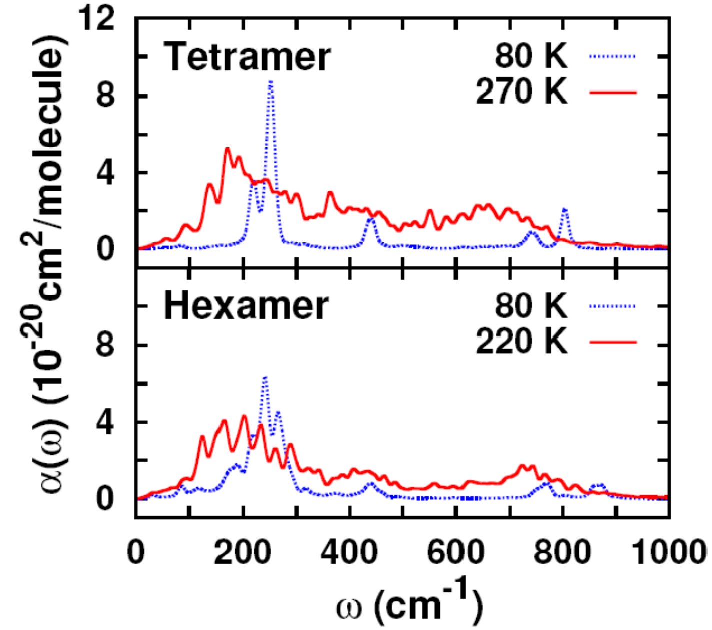
Total dipole moment

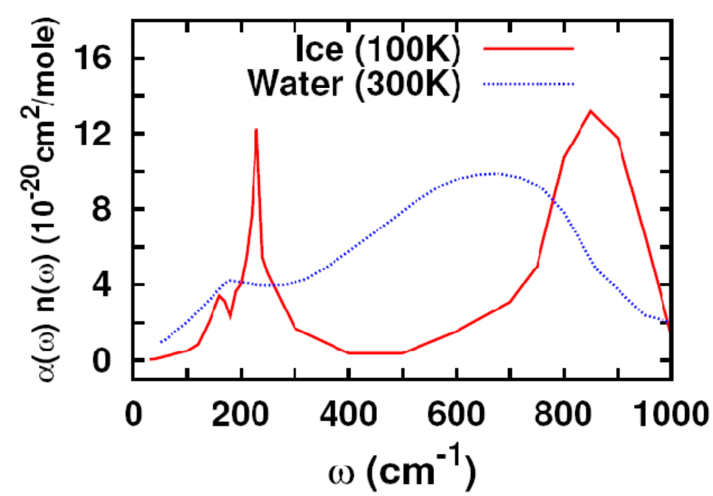
Absorption coefficient from MD trajectory

$$\alpha(\omega) = \frac{4\pi\omega \tanh(\beta\hbar\omega/2)}{3\hbar\, n(\omega)\, c\, N} \int_{-\infty}^{+\infty} dt\, e^{-i\omega t} \langle \mathbf{M}(t) \cdot \mathbf{M}(0) \rangle$$

Far-IR absorption by water nanoclusters



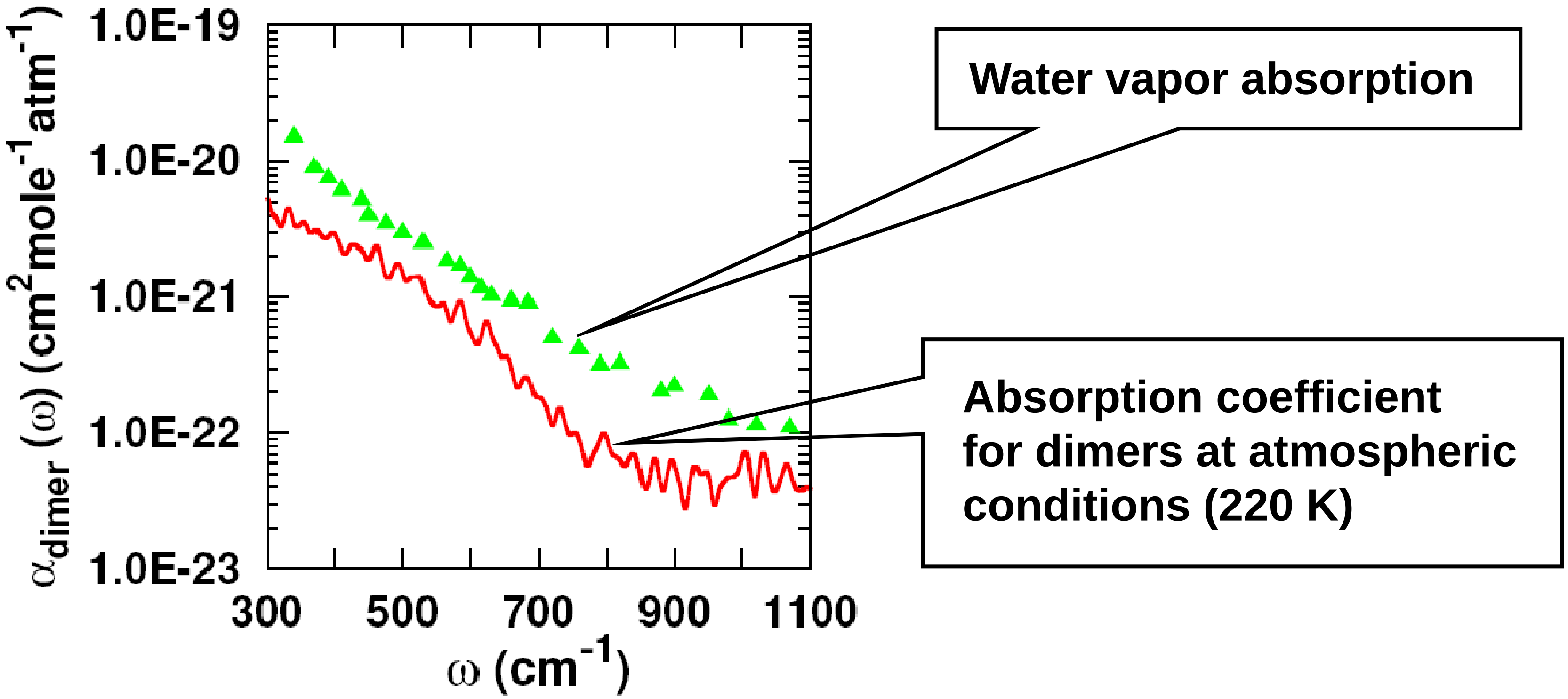




Water **dimer** **absorption is indeed different from ice and liquid water**

Emergent *atmospheric* nanoscience?

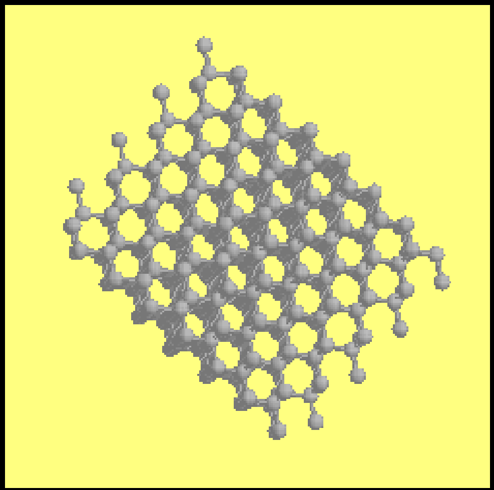
Comparison with water vapor

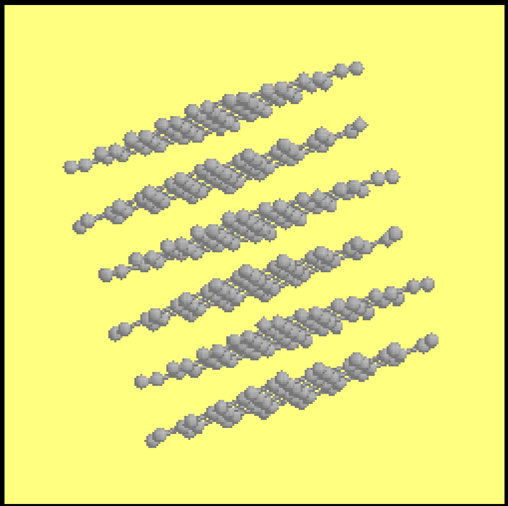


Water dimer absorption agrees qualitatively with vapor

Water dimers could be responsible for vapor absorption if their concentration was higher than currently estimated

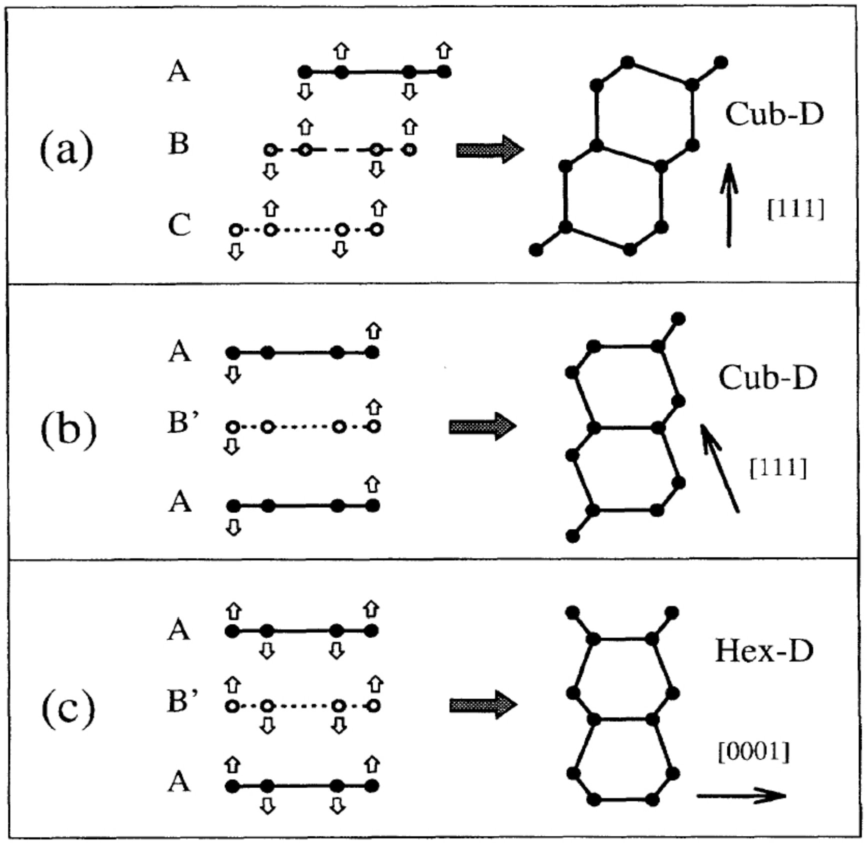
Diamond **Graphite**

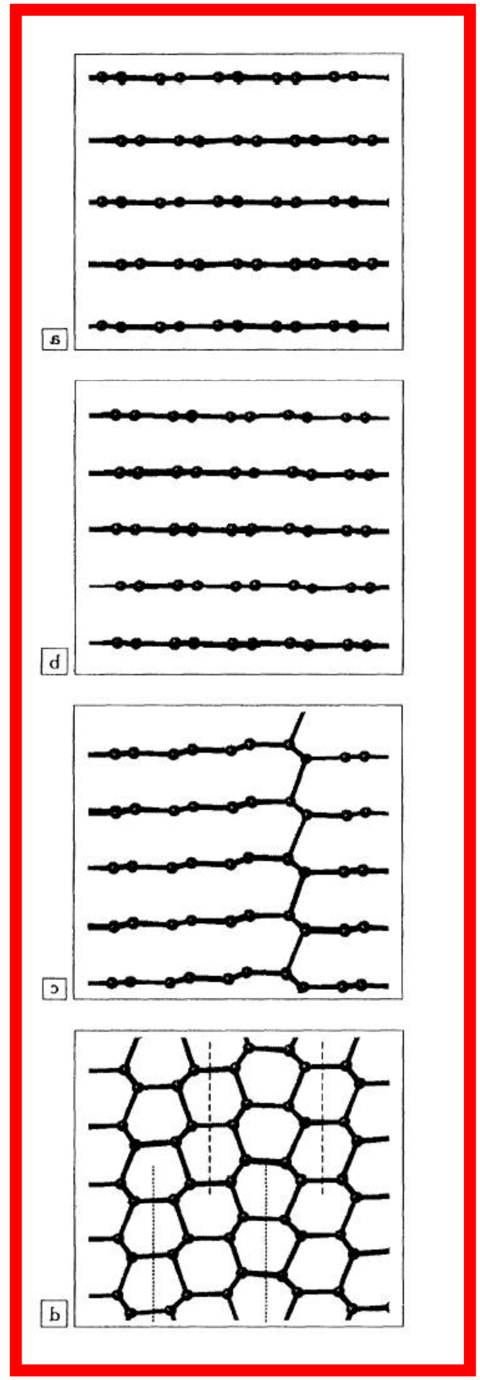




Atomistic mechanism of the graphite to diamond transition

Possible paths

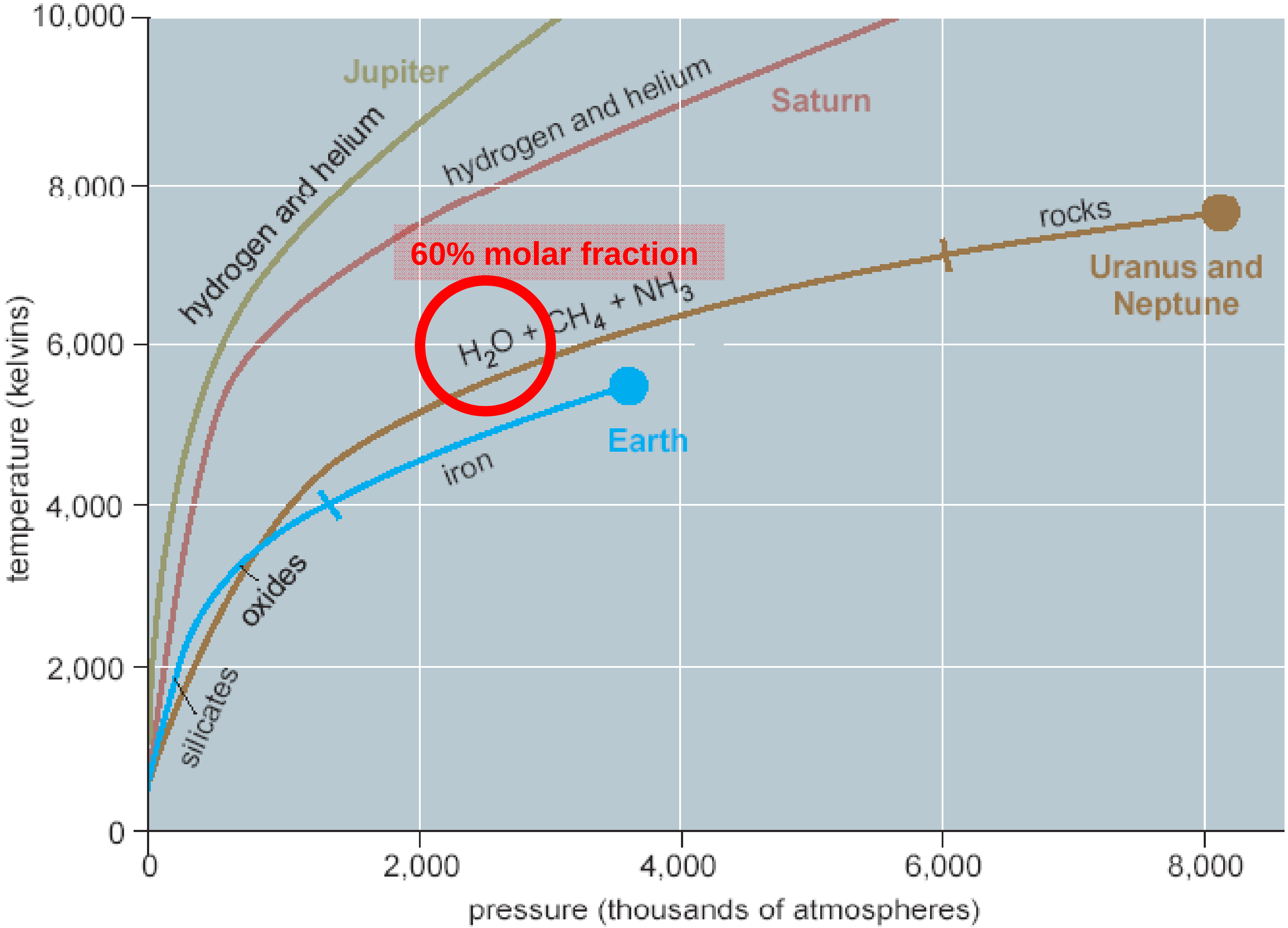




1 picosecond

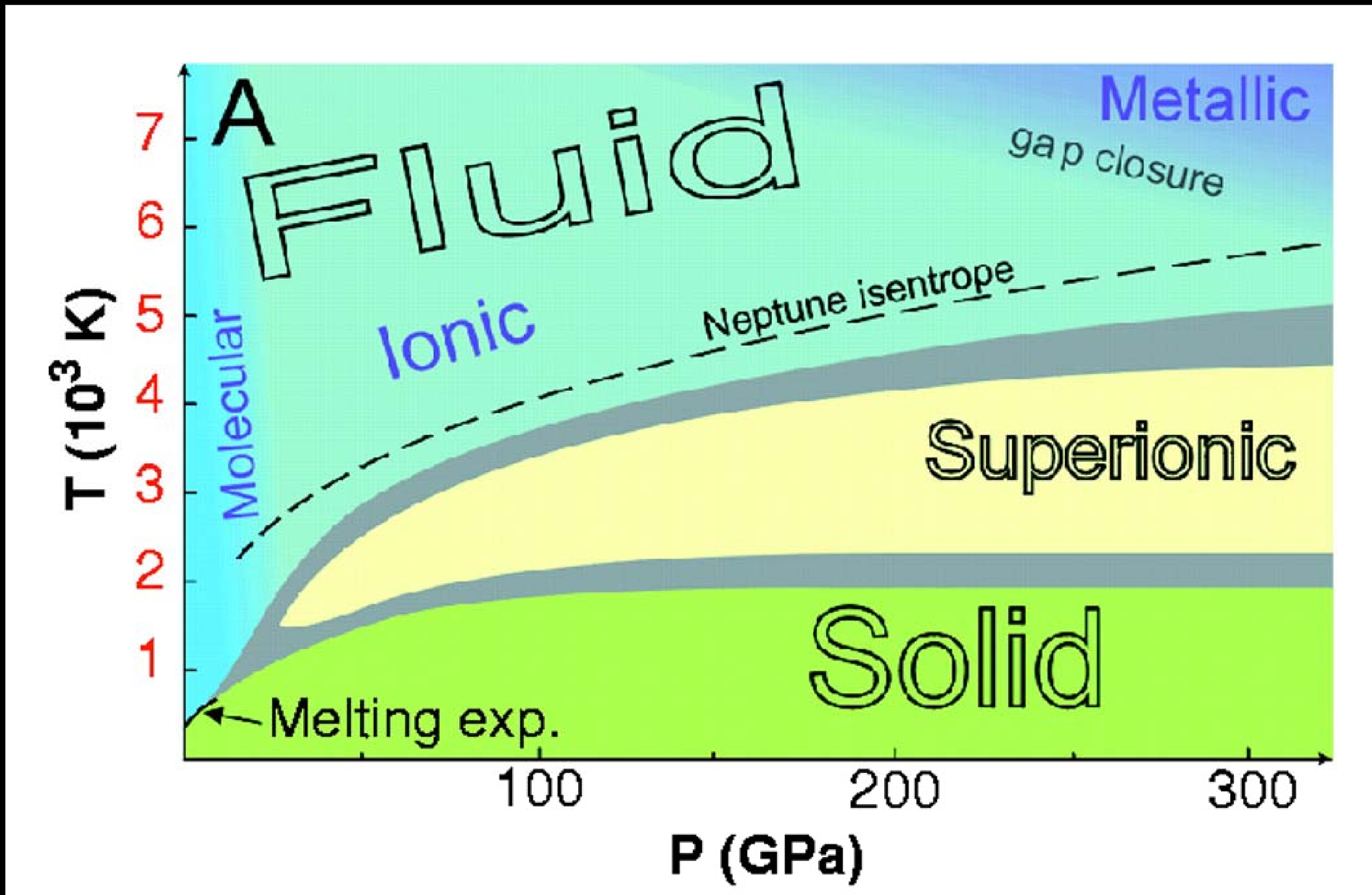
S. Scandolo et al., PRL 74, 4015 (1995)

Water and hydrogen 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
rocks
60% molar fraction
$H_2O + CH_4 + NH_3$
Uranus and Neptune
Earth
iron
oxides
silicates

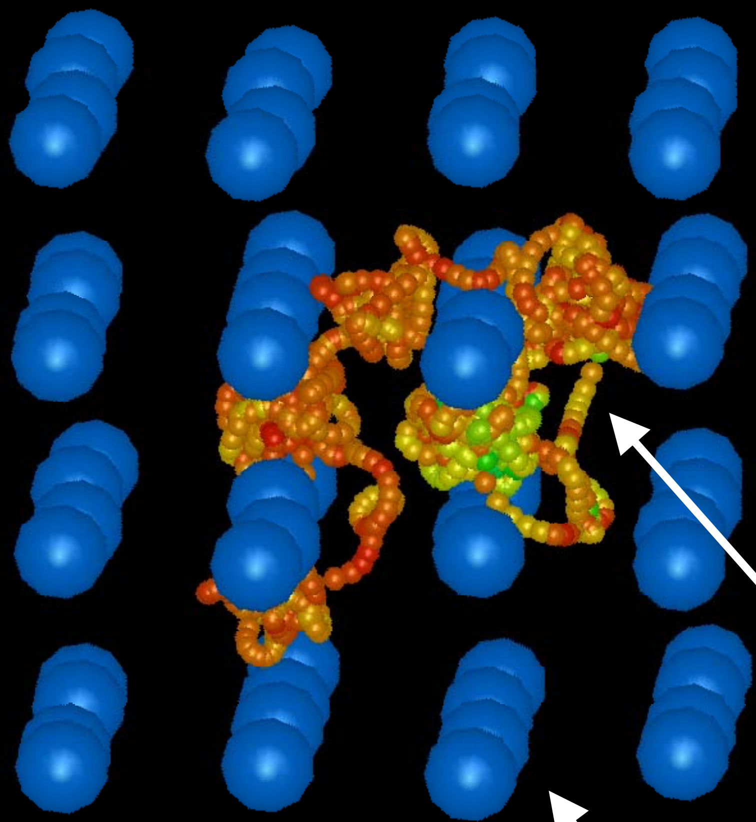
phase diagram of water from first principles



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)

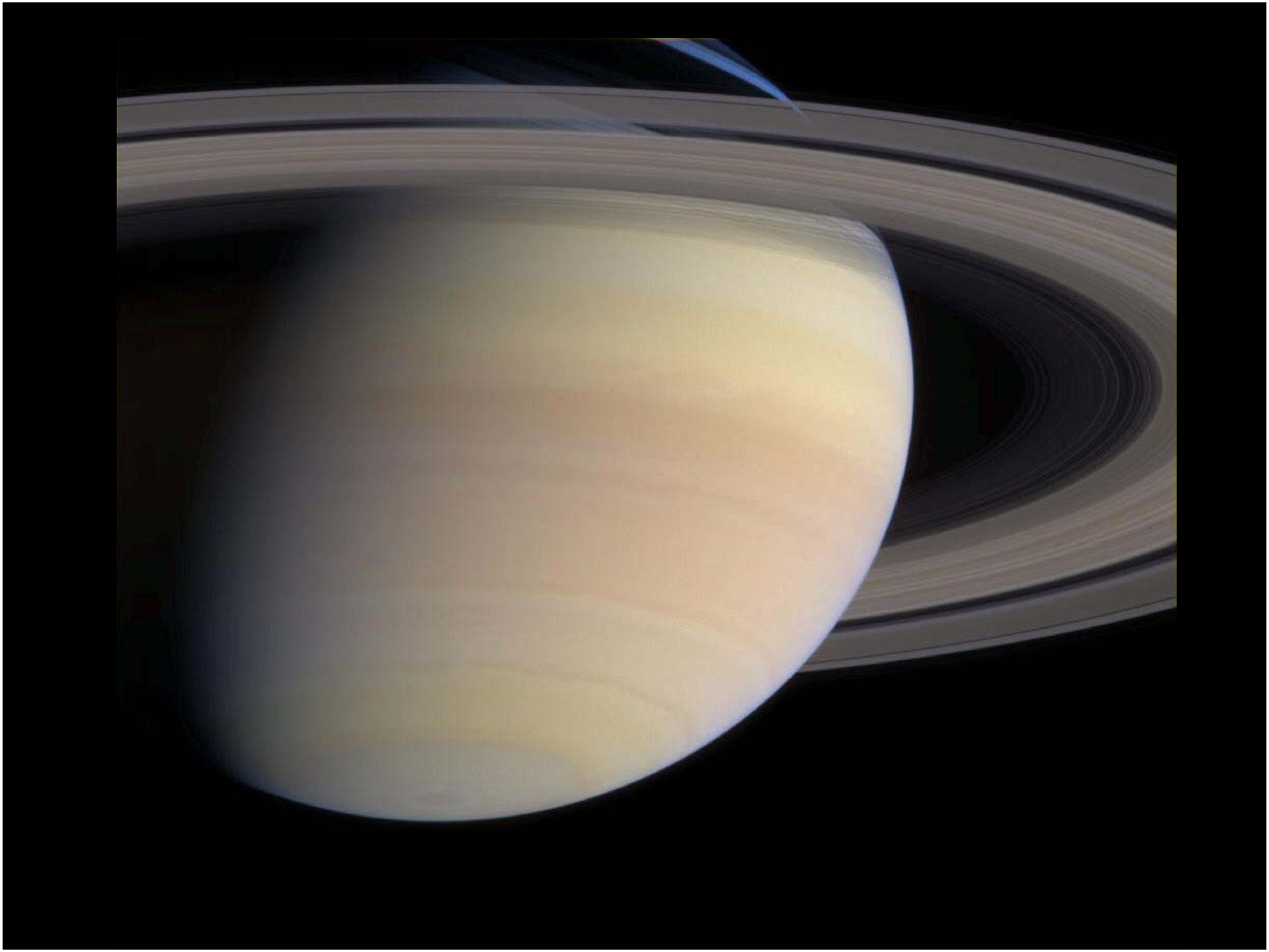


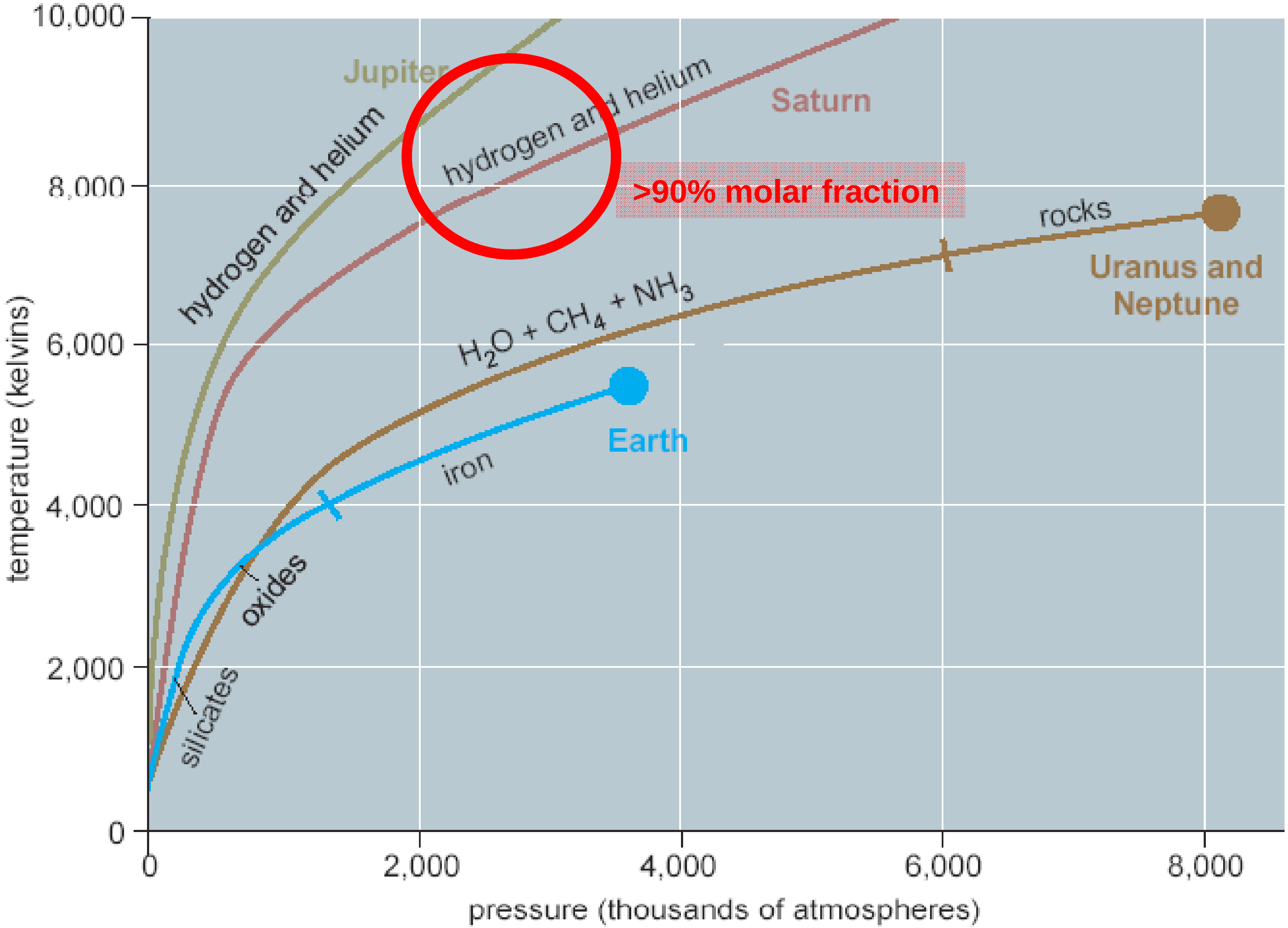
Superionic Water

P = 150 GPa
T = 2500 K

Proton diffusion by hopping

Oxygen sublattice remains crystalline



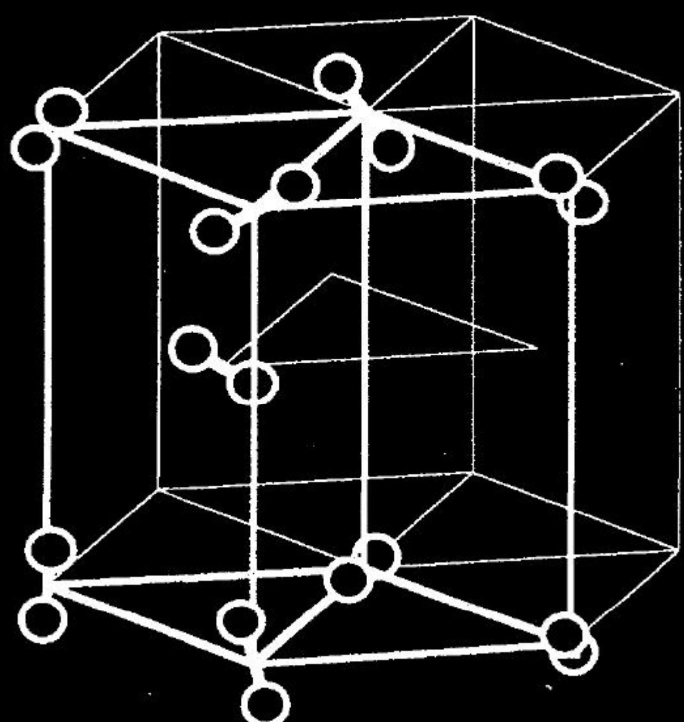


10,000
8,000
6,000
4,000
2,000
0
temperature (kelvins)
Jupiter
hydrogen and helium
hydrogen and helium
Saturn
>90% molar fraction
rocks
Uranus and
Neptune
H2O + CH4 + NH3
Earth
iron
oxides
silicates
0
2,000
4,000
6,000
8,000
pressure (thousands of atmospheres)

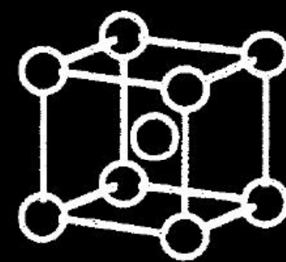
E. Wigner and H.B. Huntington

"On the possibility of a metallic modification of hydrogen"

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

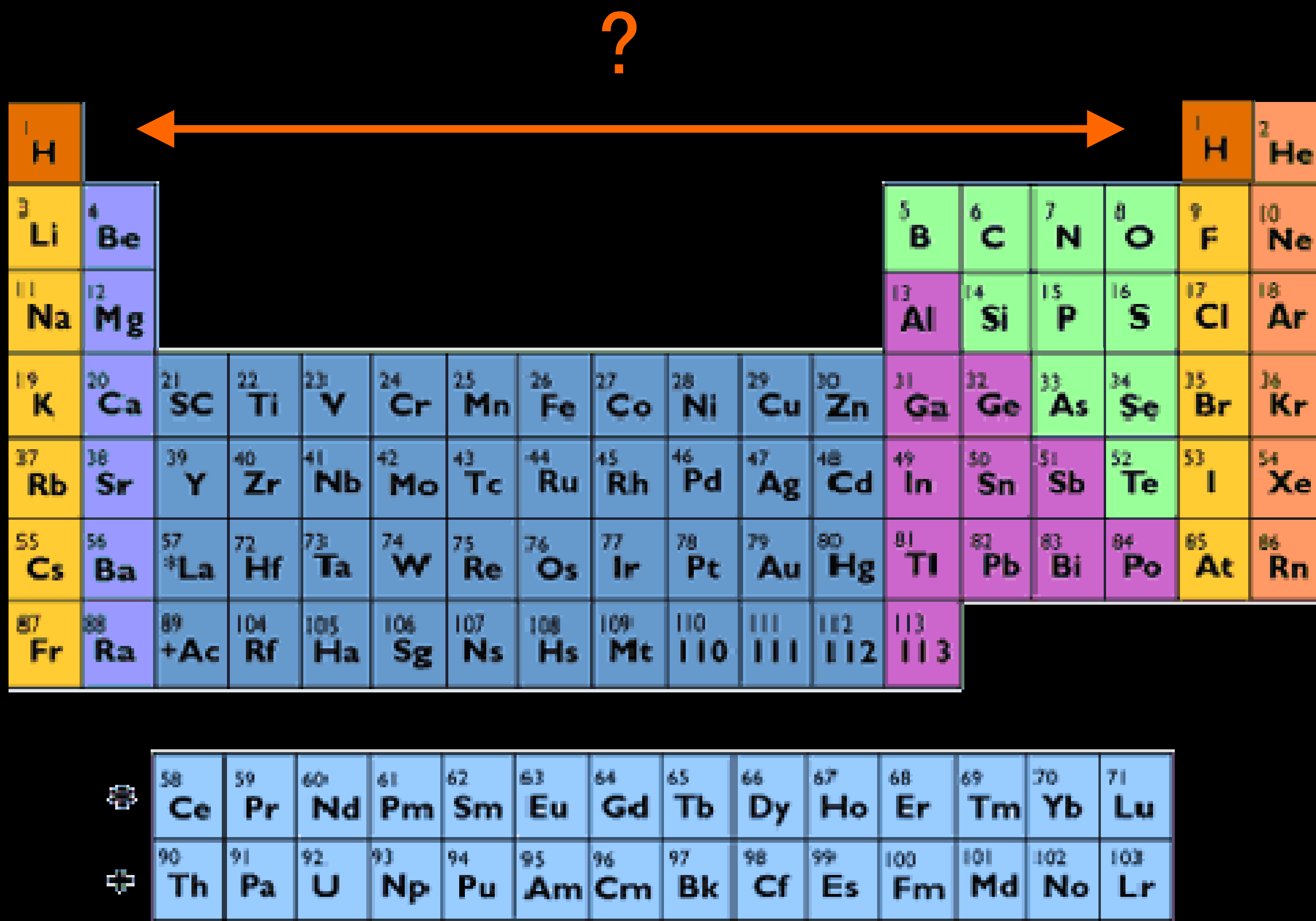


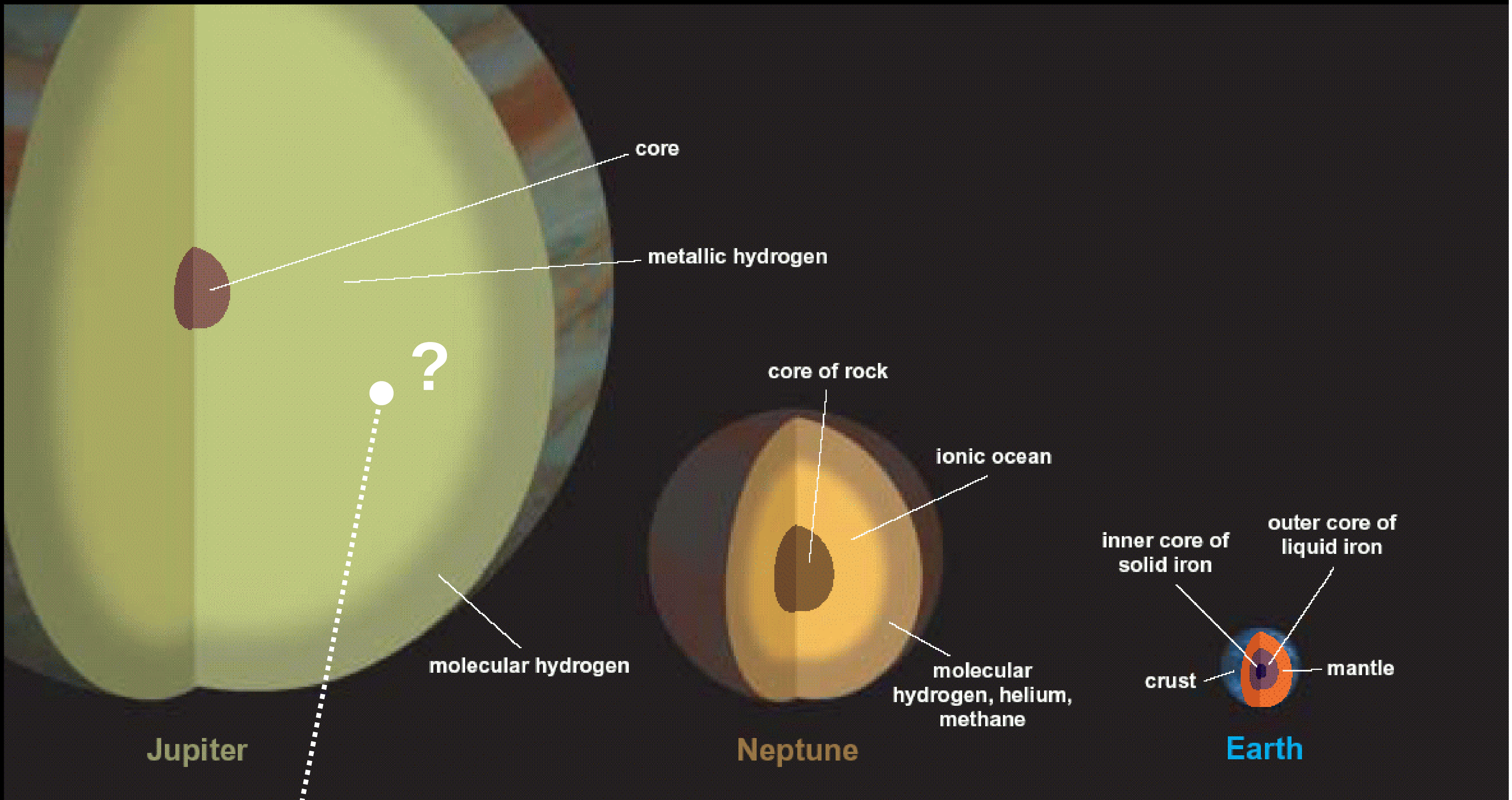
Molecular hydrogen



Monatomic hydrogen

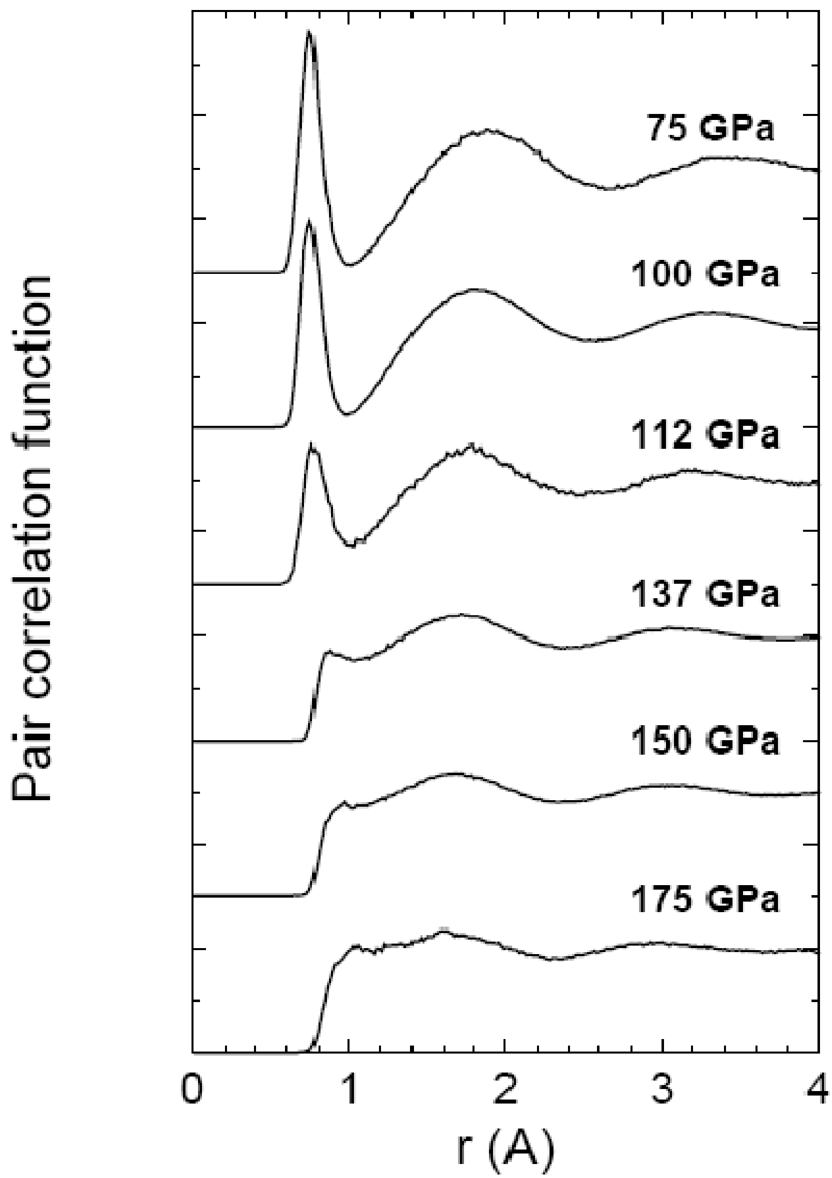
Hemley and Mao, Rev Mod Phys

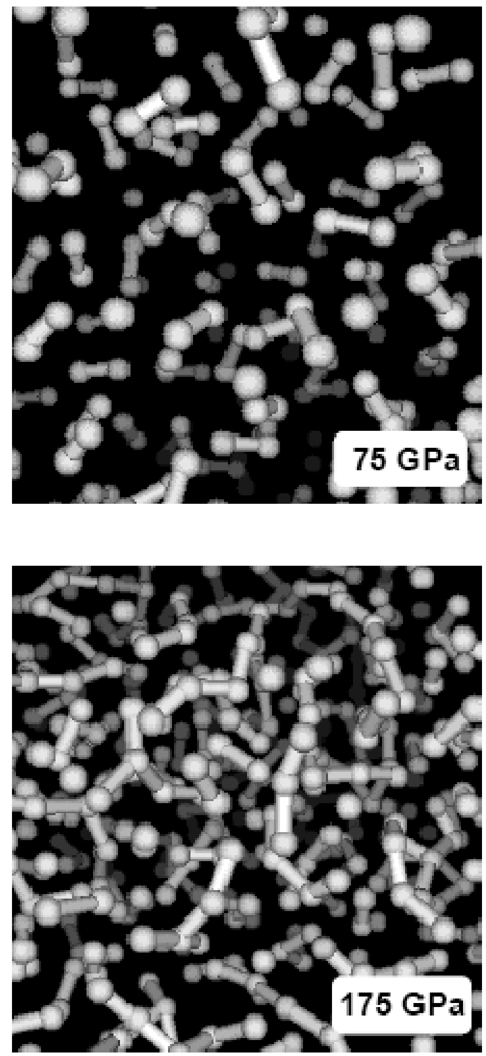

?
1 H
1 H 2 He
3 Li 4 Be 5 B 6 C 7 N 8 O 9 F 10 Ne
11 Na 12 Mg 13 Al 14 Si 15 P 16 S 17 Cl 18 Ar
19 K 20 Ca 21 SC 22 Ti 23 V 24 Cr 25 Mn 26 Fe 27 Co 28 Ni 29 Cu 30 Zn 31 Ga 32 Ge 33 As 34 Se 35 Br 36 Kr
37 Rb 38 Sr 39 Y 40 Zr 41 Nb 42 Mo 43 Tc 44 Ru 45 Rh 46 Pd 47 Ag 48 Cd 49 In 50 Sn 51 Sb 52 Te 53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

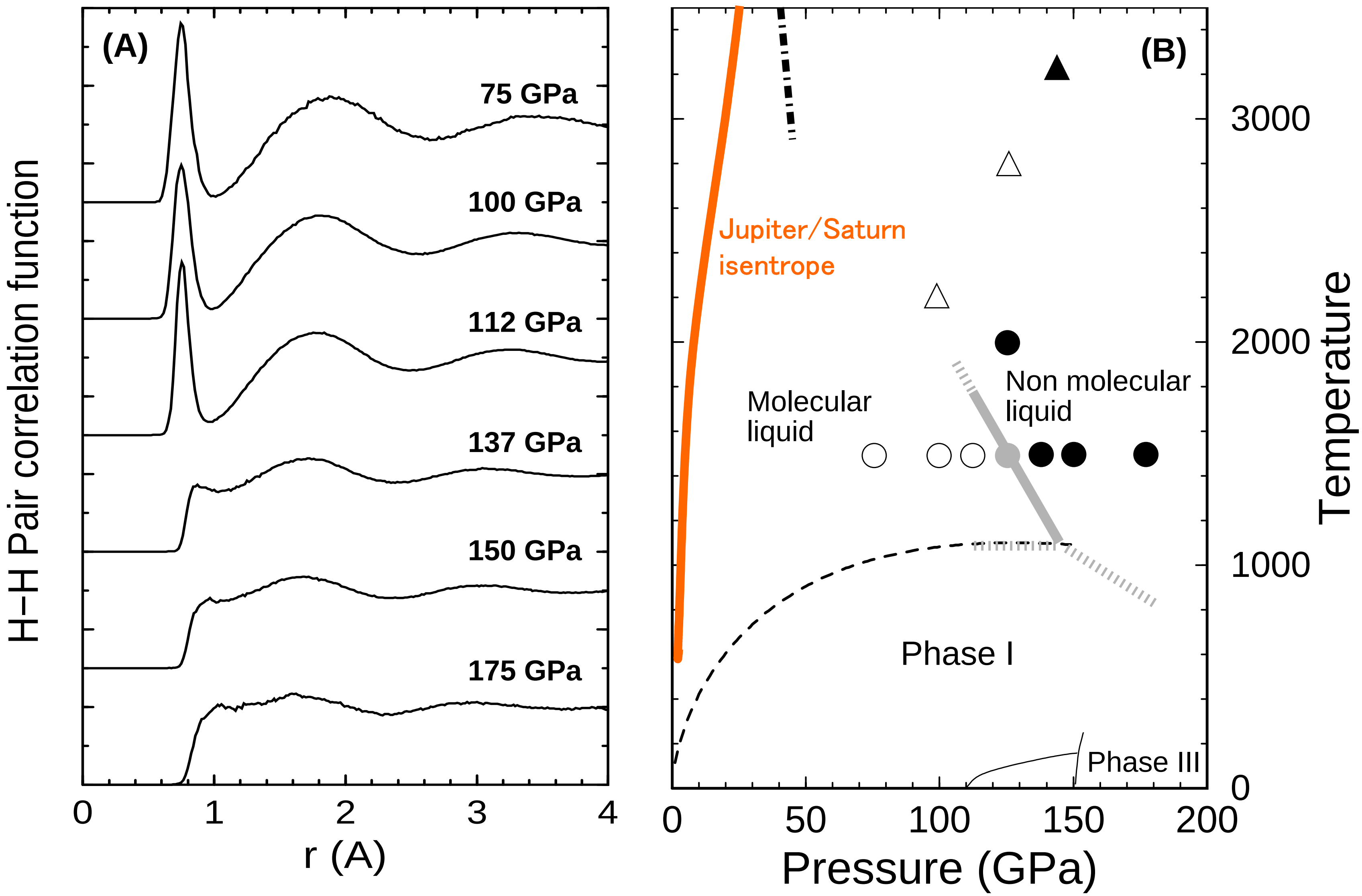




S. Scandolo, Proc. Natl. Acad. Sci. USA, 2003

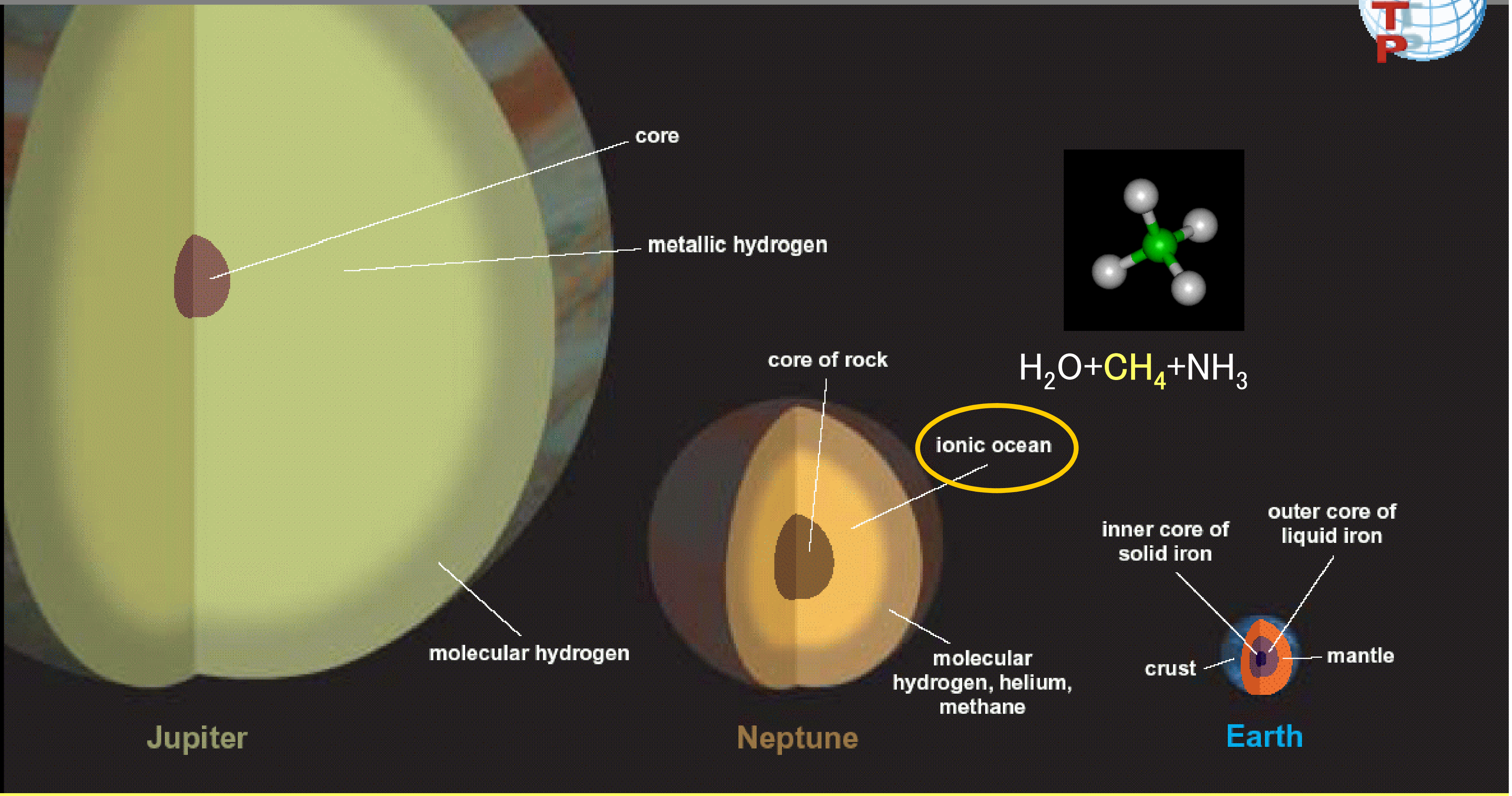
Is there a first-order phase transition inside Jupiter/Saturn?

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



Diamonds in the sky?

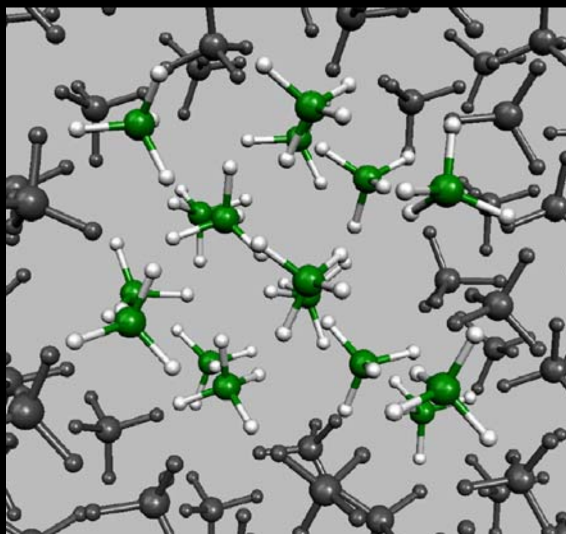
Scandolo & Jeanloz, American Scientist (2003)



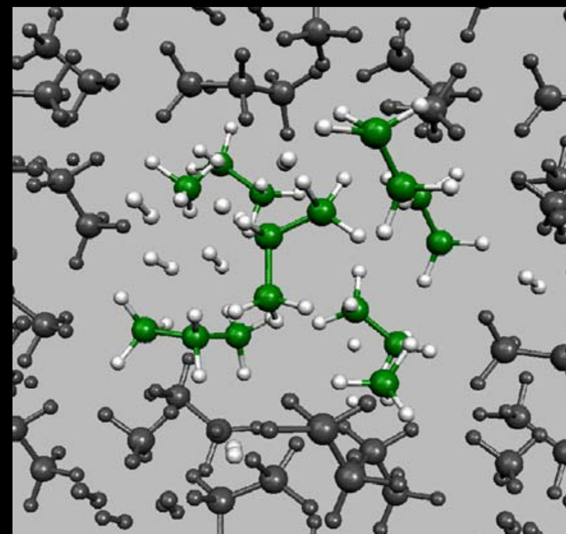
Marvin Ross, “Diamonds in the sky”
Nature (1981)

Methane was found to dissociate under a shock wave

Dissociation of methane at extreme (planetary) conditions

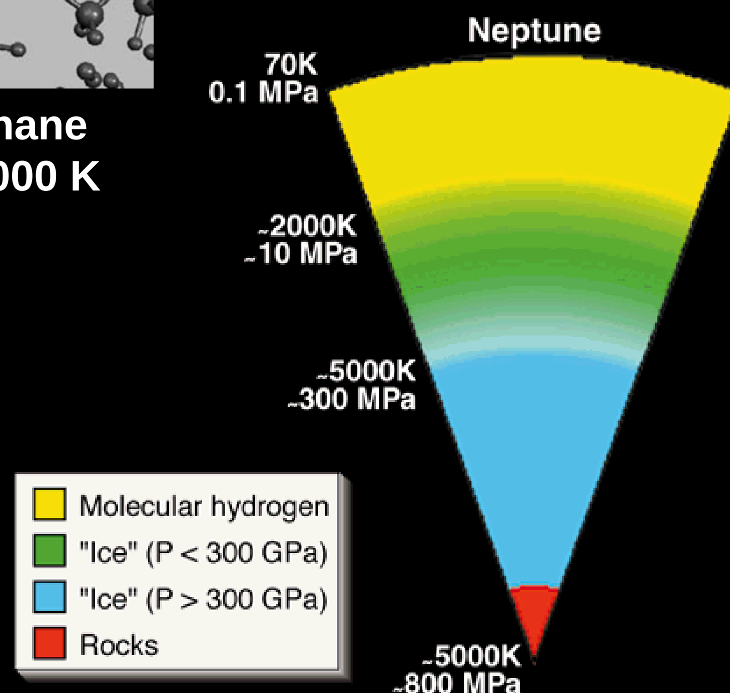


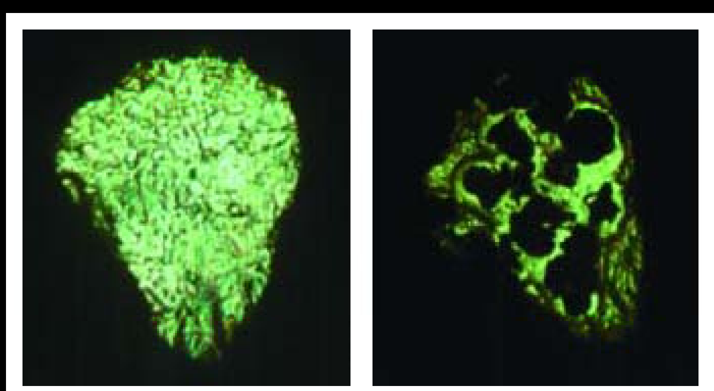
Compressed methane



Compressed methane after heating to 4000 K

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

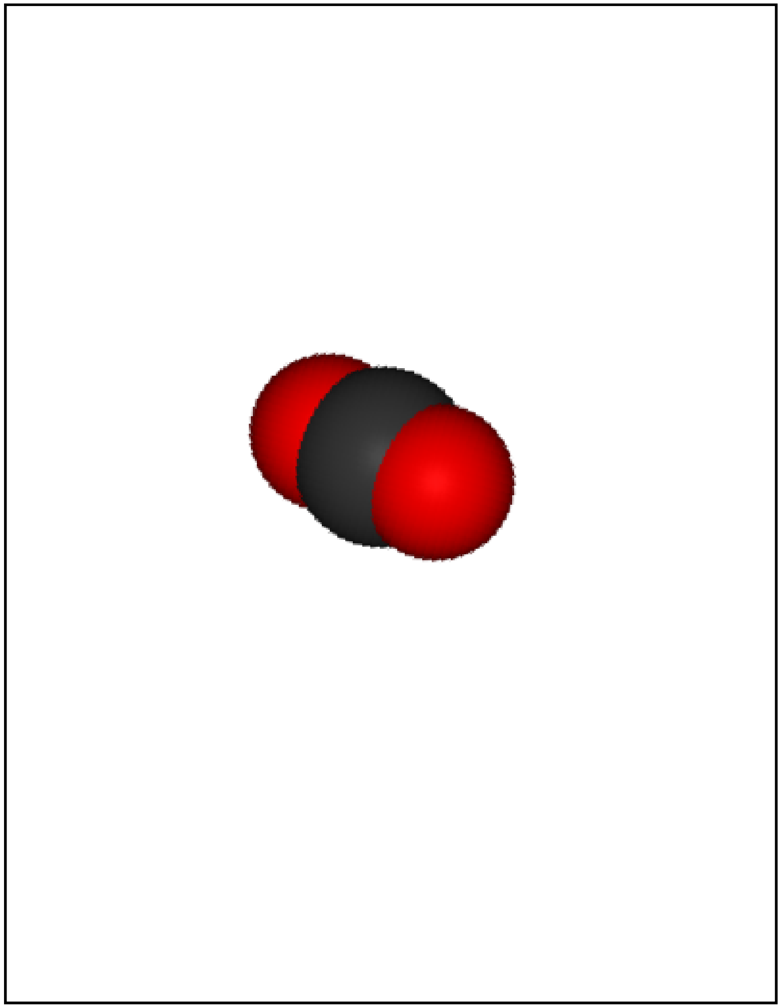




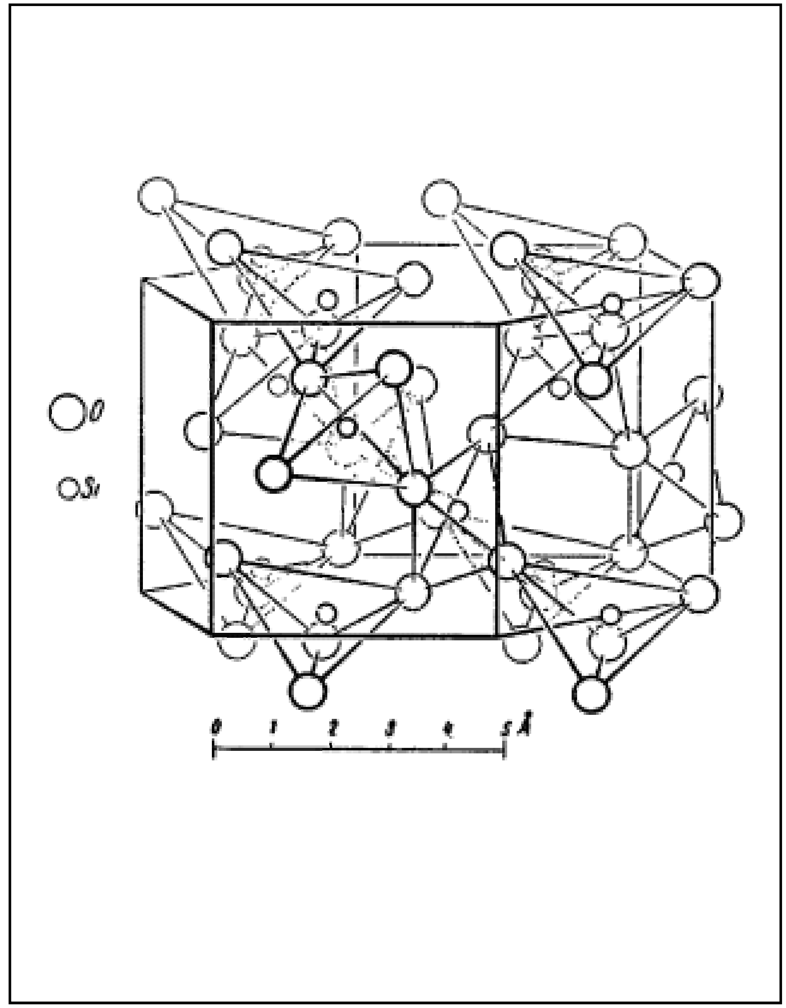
L.R. Benedetti et al., Science 283, 100 (1999)

“Polymeric” CO_2

CO_2

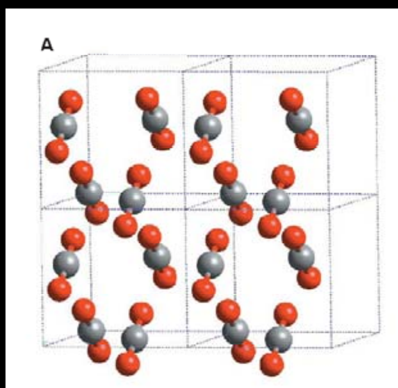


SiO_2



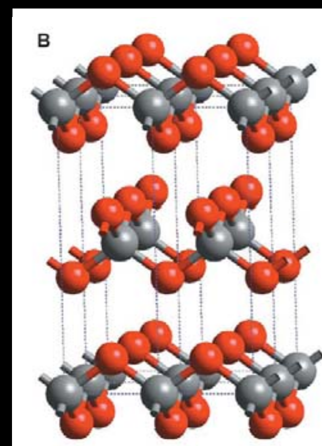
Silica-like CO_2 : the crystal phases

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



Molecular CO_2
(phase III)

1000 K
100 GPa



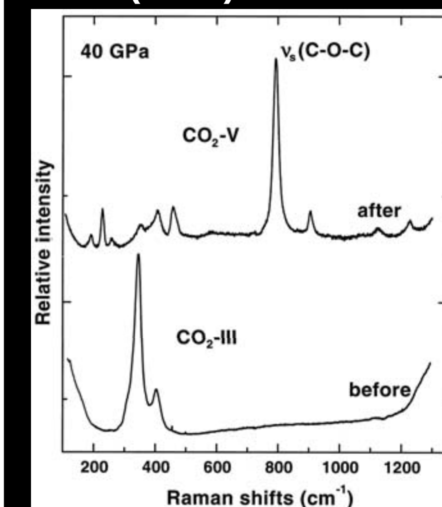
Layered tetrahedral CO_2

+ 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

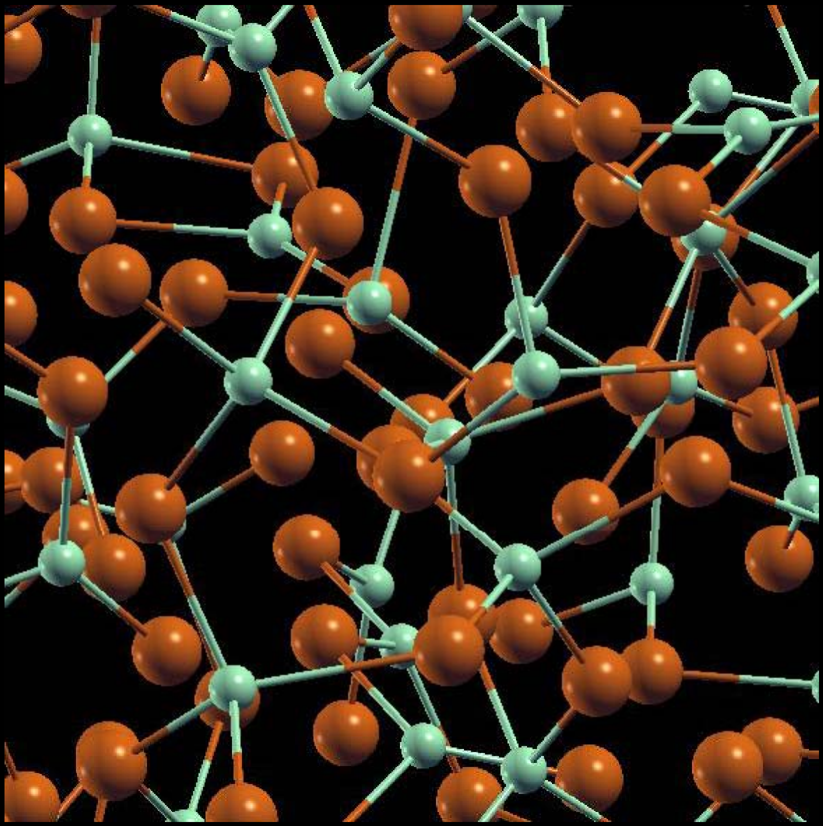
Yoo et al, Science 283, 1510 (1999)



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

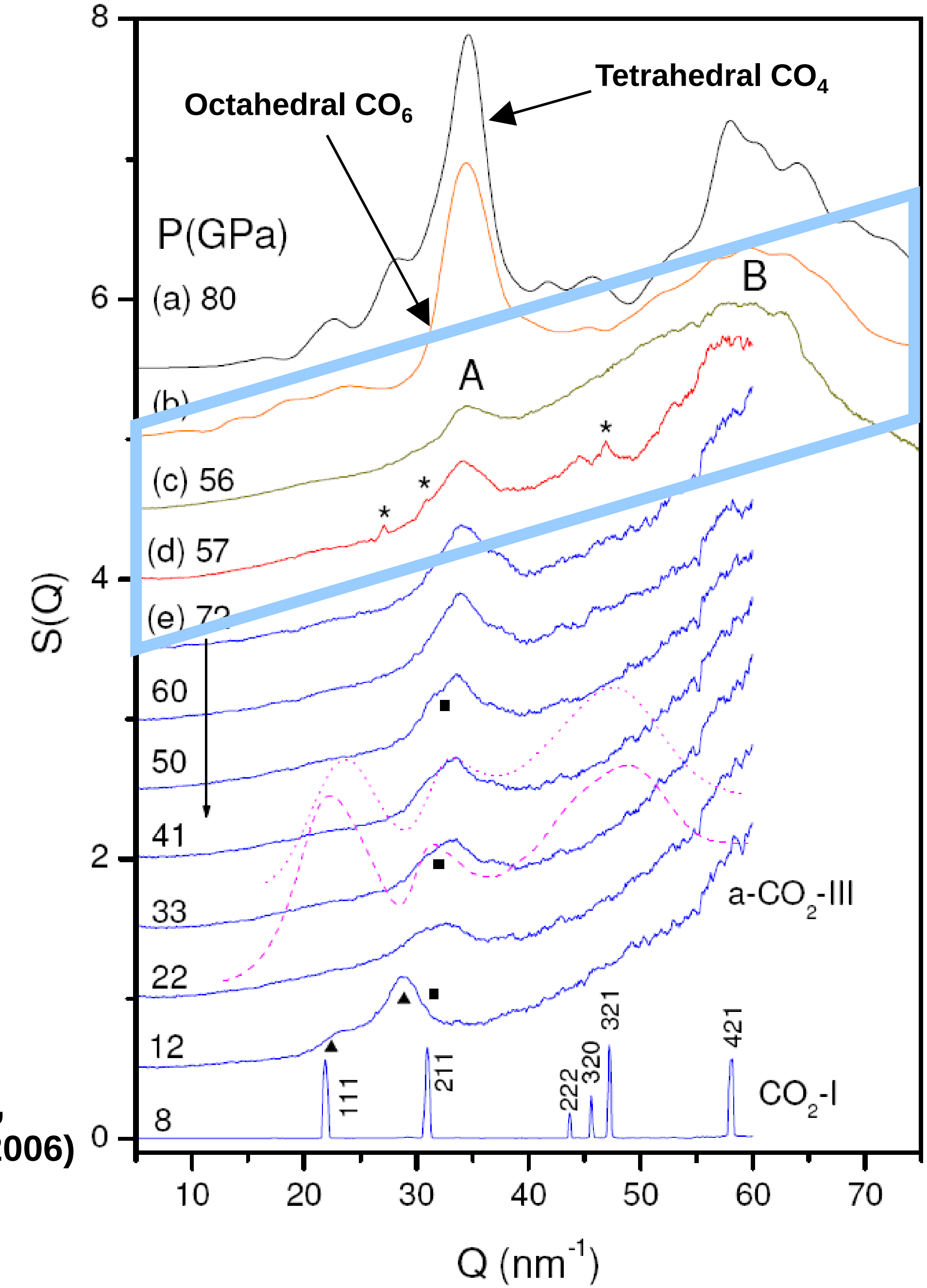
Serra, Cavazzoni, Chiarotti, Scandolo, Tosatti, Science 284, 788 (1999)

Carbonia: silica-like amorphous CO_2

Disappearance of crystalline peaks at ~50 GPa

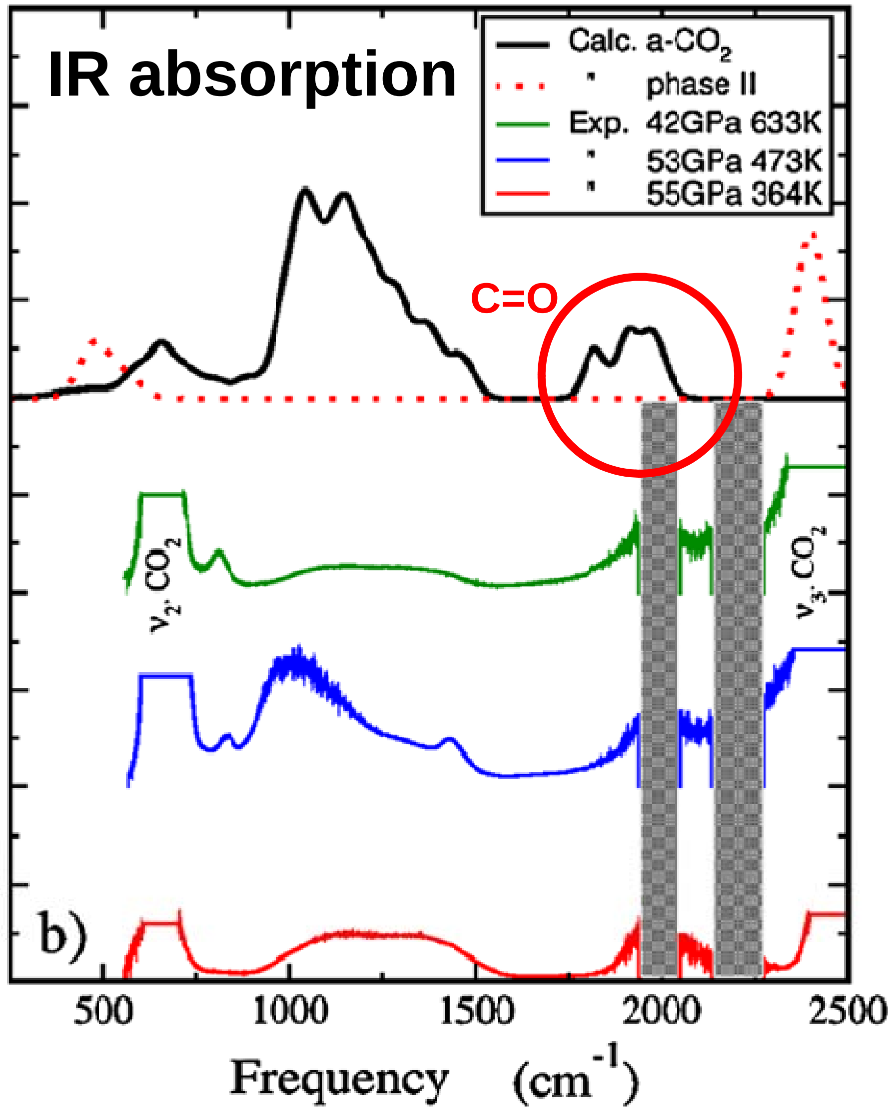
Impossible to distinguish between tetrahedral and octahedral coordination from diffraction

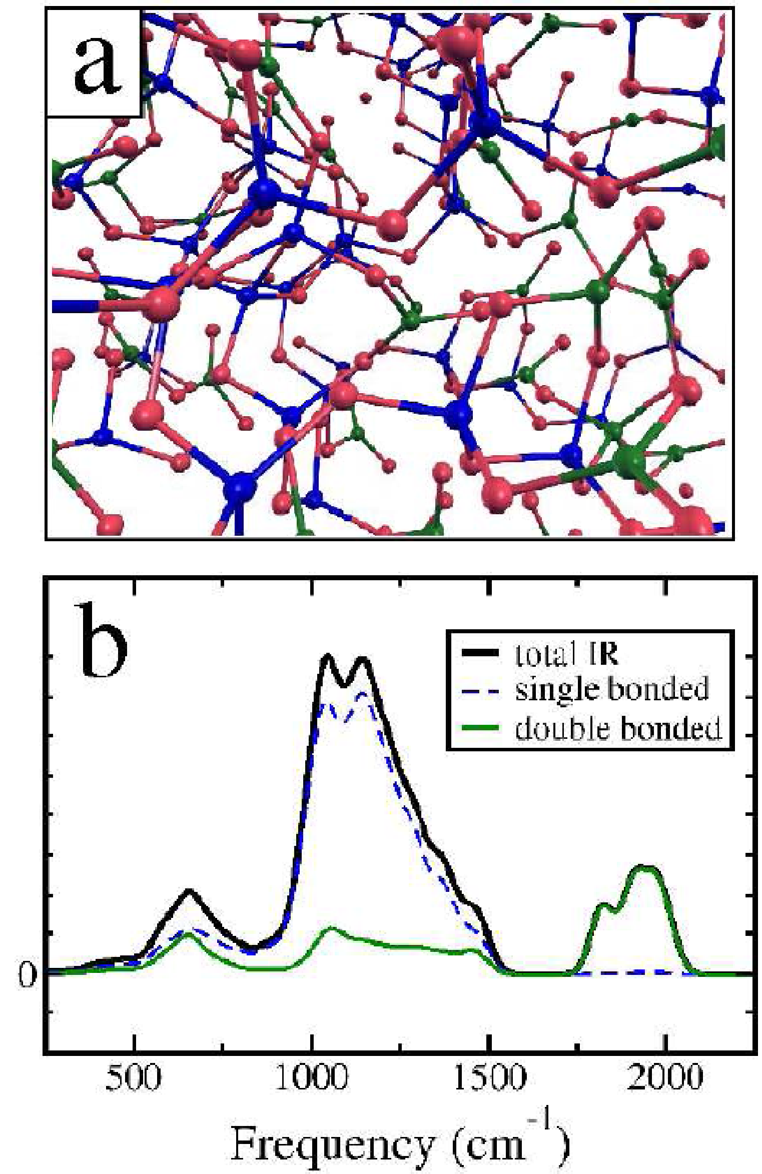
M. Santoro, F. Gorelli, R. Bini, S. Scandolo, G. Ruocco, W. Crichton, Nature 441, 857 (2006)



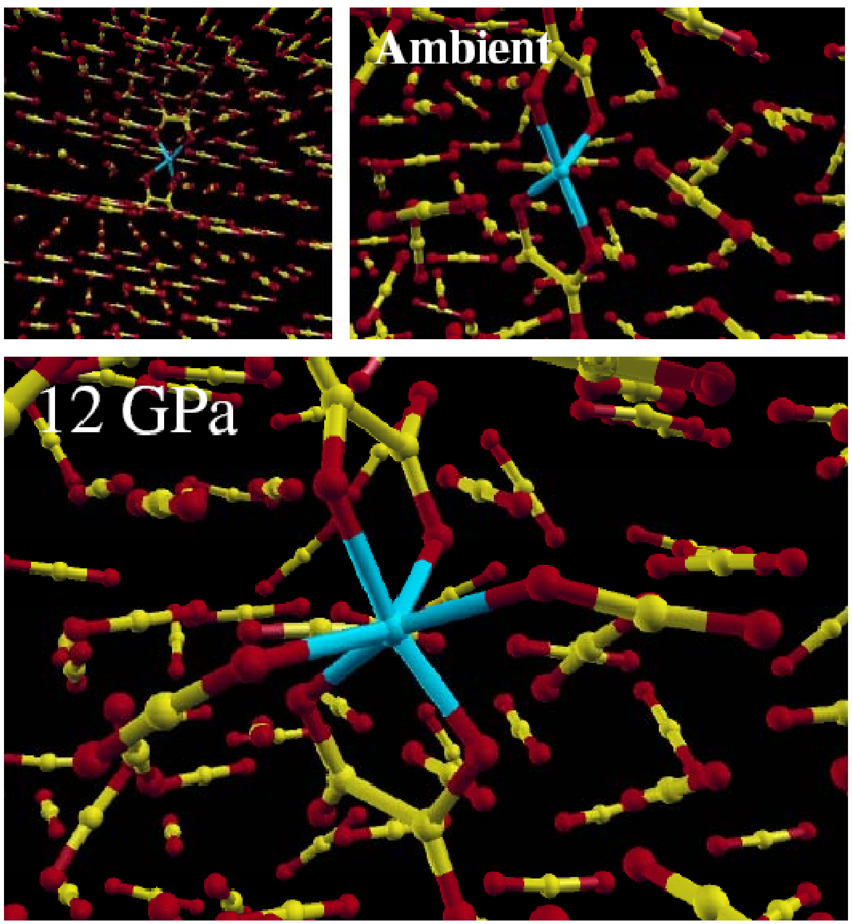
Carbonia: Mixed 3- and 4-fold coordination

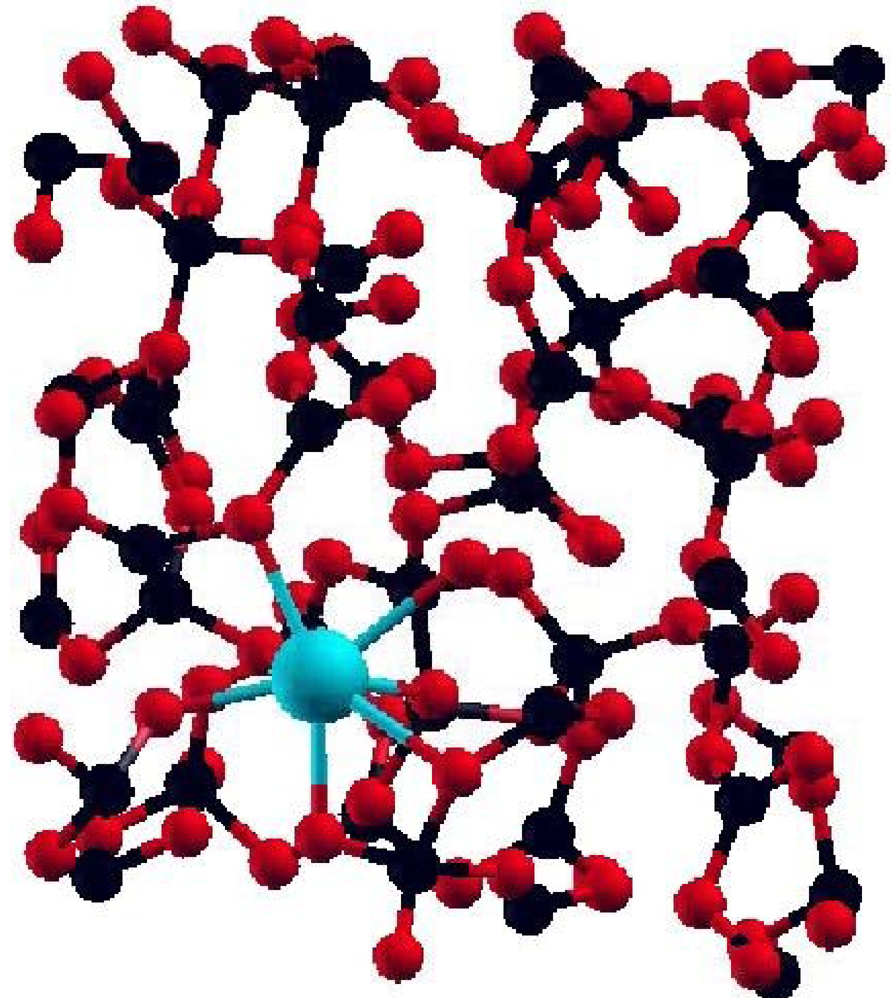
J.A. Montoya, R. Rousseau, M. Santoro, F. Gorelli, S. Scandolo, Phys. Rev. Lett., 100, 163002 (2008)





Can we catalyze the reaction?





Insertion of $Ti(CO_2)_4$ lowers transition pressure and stabilizes carbonia at ambient P

J. Montoya, R. Rousseau, SS, to be published

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.

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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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