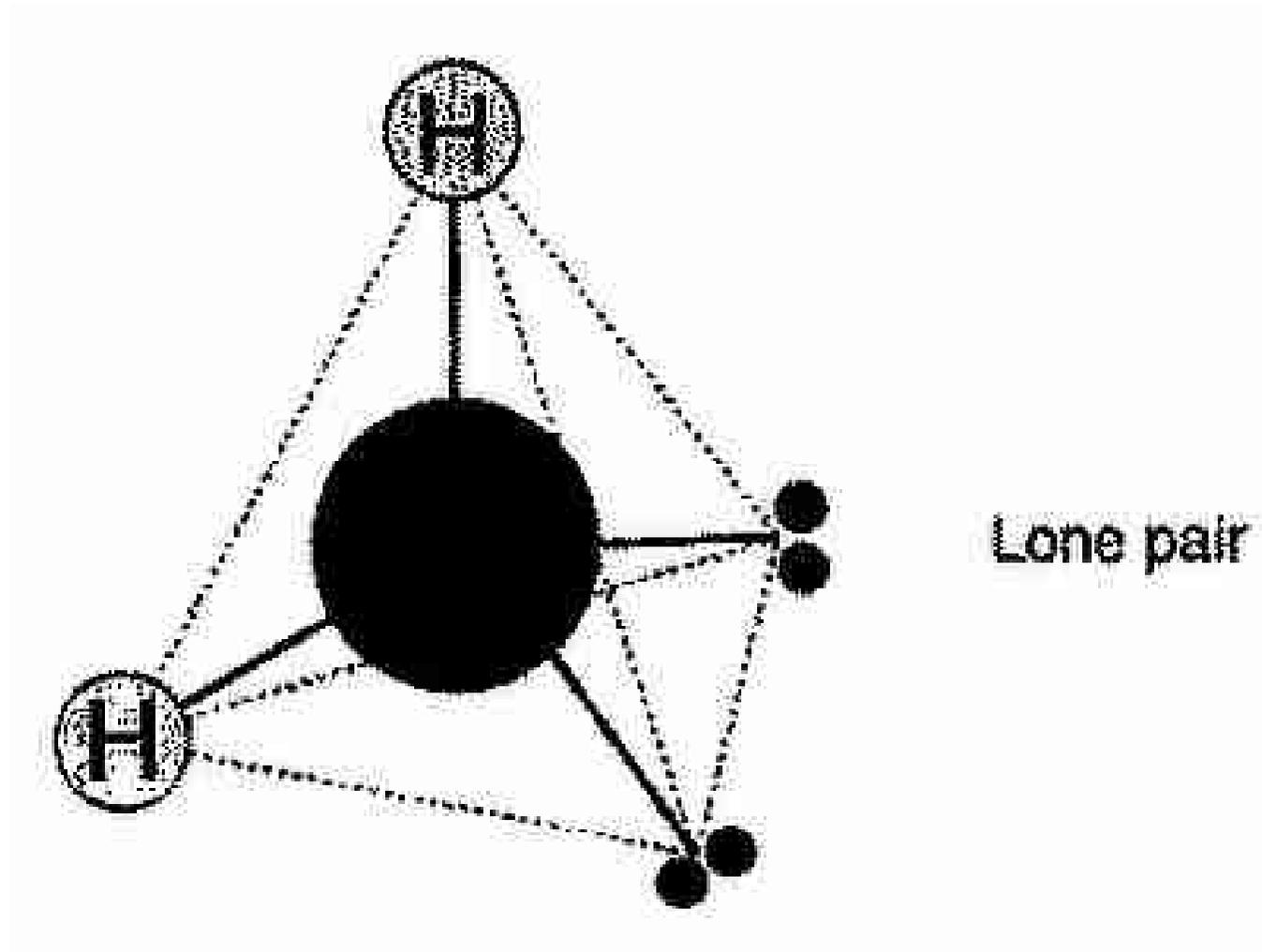


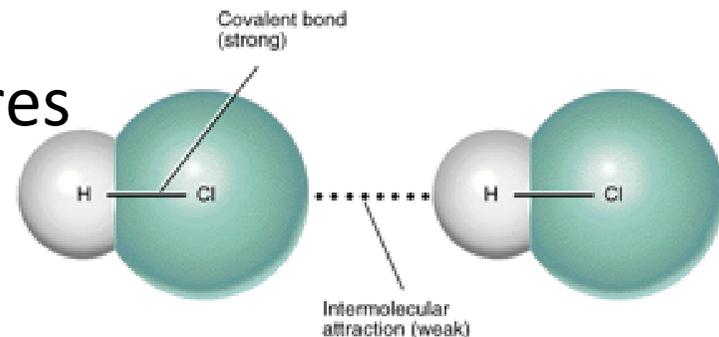
Estrutura molecular e  
supramolecular da água.  
Gelo e clatratos.

# Quatro pontos de conexão



# Interações entre moléculas

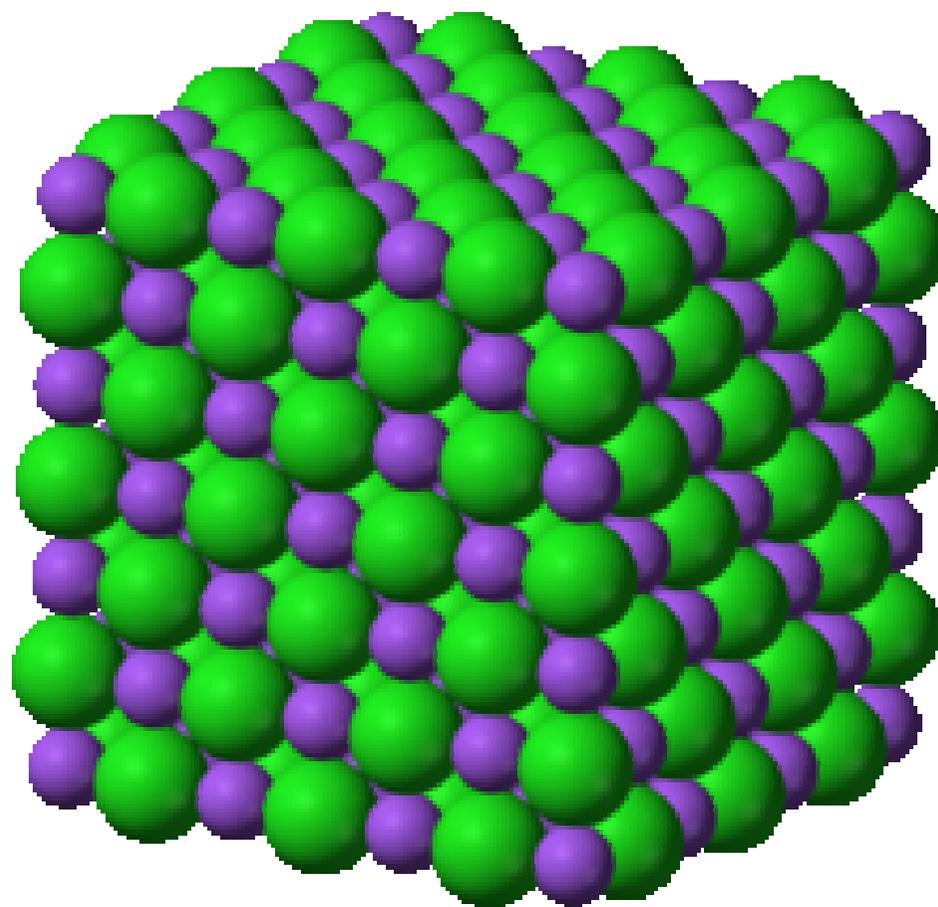
- Átomos em moléculas: forças "químicas", intramoleculares.
  - Muito intensas ( $\sim 100 \text{ kJ mol}^{-1}$ )
  - Pequenas distâncias ( $< 0,1 \text{ nm}$ )
- Força entre moléculas: forças "físicas", intermoleculares.
  - Menos intensas, não permitem grande proximidade.
  - Atuam em distâncias maiores



# Íon – íon (Coulombianas)

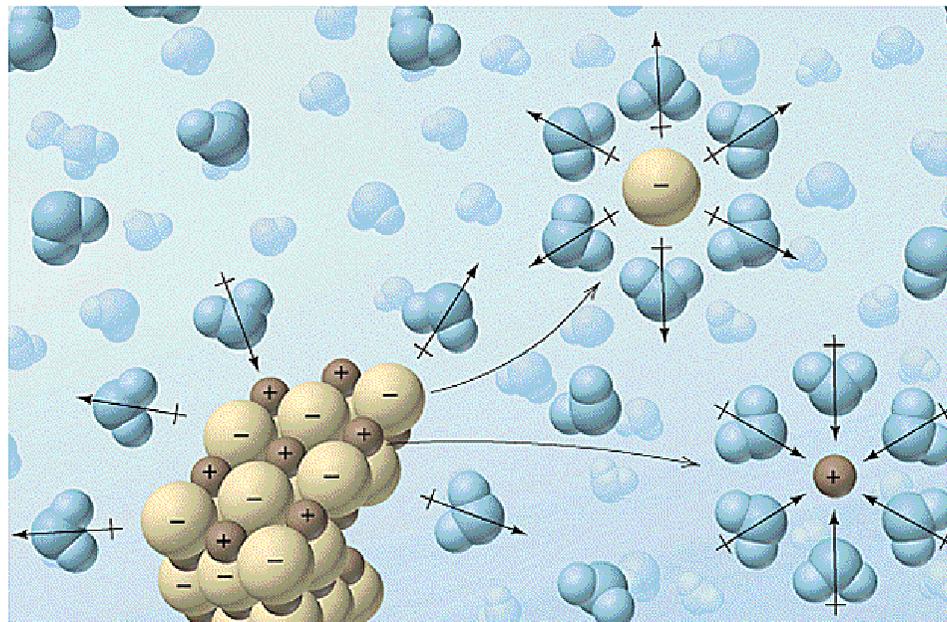
- As forças intermoleculares de maior alcance são as eletrostáticas.
- As interações entre monopolos de cargas são as de máximo alcance.
- Podem ser atrativas (+,+ ou -,-) ou repulsivas (+,-).
- Em cristais: energia de Madelung.
  - Princípio de superposição?

$$U_{ion-ion} = \frac{1}{2} \sum_{I \neq J} \frac{Q_I Q_J}{|\mathbf{R}_I - \mathbf{R}_J|}$$



# Interações íon-dipolo

- Uma molécula neutra (sem carga) pode ter um momento dipolar, resultante da separação de cargas.
- Moléculas que têm um momento dipolar são chamadas de polares.
- Água tem um momento dipolar de 1,85 Debye ( $3.3 \times 10^{-30}$  Coulomb meter).
- Água solvata íons, dissolvendo sais e formando soluções eletrolíticas.

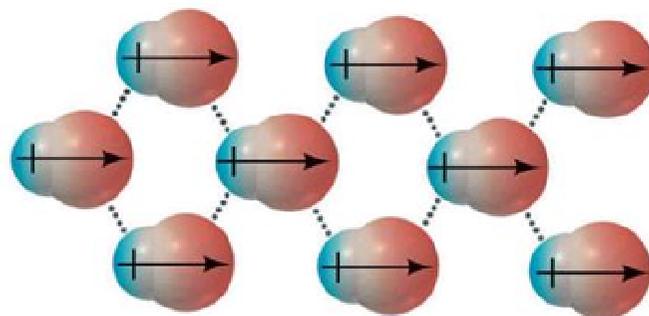
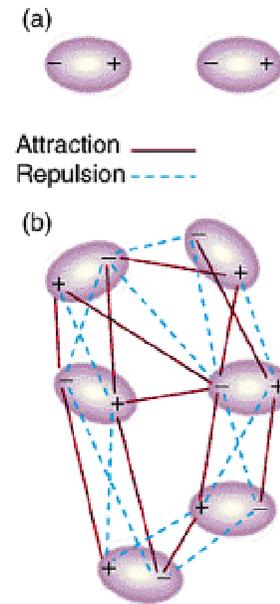


# Orientação

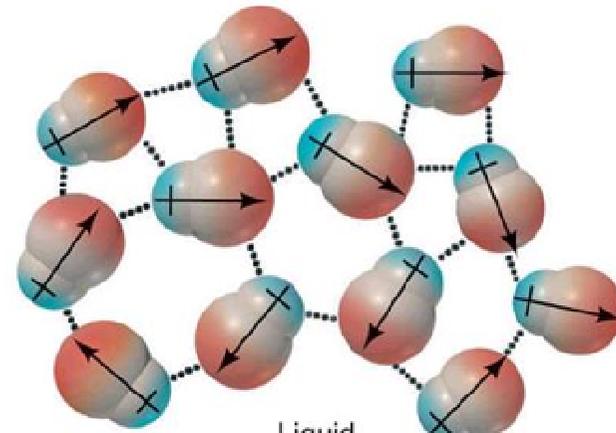
- Calcula-se a energia de interação entre íons e moléculas polares admitindo que estas são formadas por duas cargas separadas, iguais e opostas.
- As forças entre cargas e dipolos dependem da orientação das moléculas.
- As forças podem ser atrativas ou repulsivas, dependendo da orientação.
- Na média, os dipolos orientam-se de maneira a alcançarem um mínimo de energia.
- Configurações repulsivas ocorrer, como flutuações.

# Dipolo-dipolo

- Forças dipolo-dipolo são também calculadas decompondo cada dipolo em duas cargas iguais e opostas e somando o resultado das interações entre cargas.



Solid

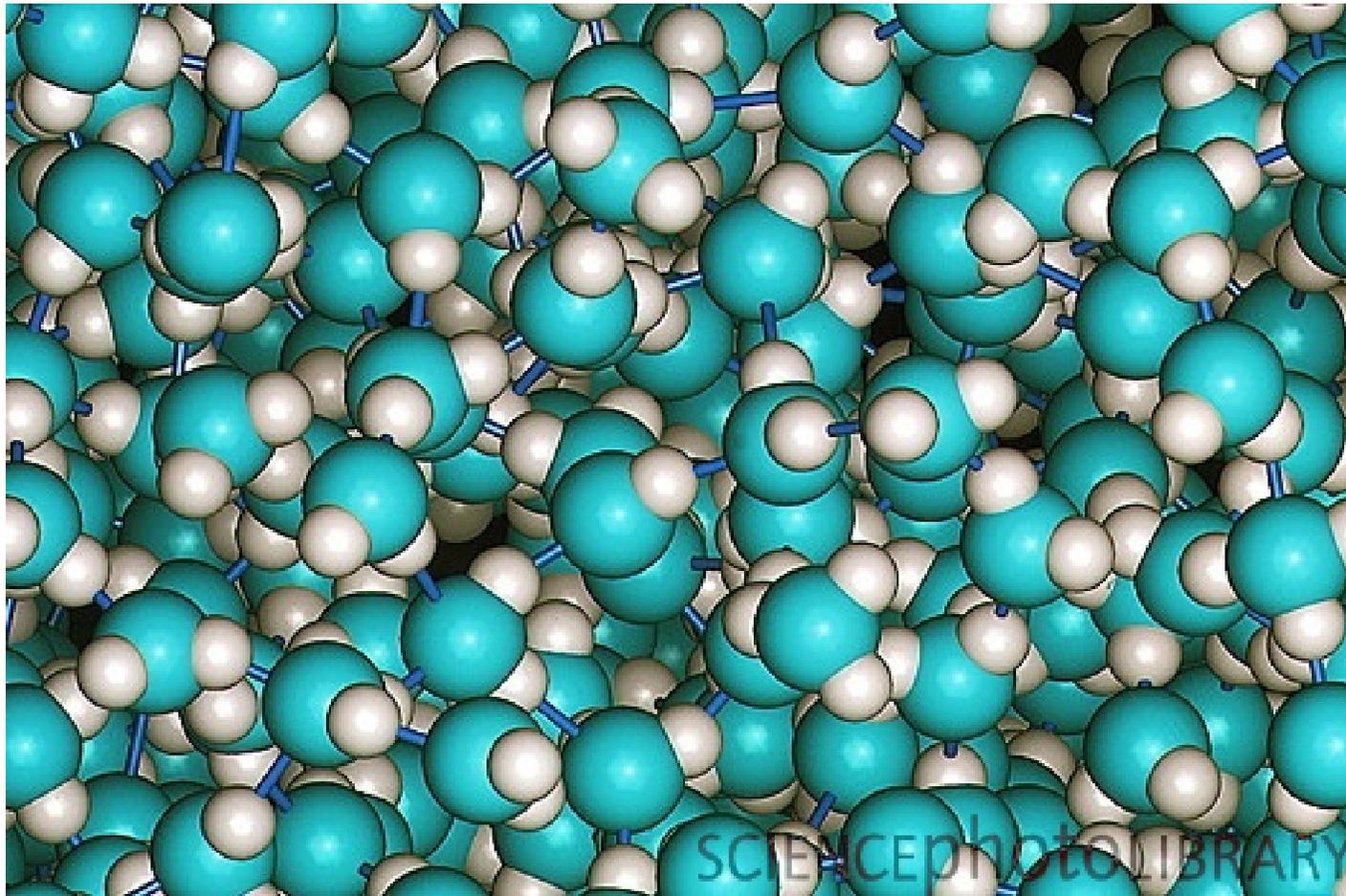


Liquid

# Efeito de interações dipolo-dipolo

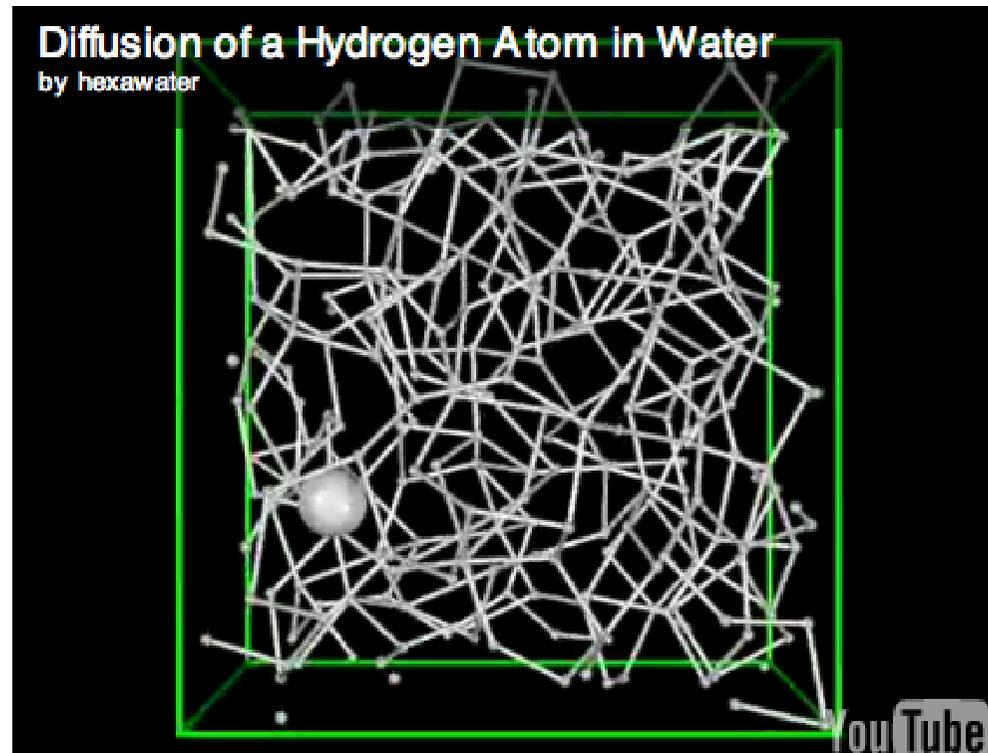
Substância	Massa molar [g/mol]	Momento dipolar [Debye]	Ponto de ebulição normal [ K ]
Propano	44	0,1	231
Éter dimetílico	46	1,3	248
Clorometano	50	2,0	249
Acetaldeído	44	2,7	294
Acetonitrila	41	3,9	355

# Água: forte associação



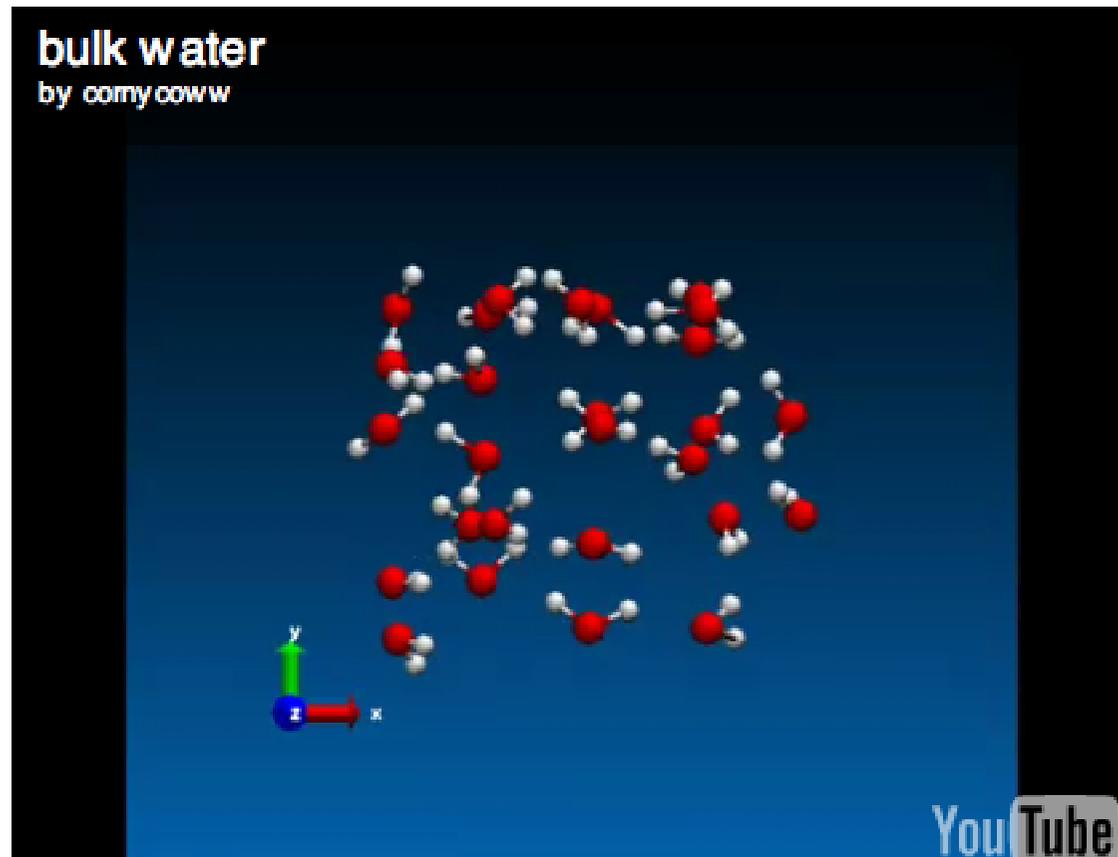
# Difusão de átomo de hidrogênio

- [http://www.theallined.com/video/diffusion-hydrogen-atom-water/B944o4m3Rp4&feature=youtube\\_gdata/](http://www.theallined.com/video/diffusion-hydrogen-atom-water/B944o4m3Rp4&feature=youtube_gdata/)

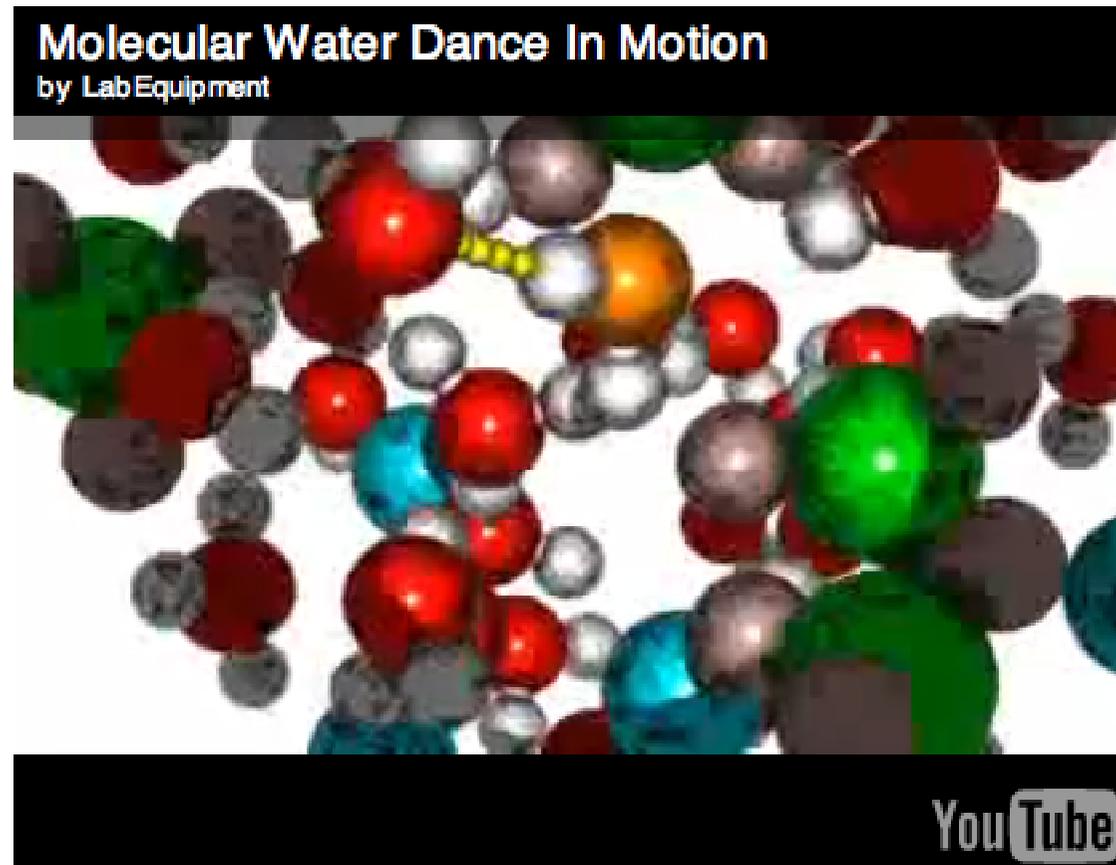


# Associação e dissociação

- [http://www.theallined.com/video/bulk-water-/CeRLggic5I0&feature=youtu\\_be\\_gdata/](http://www.theallined.com/video/bulk-water-/CeRLggic5I0&feature=youtu_be_gdata/)

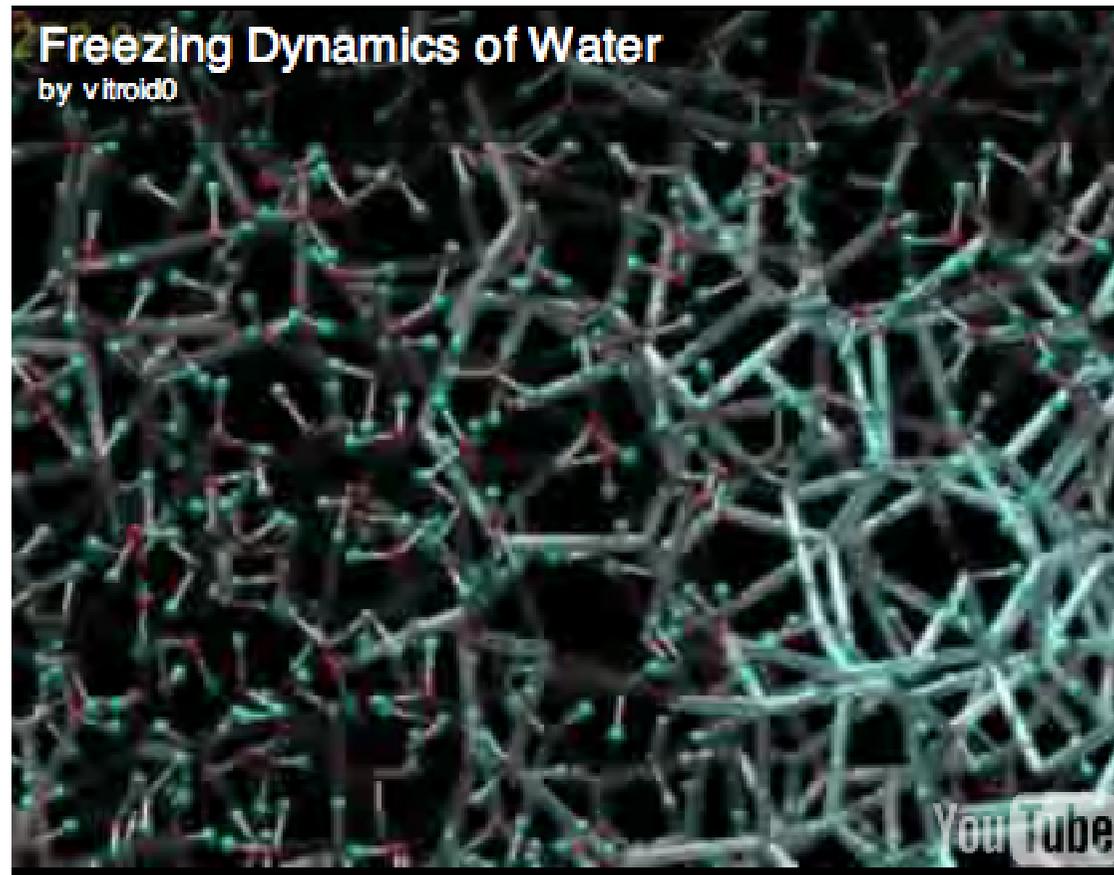


- [http://www.theallined.com/video/molecular-water-dance-motion/cThvGD-o\\_90&feature=youtu\\_gdata/](http://www.theallined.com/video/molecular-water-dance-motion/cThvGD-o_90&feature=youtu_gdata/)

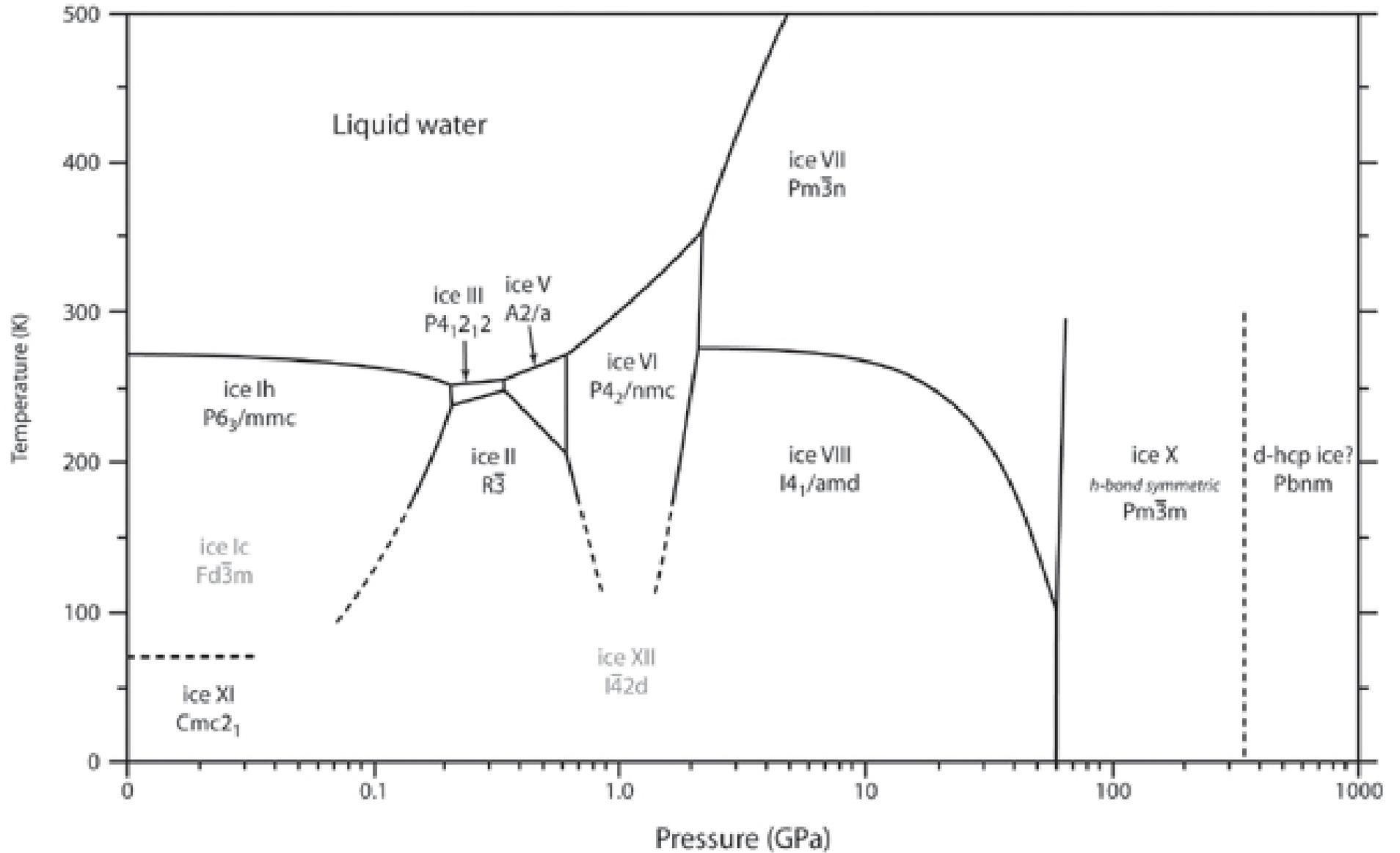


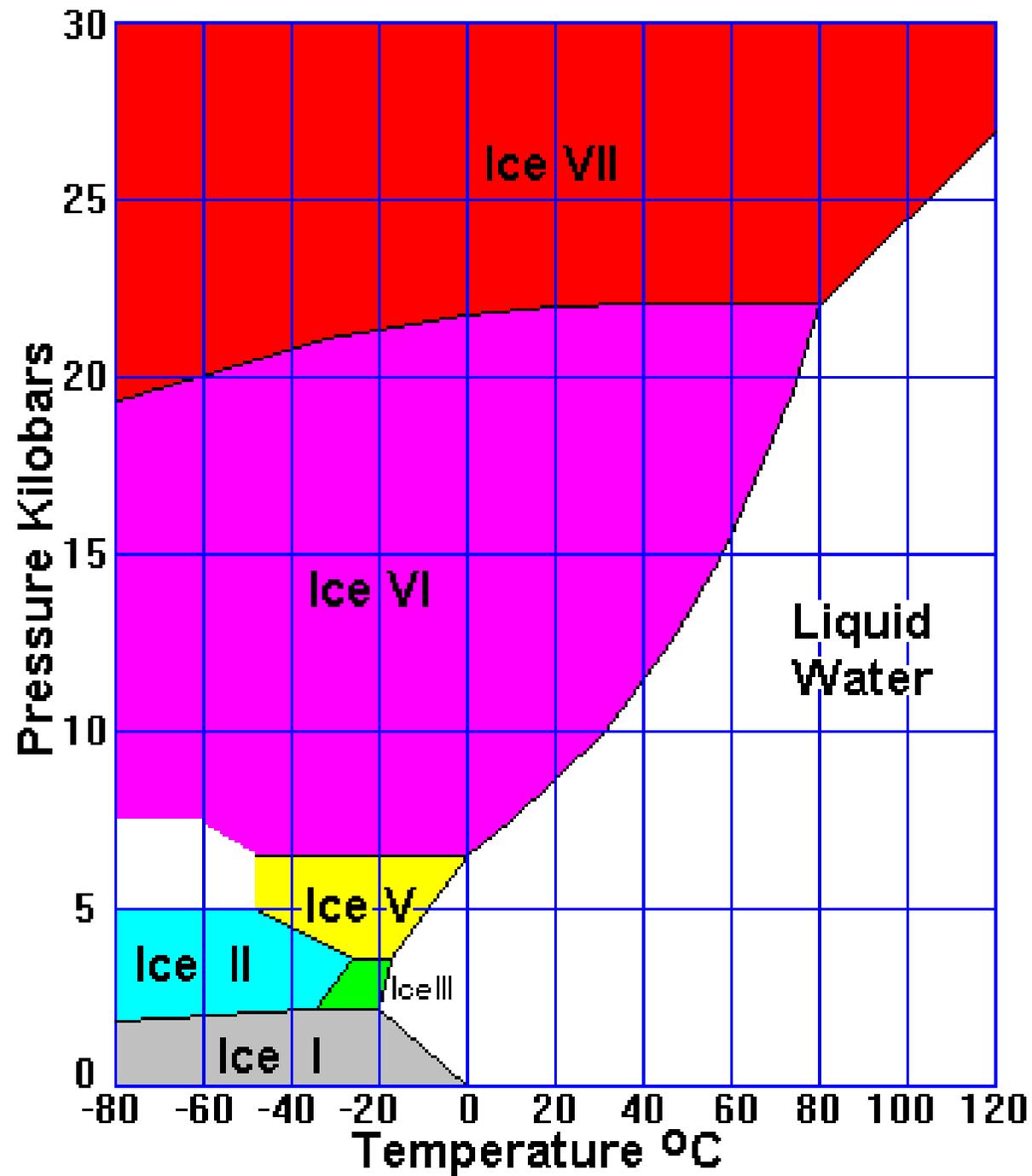
# Dinâmica de congelamento

- [http://www.theallined.com/video/molecular-water-dance-motion/cThvGD-o\\_90&feature=youtube\\_gdata/](http://www.theallined.com/video/molecular-water-dance-motion/cThvGD-o_90&feature=youtube_gdata/)



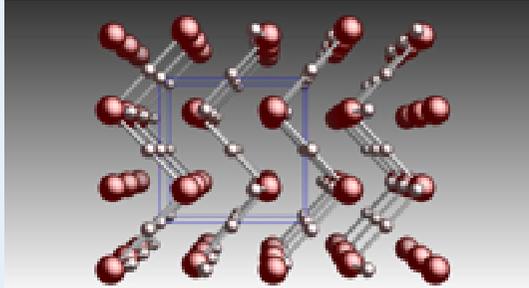
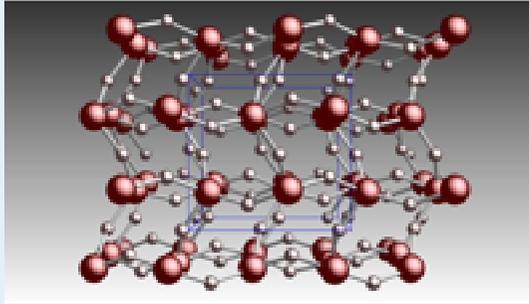
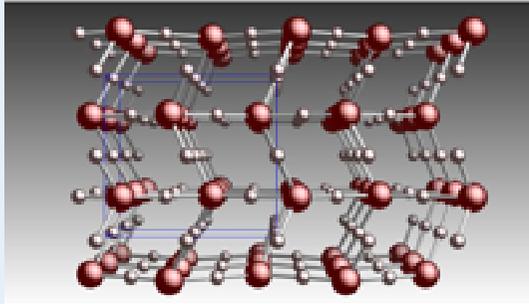
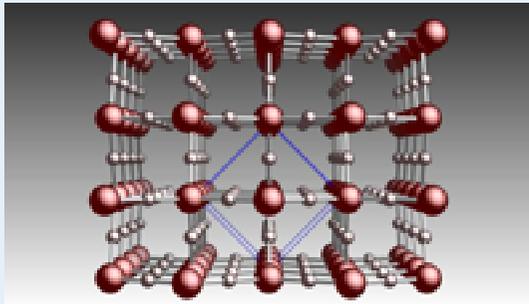
# Muitos gelos





## EPS Research Spotlight Archive

### DEC 2010 - Simulations predict water ice to become a metal at megabar pressures

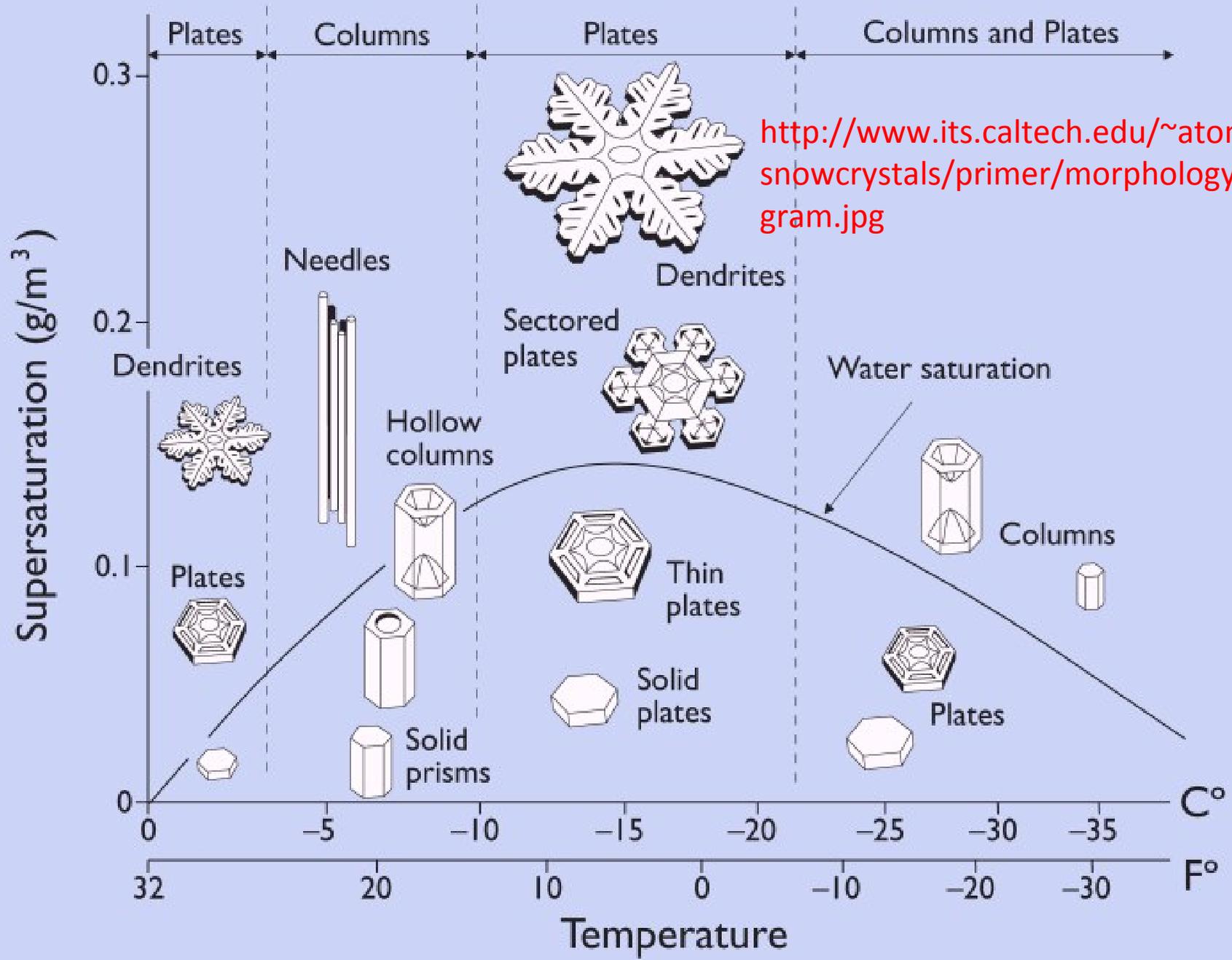


Water ice is one of the most prevalent substances in the solar system, with the majority of it existing at high pressures in the interiors of giant planets. The known phase diagram of water is extremely rich, with at least fifteen crystal phases observed experimentally. In our [article](#) in *Physical Review Letters* (see also [cond-mat](#)), Hugh Wilson and I ([Burkhard Militzer](#)) explore the phase diagram of water ice by means of *ab initio* computer simulations and predict two new phases to occur at megabar pressures. In the figure from top to bottom, you see

- 1) ice X the highest pressure phase seen in experiments,
- 2) the *Pbcm* phase that was predicted with computer simulations in 1996,
- 3) our new *PbcA* phase that transforms out of the *Pbcm* phase via a phonon instability at 7.6 Mbar, and finally
- 4) our new *Cmcm* structure that is metallic and predicted to occur at 15.5 Mbar.

The known high pressure ice phases VII, VIII, X and *Pbcmas* well as our *PbcA* phase are all insulating and composed of two interpenetrating hydrogen bonded networks, but the *Cmcm* structure is metallic and consists of corrugated sheets of H and O atoms. The H atoms are squeezed into octahedral positions between next-nearest O atoms while they occupy tetrahedral positions between nearest O atoms in the ice X, *Pbcm*, and *PbcA* phases.

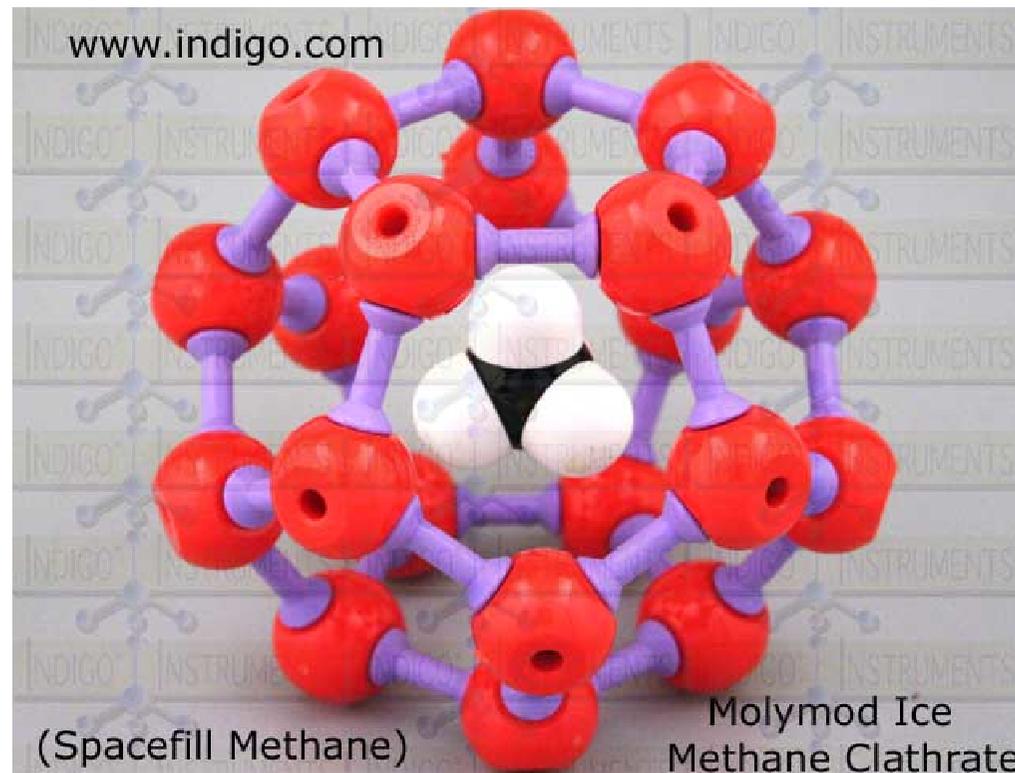
[http://eps.berkeley.edu/research/spotlight\\_list.php](http://eps.berkeley.edu/research/spotlight_list.php)



<http://www.its.caltech.edu/~atomic/snowcrystals/primer/morphologydiagram.jpg>

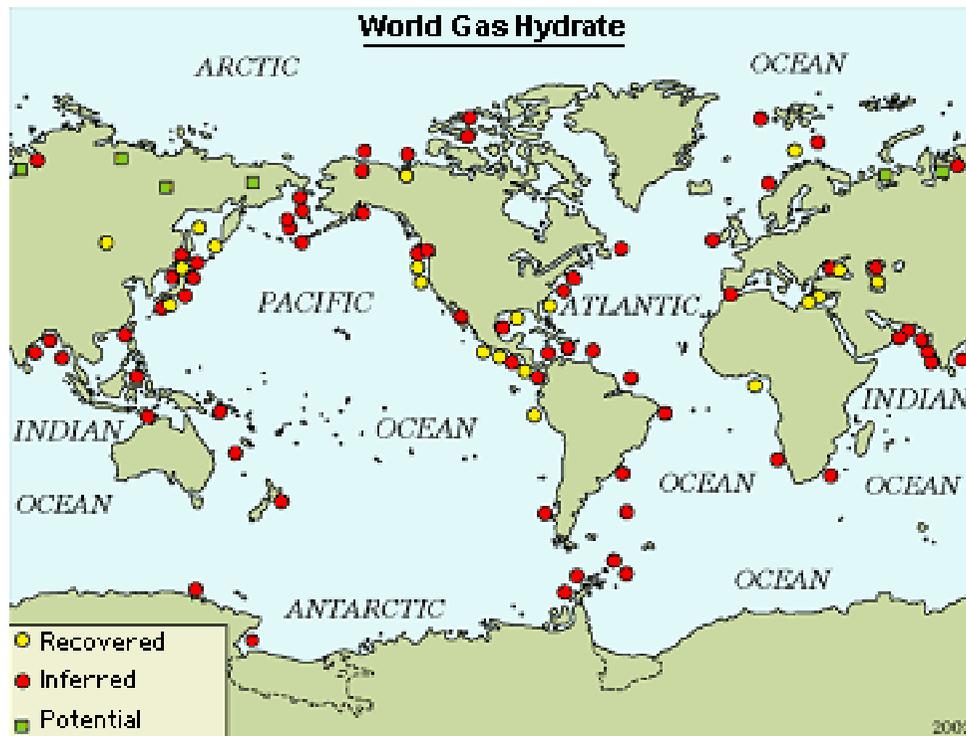
# Clatrato de metano

- <http://www.indigo.com/models/gphmodel/molymod-hydrate-methane-clathrate-structure.html>



# Ocorrências de clatratos de metano

- [http://www.geologyinmotion.com/2010\\_06\\_01\\_archive.html](http://www.geologyinmotion.com/2010_06_01_archive.html)



# Resultado controverso: estruturas duráveis, de Emoto

- [http://www.theallined.com/video/messages-water-/mIPQSeKHh0E&feature=youtube\\_gdata/](http://www.theallined.com/video/messages-water-/mIPQSeKHh0E&feature=youtube_gdata/)
- "The James Randi Educational Foundation has a standing offer to Emoto since 2003 to give him 1 million U.S. dollars if he can demonstrate his claims with a double blind procedure. Emoto has not responded to the offer."



Love

Demon



# Exercícios

- Compare, quantitativamente, a viscosidade e a densidade da água líquida à de três outros líquidos, à sua escolha. Procure explicar as diferenças observadas.
- Calcule a temperatura de equilíbrio entre água e gelo a 1 kbar. Em um ambiente de indústria química, onde se encontra pressões dessa ordem?
- Faça uma estimativa da diferença de densidades entre as formas II e V do gelo.