# FÍSICA EM CASA

outreach.ictp-saifr.org

ICTP SAIFR
International Centre for Theoretical Physics
South American Institute for Fundamental Research

FAPESP ICTP unesp IFT - UNESP PERIMETER INSTITUTE

@ictpsaifr

FÍSICA EM CASA

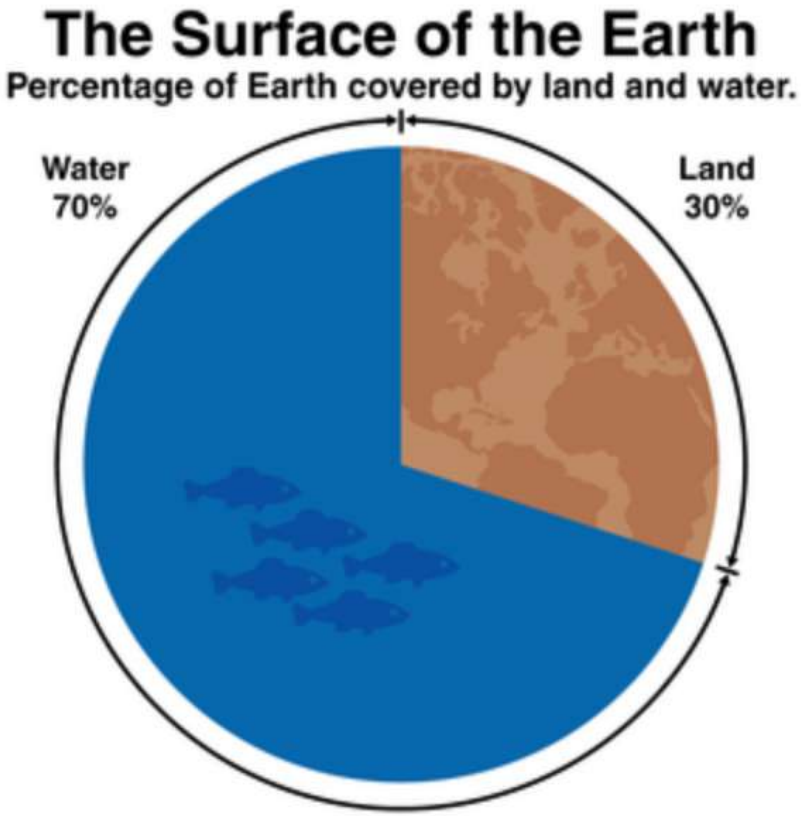
outreach.ictp-saifr.org

# DENTRO DO COPO DE ÁGUA

Luana Pedroza
CCNH - UFABC
l.pedroza@ufabc.edu.br

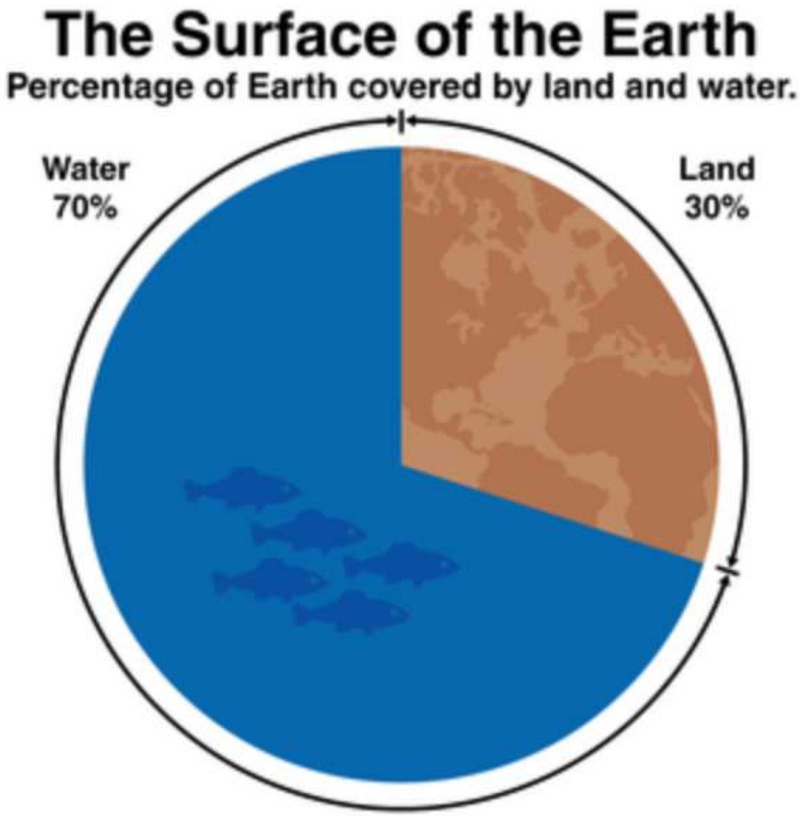
UFABC FAPESP

# PLANETA ÁGUA ?




Superfície da Terra
70% água

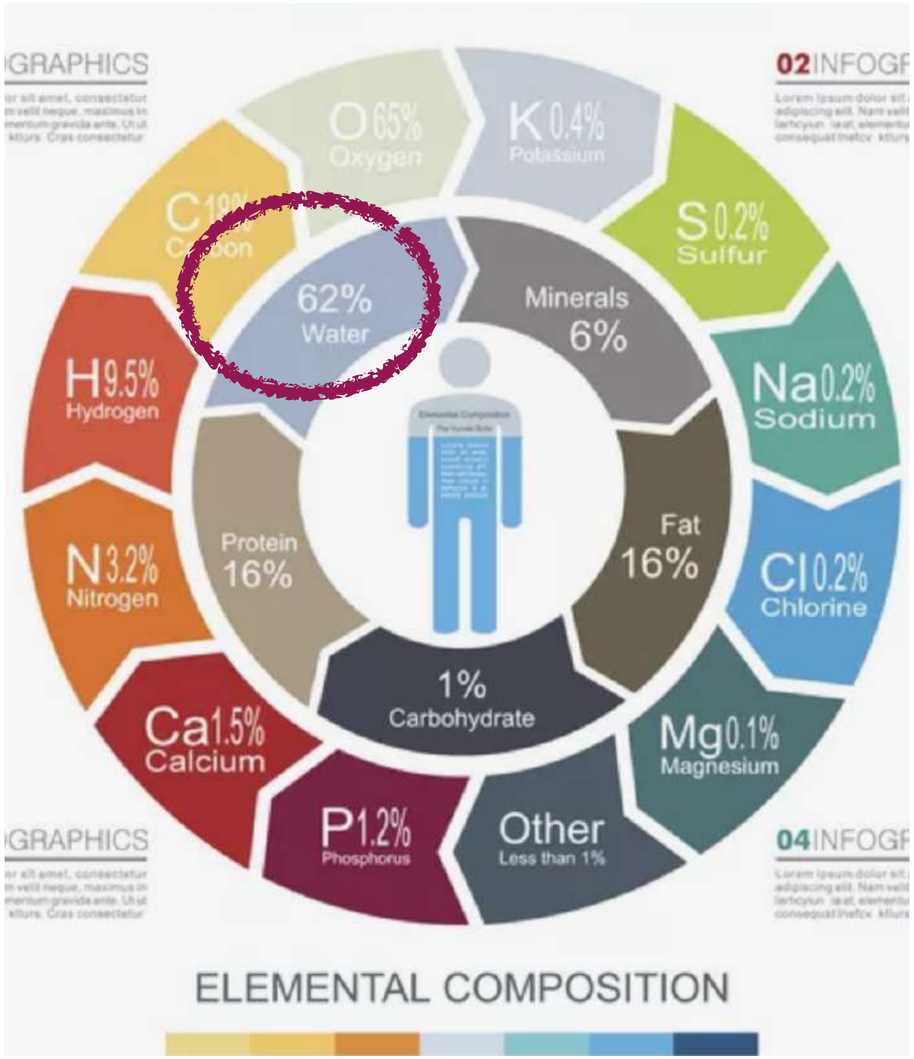
# PLANETA ÁGUA ?




Superfície da Terra
70% água

# CORPO HUMANO

62% água



# LÍQUIDO SIMPLES...

$H_2O$

# LÍQUIDO SIMPLES...

# LÍQUIDO SIMPLES...

# MAS NEM TANTO!

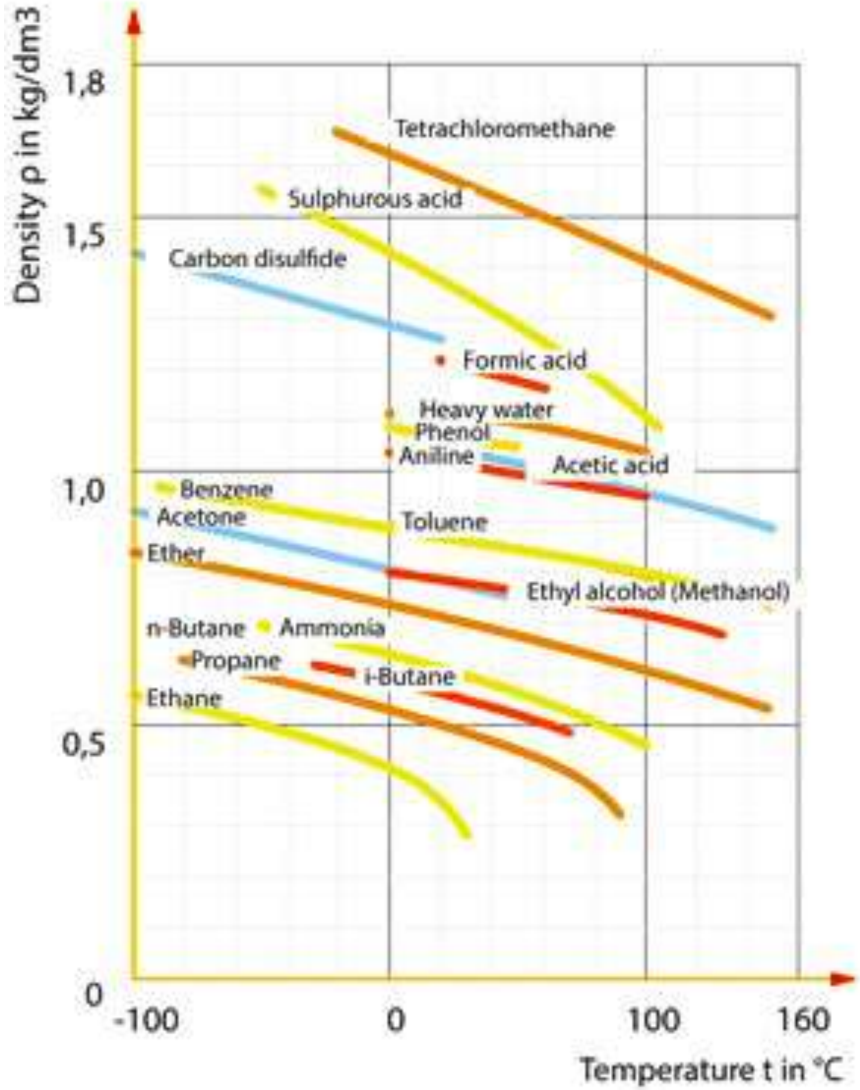
# LÍQUIDO SIMPLES...

ESSENCIAL PARA A VIDA

# MAS NEM TANTO!

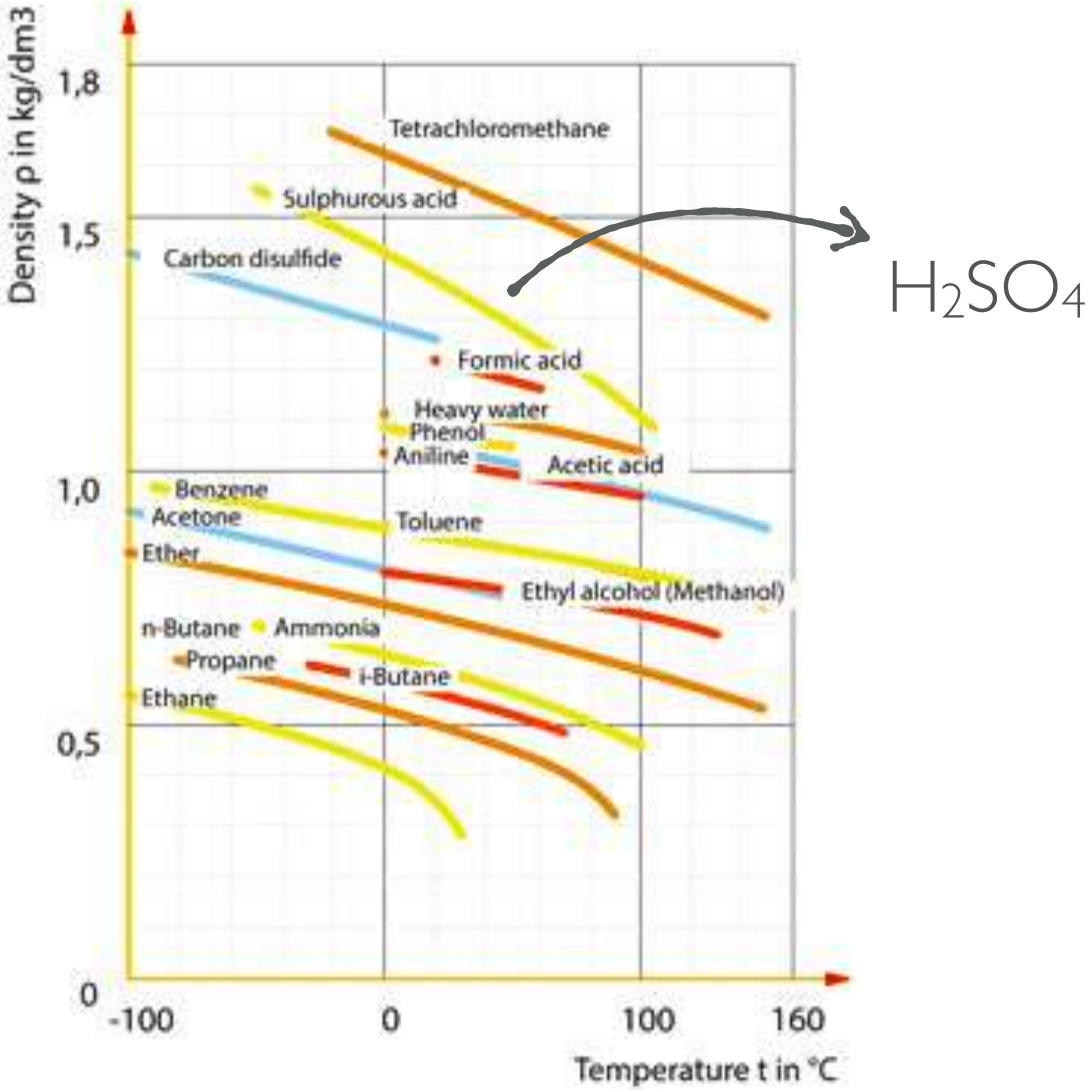
# ANOMALIAS DA ÁGUA

- Densidade em função da temperatura



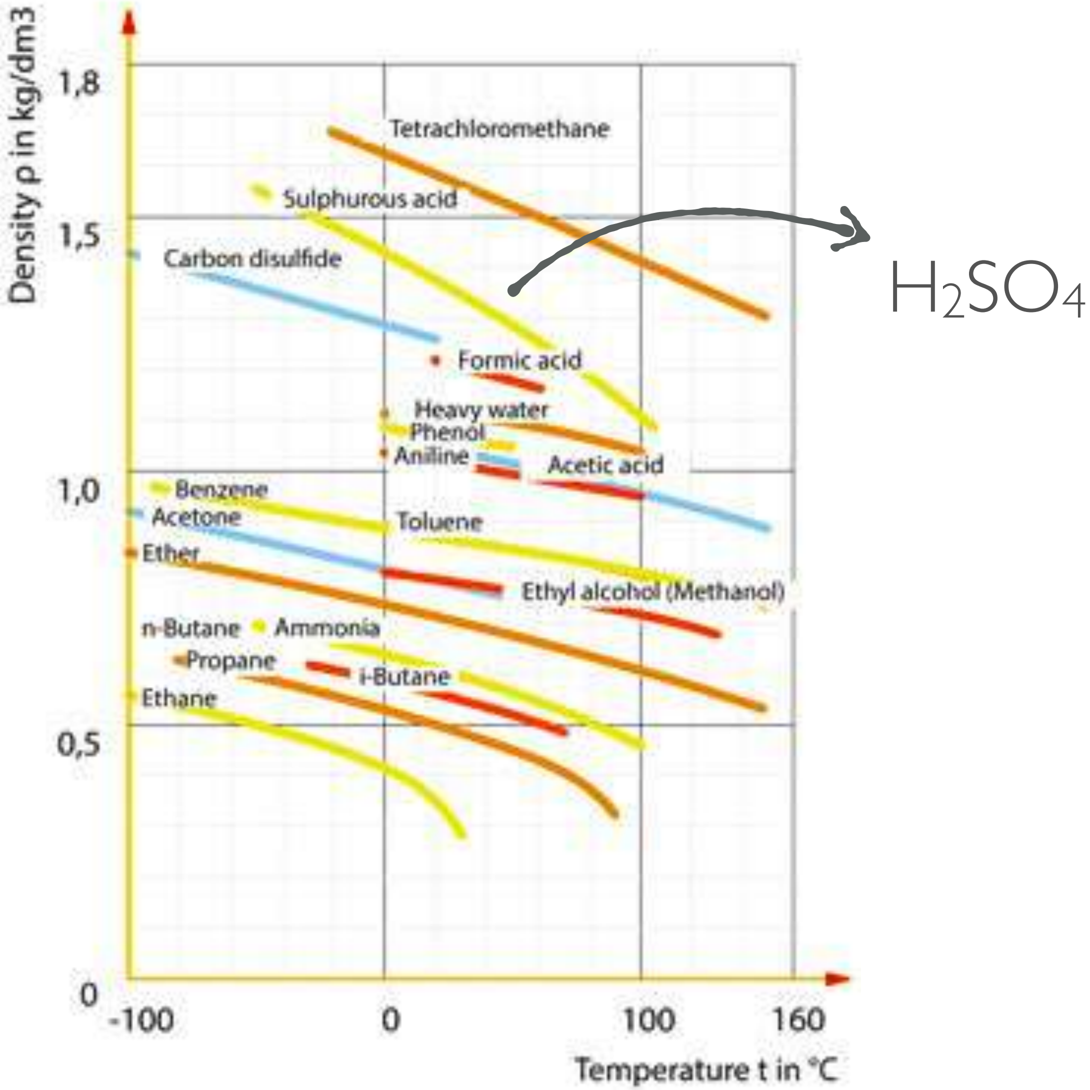
# ANOMALIAS DA ÁGUA

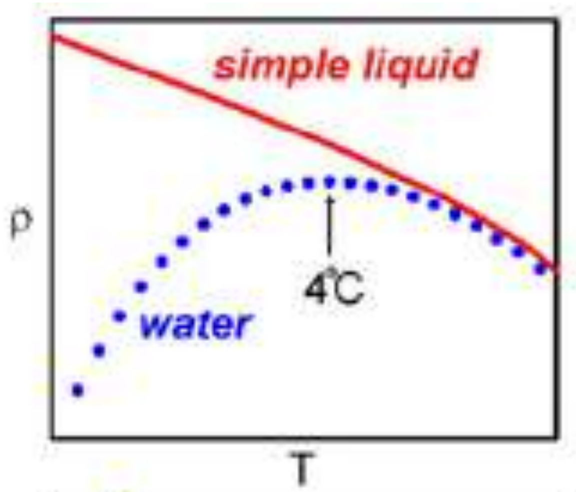
- Densidade em função da temperatura



# ANOMALIAS DA ÁGUA

- Densidade em função da temperatura

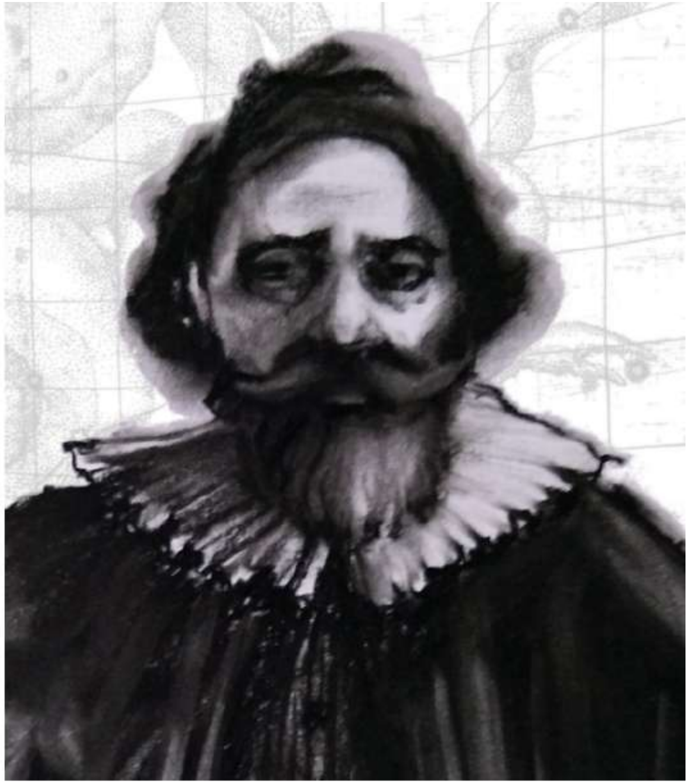


# ANOMALIAS DA ÁGUA

Galileo

×



Ludovico delle Colombe

1611

# ANOMALIAS DA ÁGUA

PHYSIOGRAPHERS lead us to believe that the earth is defended from a profound glaciation, cumulative from year to year, by the law that water is heaviest at a temperature of four degrees above centigrade zero. If the main cause lies here, it is desirable that this measure should have its peculiar power set forth with more precision than has been customary.

W. B. Croft

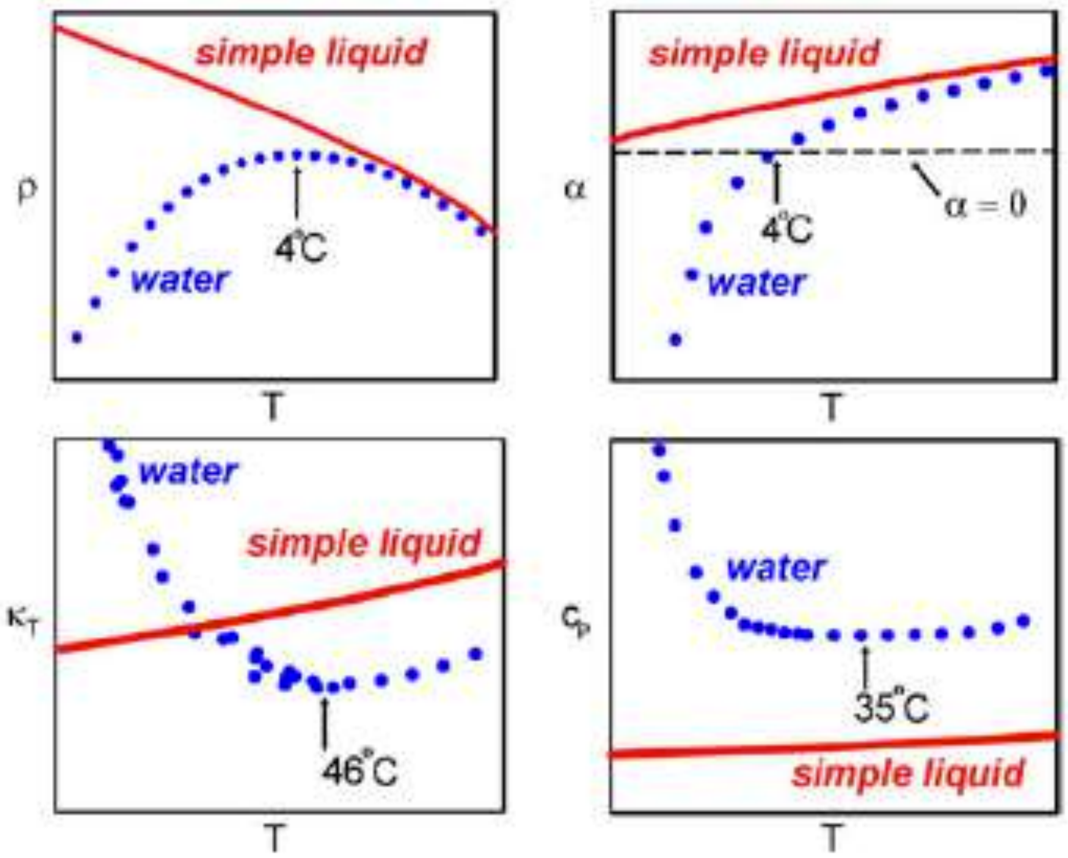
**The Maximum Density of Water.**

I FEAR Mr. W. B. Croft will get few to agree with him in supposing that it would make little difference in the conditions existing on the earth whether water was at its maximum density at $0^{\circ}$ or at $4^{\circ}$ above it (NATURE, July 17). If water was densest at $0^{\circ}$ there would be little surface ice, as water does not change to ice at $0^{\circ}$ unless in the presence of ice crystals or other solids. The ice-cold water would therefore, after sinking, freeze when it came in contact with the solid bottom, and we would have much anchor ice and but little on the surface. The small margin of only $4^{\circ}$ does not seem to be quite enough entirely to prevent anchor ice; still we have reason to be thankful for these few degrees.

JOHN AITKEN.

Nature, 1913

# ANOMALIAS DA ÁGUA




Propriedades da água são distintas das esperadas, comparadas com outros substâncias

# ANOMALIAS DA ÁGUA

**Water phase anomalies** [d]

1. Water has an unusually high melting point. [Explanation]
2. Water has an unusually high boiling point. [Explanation]
3. Water has an unusually high critical point. [Explanation]
4. Solid water exists in a wider variety of stable (and metastable) crystal and amorphous structures than othe materials. [Explanation]
5. The thermal conductivity, shear modulus and transverse sound velocity of ice reduce with increasing press [Explanation]
6. The structure of liquid water changes at high pressure. [Explanation]
7. Supercooled water has two phases and a second critical point at about -91 °C. [Explanation]
8. Liquid water is easily supercooled but glassified with difficulty. [Explanation]
9. Liquid water exists at very low temperatures and freezes on heating. [Explanation]
10. Liquid water may be easily superheated. [Explanation]
11. Hot water may freeze faster than cold water; the Mpemba effect. [Explanation]
12. Warm water vibrates longer than cold water. [Explanation]
13. Water molecules shrink as the temperature rises and expand as the pressure increases. [Explanation]

http://www1.lsbu.ac.uk/water/water_anomalies.html#bi

# ANOMALIAS DA ÁGUA

**Water phase anomalies** d

1. Water has an unusually high melting point. [Explanation]
2. Water has an unusually high boiling point. [Explanation]
3. Water has an unusually high critical point. [Explanation]
4. Solid water exists in a wider variety of stable (and metastable) cryst materials. [Explanation]
5. The thermal conductivity, shear modulus and transverse sound velo [Explanation]
6. The structure of liquid water changes at high pressure. [Explanatior
7. Supercooled water has two phases and a second critical point at ab
8. Liquid water is easily supercooled but glassified with difficulty. [Expl
9. Liquid water exists at very low temperatures and freezes on heating
10. Liquid water may be easily superheated. [Explanation]
11. Hot water may freeze faster than cold water; the Mpemba effect. [E
12. Warm water vibrates longer than cold water. [Explanation]
13. Water molecules shrink as the temperature rises and expand as the

**Water material anomalies**

1. No aqueous solution is ideal. [Explanation]
2. $D_2O$ and $T_2O$ differ significantly from $H_2O$ in their physical properties. [Explanation]
3. Liquid $H_2O$ and $D_2O$ differ significantly in their phase behavior. [Explanation]
4. $H_2O$ and $D_2O$ ices differ significantly in their quantum behavior. [Explanation]
5. The mean kinetic energy of water's hydrogen atoms increases at low temperature (disputed). [Explanation]
6. Solutes have varying effects on properties such as density and viscosity. [Explanation]
7. The solubilities of non-polar gases in water decrease with temperature to a minimum and then rise. [Explanation]
8. The dielectric constant of water and ice are high. [Explanation]
9. The relative permittivity shows a temperature maximum. [Explanation]
10. The relative permittivity shows a 'kink' in its behavior with the temperature at 60 °C. [Explanation]
11. The imaginary part of the dielectric constant shows a minimum near 20 K. [Explanation]
12. Proton and hydroxide ion mobilities are anomalously fast in an electric field. [Explanation]
13. The electrical conductivity of water rises to a maximum at about 230 °C. [Explanation]
14. The electrical conductivity of water rises considerably with frequency. [Explanation]
15. Acidity constants of weak acids show temperature minima. [Explanation]
16. X-ray diffraction shows an unusually detailed structure. [Explanation]
17. Under high pressure water molecules move further away from each other with increasing pressure; a density-distance paradox. [Explanation]
18. Water adsorption may cause negative electrical resistance. [Explanation]

http://www1.lsbu.ac.uk/water/water_anomalies.html#bi

# ANOMALIAS DA ÁGUA

### Water phase anomalies [d]

1. Water has an unusually high melting point. [Explanation]
2. Water has an unusually high boiling point. [Explanation]
3. Water has an unusually high critical point. [Explanation]
4. Solid water exists in a wider variety of stable (and metastable) cryst materials. [Explanation]
5. The thermal conductivity, shear modulus and transverse sound velo [Explanation]
6. The structure of liquid water changes at high pressure. [Explanatior
7. Supercooled water has two phases and a second critical point at ab
8. Liquid water is easily supercooled but glassified with difficulty. [Expl
9. Liquid water exists at very low temperatures and freezes on heating
10. Liquid water may be easily superheated. [Explanation]
11. Hot water may freeze faster than cold water; the Mpemba effect. [E
12. Warm water vibrates longer than cold water. [Explanation]
13. Water molecules shrink as the temperature rises and expand as the

### Water material anomalies

1. No aqueous solution is ideal. [Explanation]
2. $D_2O$ and $T_2O$ differ significantly from $H_2O$ in their physical properties. [Explanation]
3. Liquid $H_2O$ and $D_2O$ differ significantly in their phase behavior. [Explanation]
4. $H_2O$ and $D_2O$ ices differ significantly in their quantum behavior. [Explanation]
5. The mean kinetic energy of water's hydrogen atoms increases at low temperature (disputed). [Explanation]
6. Solutes have varying effects on properties such as density and viscosity. [Explanation]
7. The solubilities of non-polar gases in water decrease with temperature to a minimum and then rise. [Explanation]
8. The dielectric constant of water and ice are high. [Explanation]
9. The relative permittivity shows a temperature maximum. [Explanation]
10. The relative permittivity shows a 'kink' in its behavior with the temperature at 60 °C. [Explanation]
11. The imaginary part of the dielectric constant shows a minimum near 20 K. [Explanation]
12. Proton and hydroxide ion mobilities are anomalously fast in an electric field. [Explanation]
13. The electrical conductivity of water rises to a maximum at about 230 °C. [Explanation]
14. The electrical conductivity of water rises considerably with frequency. [Explanation]
15. Acidity constants of weak acids show temperature minima. [Explanation]
16. X-ray diffraction shows an unusually detailed structure. [Explanation]
17. Under high pressure water molecules move further away from each other with increasing pressure; a density-distance paradox. [Explanation]
18. Water adsorption may cause negative electrical resistance. [Explanation]

### Water density anomalies

1. The density of ice increases on heating (up to 70 K). [Explanation]
2. Water shrinks on melting. [Explanation]
3. Pressure reduces ice's melting point. [Explanation]
4. Liquid water has a high-density that increases on heating (up to 3.984 °C). [Explanation]
5. The surface of water is denser than the bulk. [Explanation]
6. Pressure reduces the temperature of maximum density. [Explanation]
7. There is a minimum in the density of supercooled water. [Explanation]
8. Water has a low coefficient of expansion (thermal expansivity). [Explanation]
9. Water's thermal expansivity reduces increasingly (becoming negative) at low temperatures. [Expla
10. Water's thermal expansivity increases with increased pressure. [Explanation]
11. The number of nearest neighbors increases on melting. [Explanation]
12. The number of nearest neighbors increases with temperature. [Explanation]
13. Water has unusually low compressibility. [Explanation]
14. The compressibility drops as temperature increases up to 46.5 °C. [Explanation]
15. There is a maximum in the compressibility-temperature relationship. [Explanation]
16. The speed of sound increases with temperature up to 74 °C. [Explanation]
17. The speed of sound may show a minimum. [Explanation]
18. 'Fast sound' is found at high frequencies and shows a discontinuity at higher pressure. [Explanatio
19. NMR spin-lattice relaxation time is very small at low temperatures. [Explanation]
20. The NMR shift increases to a maximum at low (supercooled) temperatures [Explanation]
21. The refractive index of water has a maximum value
22. The change in volume as liquid changes to gas is v... larger [Explanation]

**http://www1.lsbu.ac.uk/water/water_anomalies.html#bi**

# ANOMALIAS DA ÁGUA

### Water phase anomalies [d]

1. Water has an unusually high melting point. [Explanation]
2. Water has an unusually high boiling point. [Explanation]
3. Water has an unusually high critical point. [Explanation]
4. Solid water exists in a wider variety of stable (and metastable) cryst materials. [Explanation]
5. The thermal conductivity, shear modulus and transverse sound velo [Explanation]
6. The structure of liquid water changes at high pressure. [Explanatior
7. Supercooled water has two phases and a second critical point at ab
8. Liquid water is easily supercooled but glassified with difficulty. [Expl
9. Liquid water exists at very low temperatures and freezes on heating
10. Liquid water may be easily superheated. [Explanation]
11. Hot water may freeze faster than cold water; the Mpemba effect. [E
12. Warm water vibrates longer than cold water. [Explanation]
13. Water molecules shrink as the temperature rises and expand as the

### Water material anomalies

1. No aqueous solution is ideal. [Explanation]
2. $D_2O$ and $T_2O$ differ significantly from $H_2O$ in their physical properties. [Explanation]
3. Liquid $H_2O$ and $D_2O$ differ significantly in their phase behavior. [Explanation]
4. $H_2O$ and $D_2O$ ices differ significantly in their quantum behavior. [Explanation]
5. The mean kinetic energy of water's hydrogen atoms increases at low temperature (disputed). [Explanation]
6. Solutes have varying effects on properties such as density and viscosity. [Explanation]
7. The solubilities of non-polar gases in water decrease with temperature to a minimum and then rise. [Explanation]
8. The dielectric constant of water and ice are high. [Explanation]
9. The relative permittivity shows a temperature maximum. [Explanation]
10. The relative permittivity shows a 'kink' in its behavior with the temperature at 60 °C. [Explanation]
11. The imaginary part of the dielectric constant shows a minimum near 20 K. [Explanation]
12. Proton and hydroxide ion mobilities are anomalously fast in an electric field. [Explanation]
13. The electrical conductivity of water rises to a maximum at about 230 °C. [Explanation]
14. The electrical conductivity of water rises considerably with frequency. [Explanation]
15. Acidity constants of weak acids show temperature minima. [Explanation]
16. X-ray diffraction shows an unusually detailed structure. [Explanation]
17. Under high pressure water molecules move further away from each other with increasing pressure; a density-distance paradox. [Explanation]
18. Water adsorption may cause negative electrical resistance. [Explanation]

### Water density anomalies

1. The density of ice increases on heating (up to 70 K). [Explanation]
2. Water shrinks on melting. [Explanation]
3. Pressure reduces ice's melting point. [Explanation]
4. Liquid water has a high-density that increases on heating (up to 3.984 °C). [Explanation]
5. The surface of water is denser than the bulk. [Explanation]
6. Pressure reduces the temperature of maximum density. [Explanation]
7. There is a r
8. Water has a
9. Water's the
10. Water's the
11. The numbe
12. The numbe
13. Water has u
14. The compre
15. There is a r
16. The speed o
17. The speed o
18. 'Fast sound'
19. NMR spin-la
20. The NMR sh
21. The refracti
22. The change

### Water physical anomalies

1. Water has unusually high viscosity. [Explanation]
2. Large viscosity and Prandtl number increase as the temperature is lowered. [Explanation]
3. Water's viscosity decreases with pressure below 33 °C. [Explanation]
4. Large diffusion decrease as the temperature is lowered. [Explanation]
5. At low temperatures, the self-diffusion of water increases as the density and pressure increase. [
6. The thermal diffusivity rises to a maximum at about 0.8 GPa. [Explanation]
7. Water has unusually high surface tension. [Explanation]
8. Some salts give a surface tension-concentration minimum; the Jones-Ray effect. [Explanation]
9. Some salts prevent the coalescence of small bubbles. [Explanation]
10. The molar ionic volumes o

**http://www1.lsbu.ac.uk/water/water_anomalies.html#bi**

# ANOMALIAS DA ÁGUA

**Water phase anomalies** [d]

1. Water has an unusually high melting point. [Explanation]
2. Water has an unusually high boiling point. [Explanation]
3. Water has an unusually high critical point. [Explanation]
4. Solid water exists in a wider variety of stable (and metastable) cryst materials. [Explanation]
5. The thermal conductivity, shear modulus and transverse sound velo [Explanation]
6. The structure of liquid water changes at high pressure. [Explanatior
7. Supercooled water has two phases and a second critical point at ab
8. Liquid water is easily supercooled but glassified with difficulty. [Expl
9. Liquid water exists at very low temperatures and freezes on heating
10. Liquid water may be easily superheated.
11. Hot water may freeze faster than cold w
12. Warm water vibrates longer than cold w
13. Water molecules shrink as the temperatu

**Water material anomalies**

1. No aqueous solution is ideal. [Explanation]
2. $D_2O$ and $T_2O$ differ significantly from $H_2O$ in their physical properties. [Explanation]
3. Liquid $H_2O$ and $D_2O$ differ significantly in their phase behavior. [Explanation]
4. $H_2O$ and $D_2O$ ices differ significantly in their quantum behavior. [Explanation]
5. The mean kinetic energy of water's hydrogen atoms increases at low temperature (disputed). [Explanation]
6. Solutes have varying effects on properties such as density and viscosity. [Explanation]
7. The solubilities of non-polar gases in water decrease with temperature to a minimum and then rise. [Explanation]
8. The dielectric constant of water and ice are high. [Explanation]
9. The relative permittivity shows a temperature maximum. [Explanation]
10. The relative permittivity shows a 'kink' in its behavior with the temperature at 60 °C. [Explanation]
11. The imaginary part of the dielectric constant shows a minimum near 20 K. [Explanation]
12. Proton and hydroxide ion mobilities are anomalously fast in an electric field. [Explanation]
13. The electrical conductivity of water rises to a maximum at about 230 °C. [Explanation]

nsity-

**Water density anomalies**

1. The density of ice increases on heati
2. Water shrinks on melting. [Explanati
3. Pressure reduces ice's melting point.
4. Liquid water has a high-density that
5. The surface of water is denser than
6. Pressure re
7. There is a r
8. Water has a
9. Water's the
10. Water's the
11. The numbe
12. The numbe
13. Water has u
14. The compre
15. There is a r
16. The speed o
17. The speed o
18. 'Fast sound'
19. NMR spin-la
20. The NMR sh
21. The refracti
22. The change

**Water thermodynamic anomalies**

1. The heat of fusion of water with temperature exhibits a maximum at -17 °C. [Explanation]
2. Water has over twice the specific heat capacity of ice or steam. [Explanation]
3. The specific heat capacity ($C_P$ and $C_V$) is unusually high. [Explanation]
4. The specific heat capacity $C_P$ has a minimum at 36 °C. [Explanation]
5. The specific heat capacity ($C_P$) has a maximum at about -45 °C. [Explanation]
6. The specific heat capacity ($C_P$) has a minimum with respect to pressure. [Explanation]
7. The heat capacity ($C_V$) has a maximum. [Explanation]

planation]

**Water physical anomalies**

1. Water has unusually high viscosity. [Explanation]
2. Large viscosity and Prandtl number increase as the temperature is lowered. [Explanation]
3. Water's viscosity decreases with pressure below 33 °C. [Explanation]
4. Large diffusion decrease as the temperature is lowered. [Explanation]
5. At low temperatures, the self-diffusion of water increases as the density and pressure increase. [
6. The thermal diffusivity rises to a maximum at about 0.8 GPa. [Explanation]
7. Water has unusually high surface tension. [Explanation]
8. Some salts give a surface tension-concentration minimum; the Jones-Ray effect. [Explanation]
9. Some salts prevent the co
10. The molar ionic volumes o

**http://www1.lsbu.ac.uk/water/water_anomalies.html#bi**

# ANOMALIAS DA ÁGUA

**Water phase anomalies** [d]

1. Water has an unusually high melting point. [Explanation]
2. Water has an unusually high boiling point. [Explanation]
3. Water has an unusually high critical point. [Explanation]
4. Solid water exists in a wider variety of stable (and metastable) cryst materials. [Explanation]
5. The thermal conductivity, shear modulus and transverse sound velo [Explanation]
6. The structure of liquid water changes at high pressure. [Explanatior
7. Supercooled water has two phases and a second critical point at ab
8. Liquid water is easily supercooled but glassified with difficulty. [Expl
9. Liquid water exists at very low temperatures and freezes on heating
10. Liquid water may be easily superheated.
11. Hot water may freeze faster than cold w
12. Warm water vibrates longer than cold w
13. Water molecules shrink as the te

**Water material anomalies**

1. No aqueous solution is ideal. [Explanation]
2. $D_2O$ and $T_2O$ differ significantly from $H_2O$ in their physical properties. [Explanation]
3. Liquid $H_2O$ and $D_2O$ differ significantly in their phase behavior. [Explanation]
4. $H_2O$ and $D_2O$ ices differ significantly in their quantum behavior. [Explanation]
5. The mean kinetic energy of water's hydrogen atoms increases at low temperature (disputed). [Explanation]
6. Solutes have varying effects on properties such as density and viscosity. [Explanation]
7. The solubilities of non-polar gases in water decrease with temperature to a minimum and then rise. [Explanation]
8. The dielectric constant of water and ice are high. [Explanation]
9. The relative permittivity shows a temperature maximum. [Explanation]
10. The relative permittivity shows a 'kink' in its behavior with the temperature at 60 °C. [Explanation]
11. The imaginary part of the dielectric constant shows a minimum near 20 K. [Explanation]
12. Proton and hydroxide ion mobilities are anomalously fast in an electric field. [Explanation]
13. The electrical conductivity of water rises to a maximum at about 230 °C. [Explanation]

**Water thermodynamic anomalies**

…nsity-
…7 °C. [Explanation]
…ation]
…ation]
… [Explanation]
…planation]

**75 ANOMALIAS**

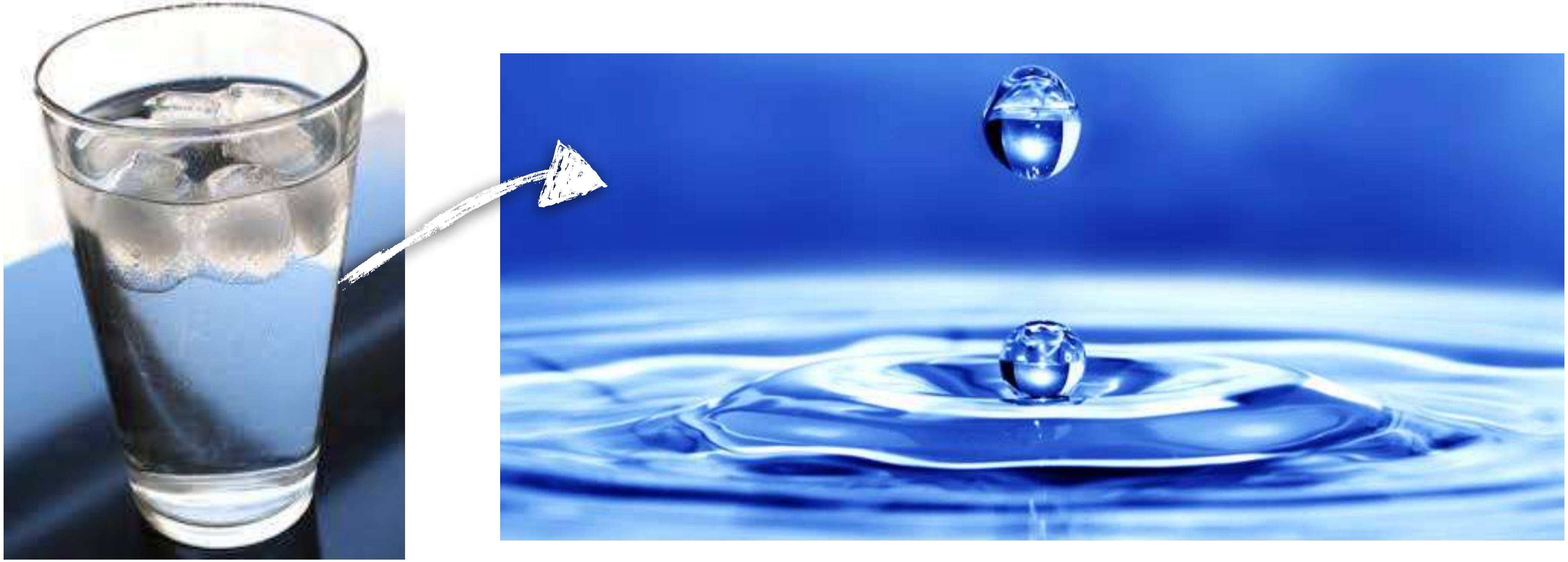
**Water density anomalies**

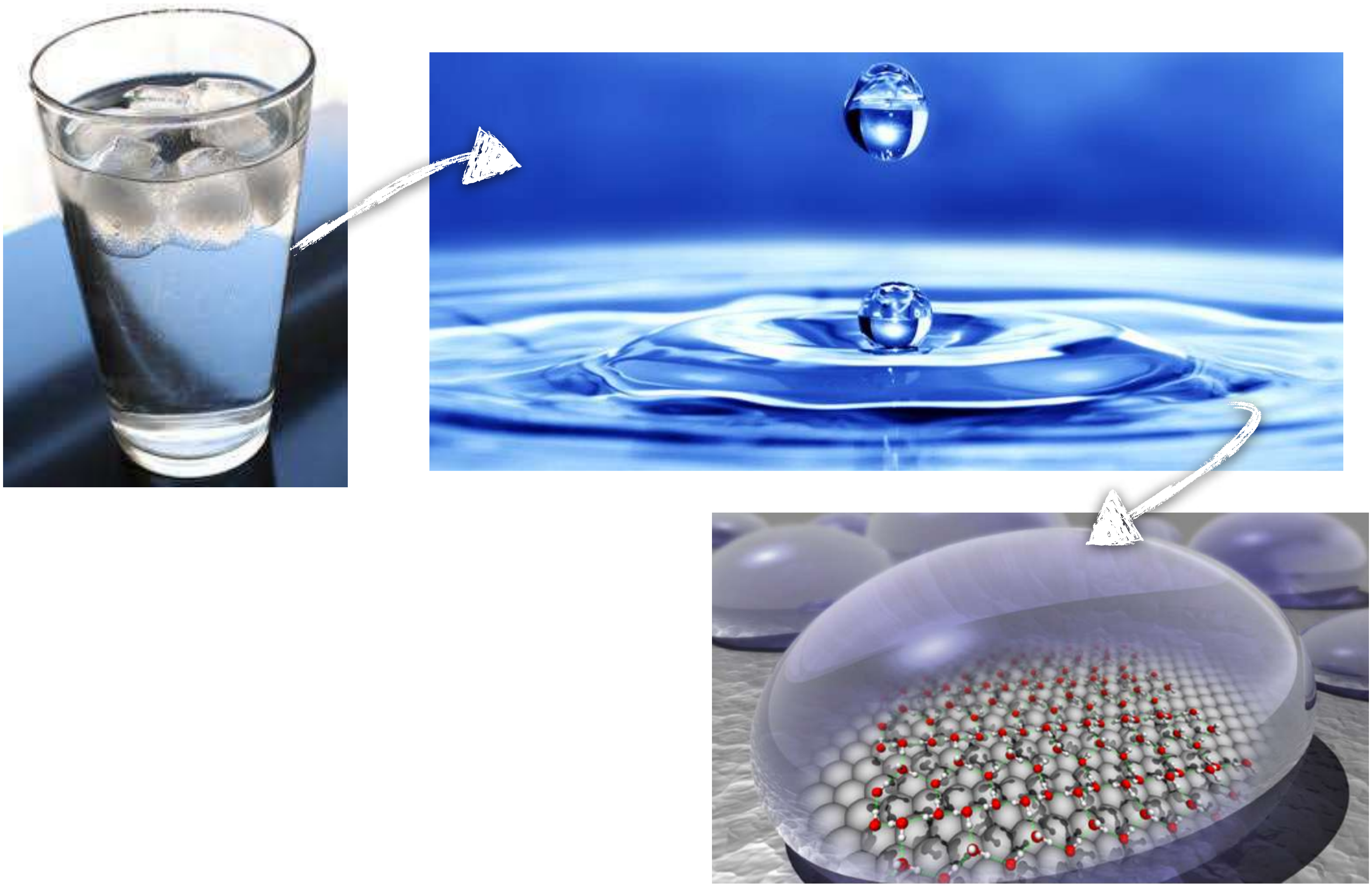
1. The density of ice increases o
2. Water shrinks on melting. [Ex
3. Pressure reduces ice's meltin
4. Liquid water has a high-dens
5. The surface of water is dense
6. Pressure reduces the temper
7. There is a n
8. Water has a
9. Water's the
10. Water's the
11. The numbe
12. The numbe
13. Water has u
14. The compre
15. There is a n
16. The speed
17. The speed
18. 'Fast sound'
19. NMR spin-la
20. The NMR sh
21. The refracti
22. The change

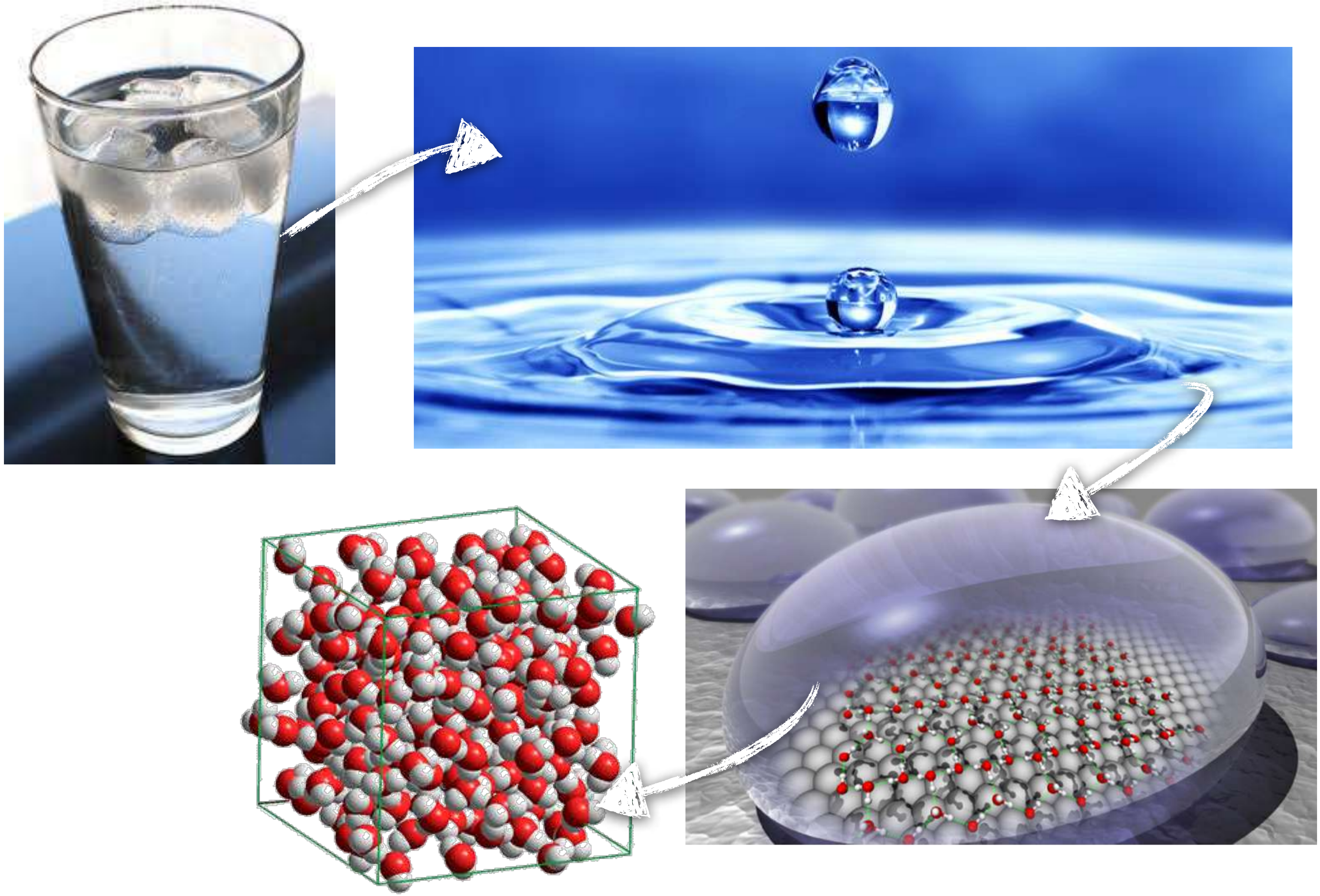
**Water physical anomalies**

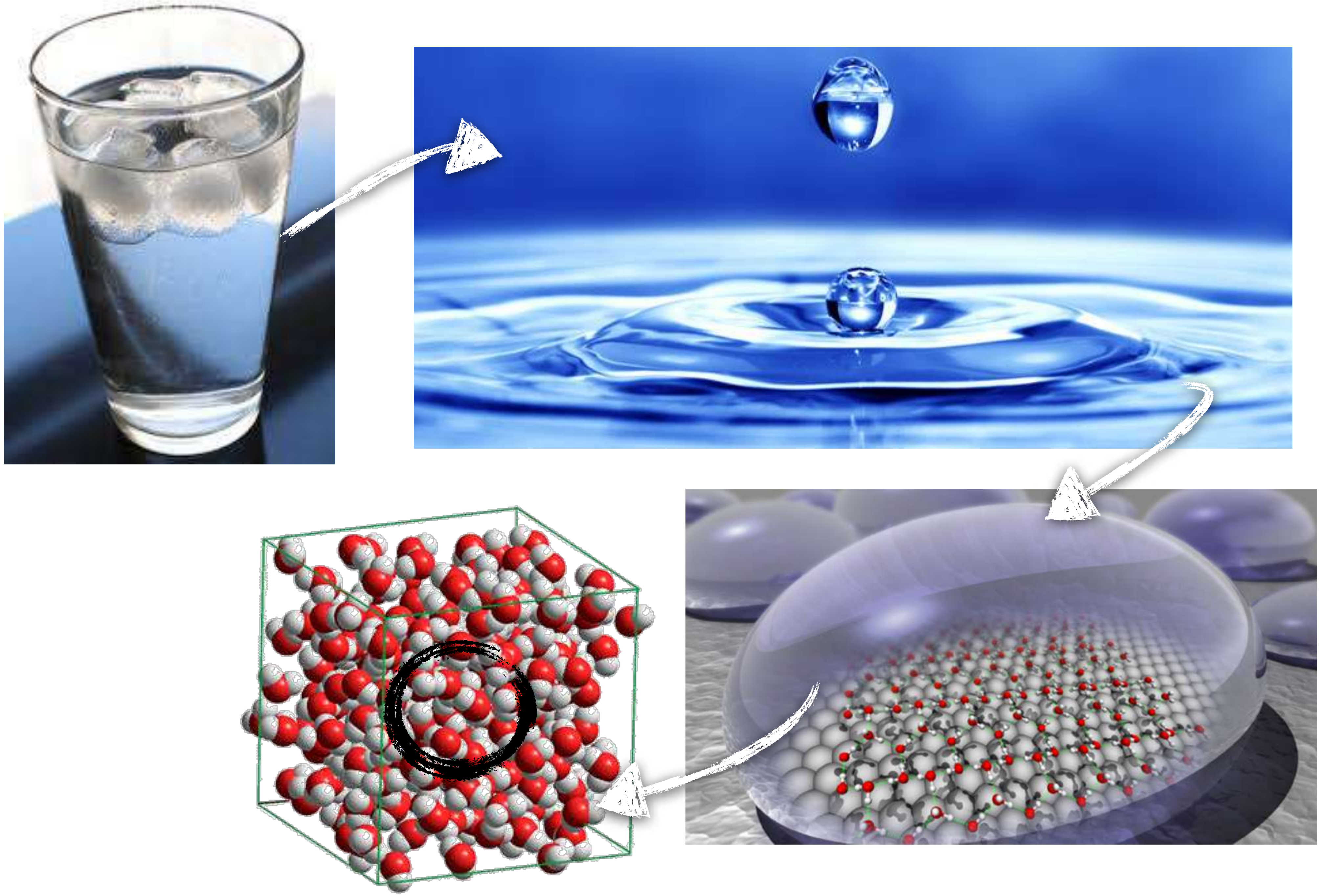
1. Water has unusually high viscosity. [Explanation]
2. Large viscosity and Prandtl number increase as the temperature is lowered. [Explanation]
3. Water's viscosity decreases with pressure below 33 °C. [Explanation]
4. Large diffusion decrease as the temperature is lowered. [Explanation]
5. At low temperatures, the self-diffusion of water increases as the density and pressure increase. [
6. The thermal diffusivity rises to a maximum at about 0.8 GPa. [Explanation]
7. Water has unusually high surface tension. [Explanation]
8. Some salts give a surface tension-concentration minimum; the Jones-Ray effect. [Explanation]
9. Some salts prevent the co
10. The molar ionic volumes o

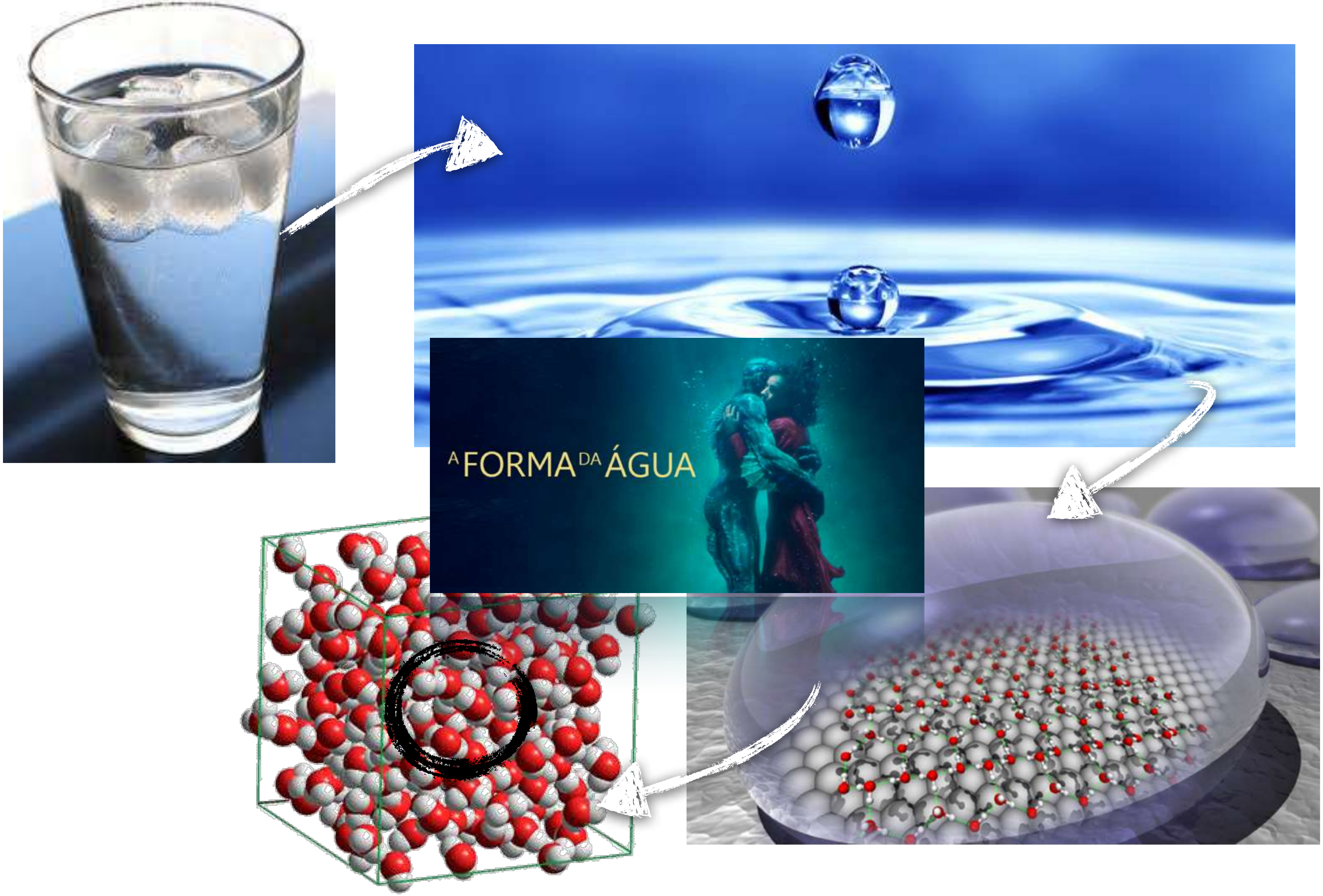
http://www1.lsbu.ac.uk/water/water_anomalies.html#bi

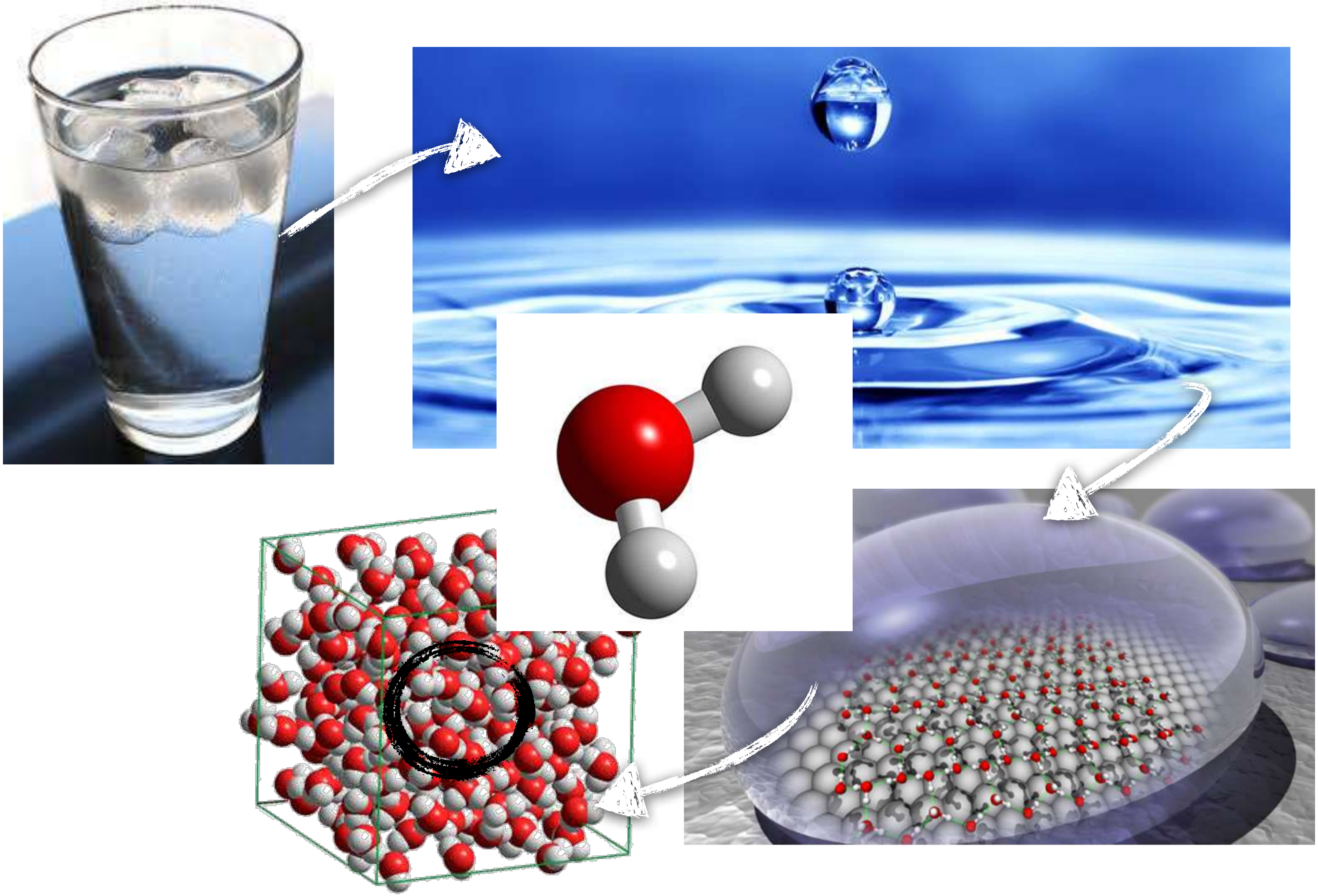


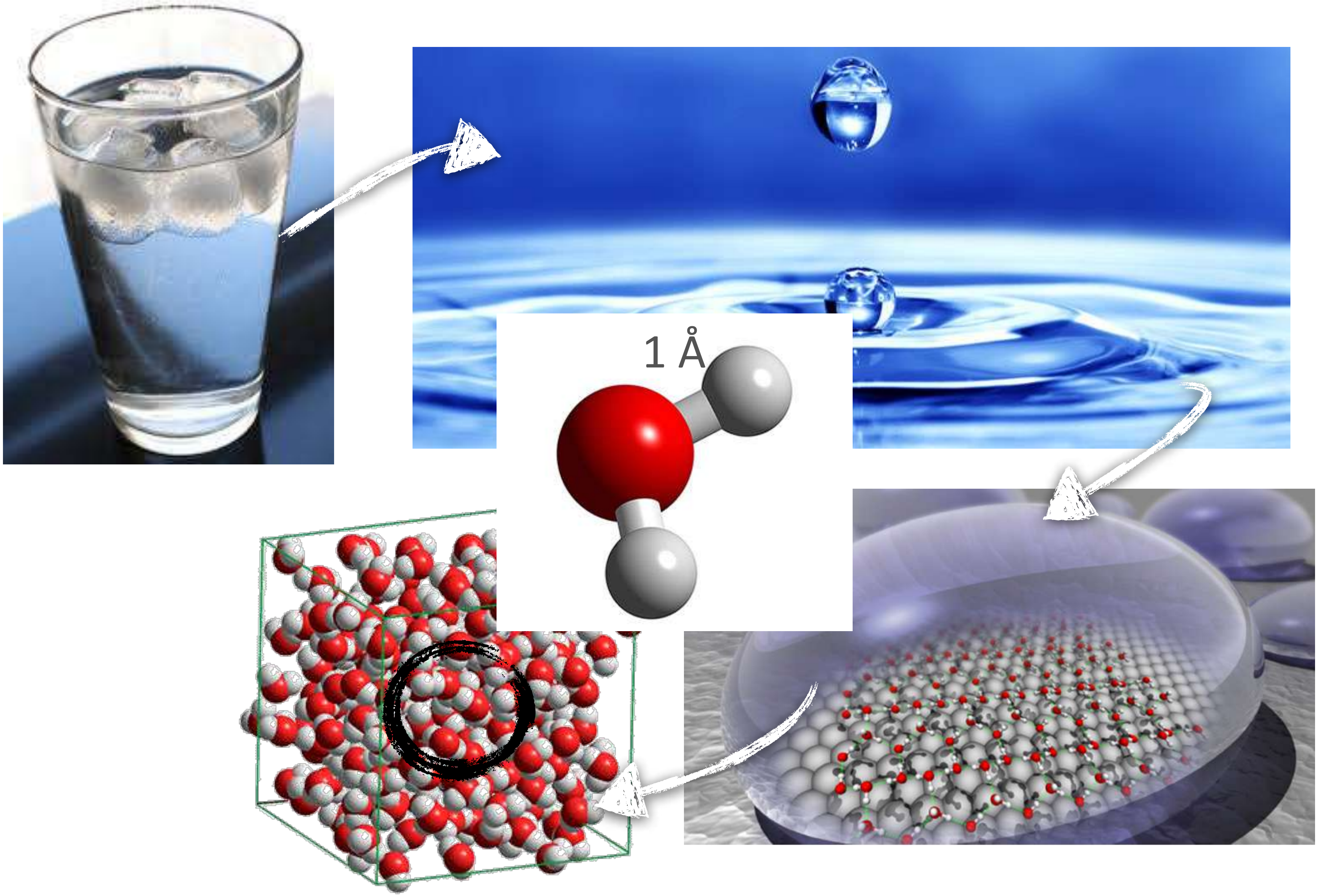




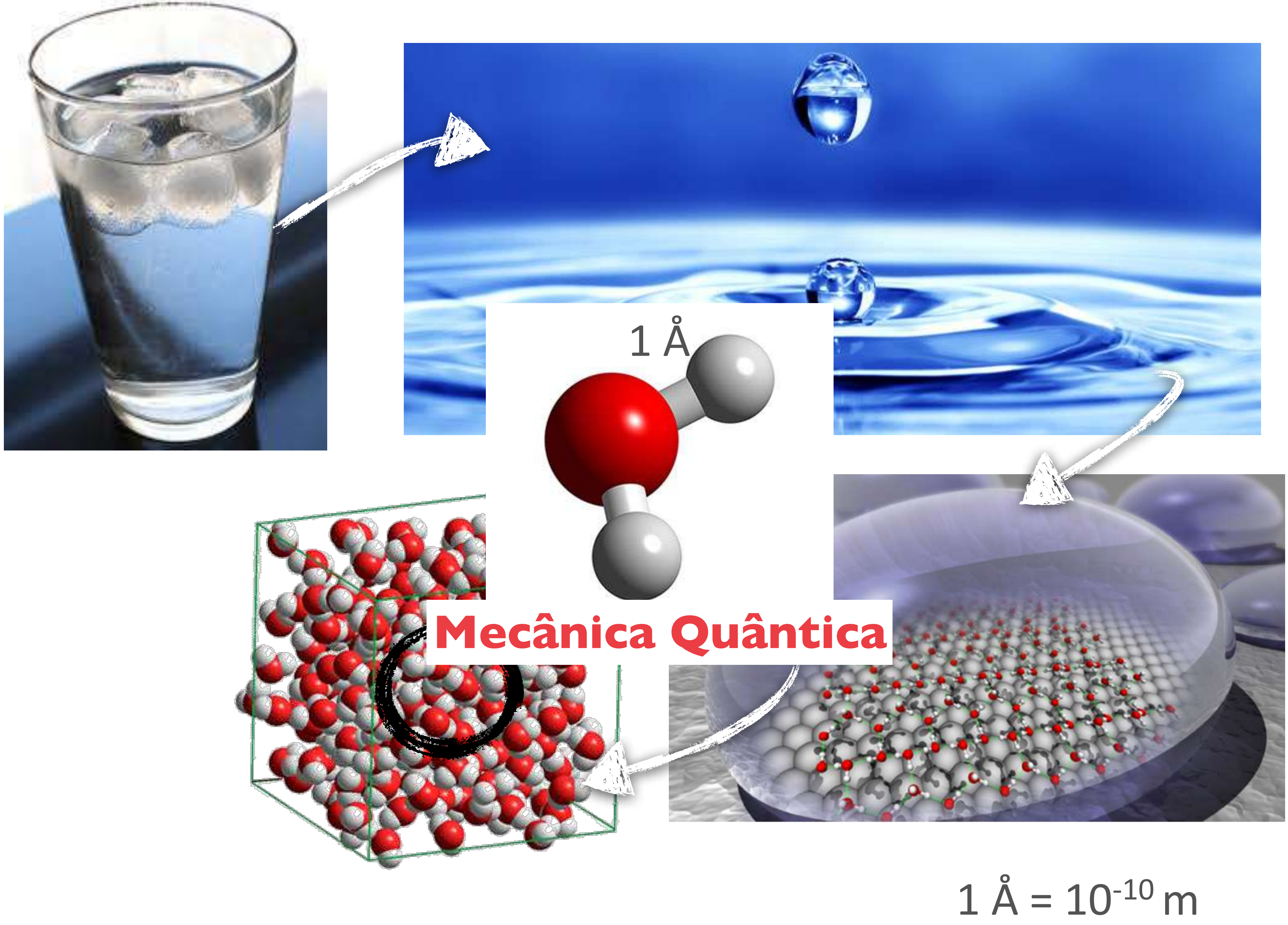



A FORMA DA ÁGUA



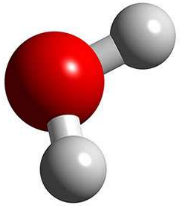



$1\ \text{Å} = 10^{-10}$ m



1 Å
Mecânica Quântica
1 Å = 10-10 m

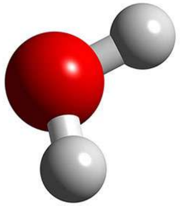
# ESTRUTURA DA (MOLÉCULA DE) ÁGUA



## Mecânica Quântica

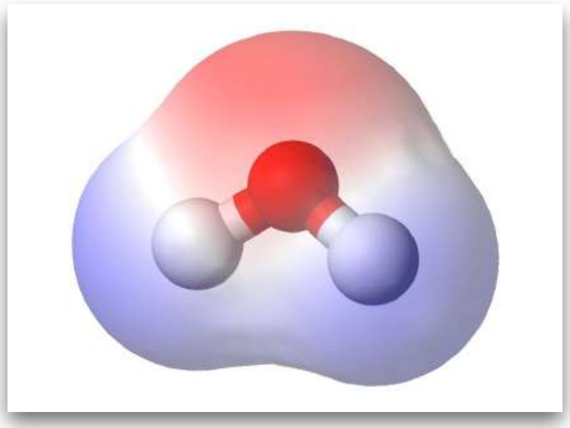
$$\left[\sum_{i}^{N}\left(-\frac{\hbar^2\nabla_i^2}{2m}+v(\mathbf{r}_i)\right)+\sum_{i<j}U(\mathbf{r}_i,\mathbf{r}_j)\right]\Psi(\mathbf{r}_1,\mathbf{r}_2\ldots,\mathbf{r}_N)=E\Psi(\mathbf{r}_1,\mathbf{r}_2\ldots,\mathbf{r}_N)$$

# ESTRUTURA DA (MOLÉCULA DE) ÁGUA

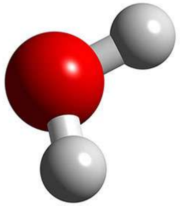


## Mecânica Quântica

$$\left[\sum_{i}^{N}\left(-\frac{\hbar^2\nabla_i^2}{2m}+v(\mathbf{r}_i)\right)+\sum_{i<j}U(\mathbf{r}_i,\mathbf{r}_j)\right]\Psi(\mathbf{r}_1,\mathbf{r}_2\ldots,\mathbf{r}_N)=E\Psi(\mathbf{r}_1,\mathbf{r}_2\ldots,\mathbf{r}_N).$$

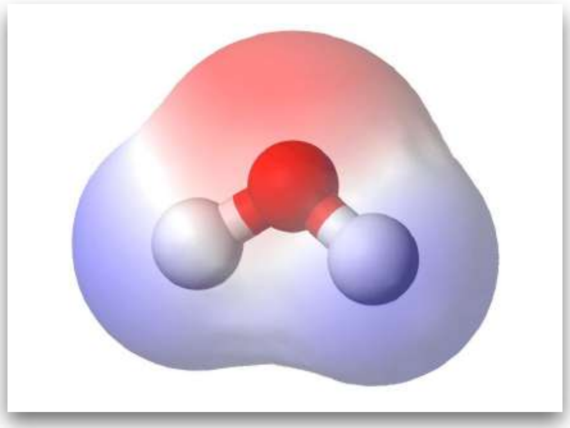


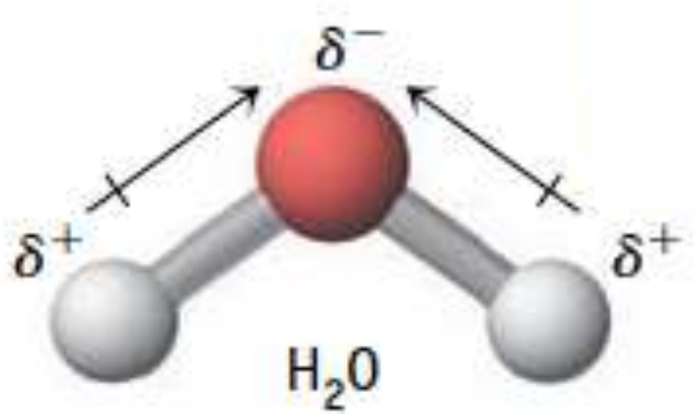
# ESTRUTURA DA (MOLÉCULA DE) ÁGUA



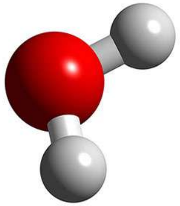
## Mecânica Quântica

$$\left[\sum_i^N \left(-\frac{\hbar^2\nabla_i^2}{2m} + v(\mathbf{r}_i)\right) + \sum_{i<j} U(\mathbf{r}_i, \mathbf{r}_j)\right] \Psi(\mathbf{r}_1, \mathbf{r}_2 \ldots, \mathbf{r}_N) = E\Psi(\mathbf{r}_1, \mathbf{r}_2 \ldots, \mathbf{r}_N).$$



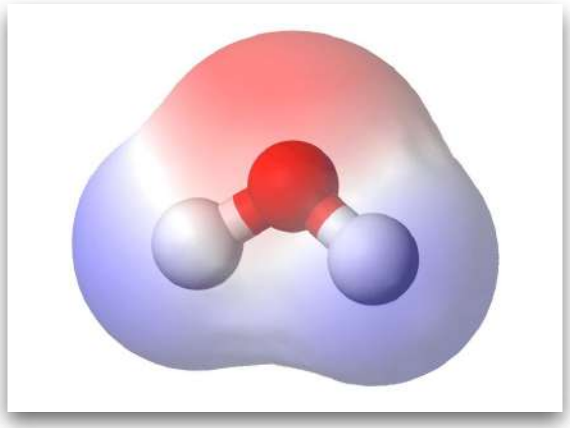


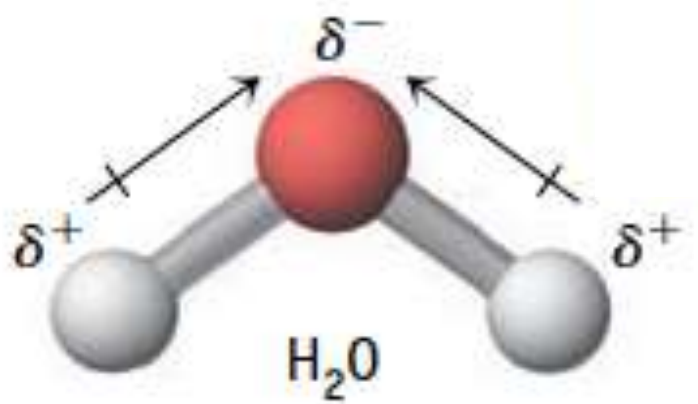
# ESTRUTURA DA (MOLÉCULA DE) ÁGUA

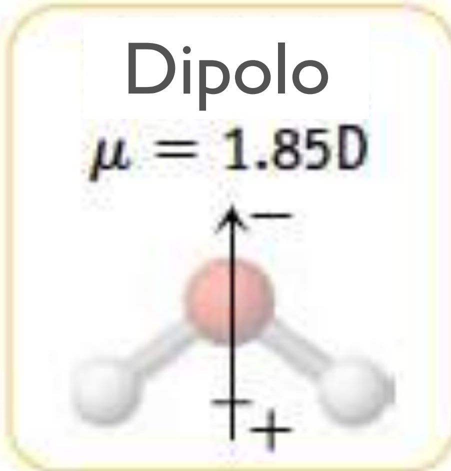


## Mecânica Quântica

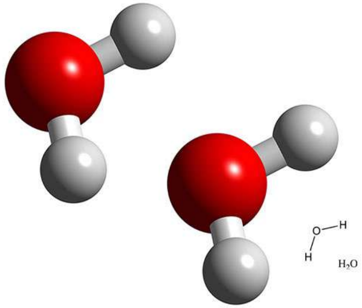
$$\left[\sum_{i}^{N}\left(-\frac{\hbar^2\nabla_i^2}{2m}+v(\mathbf{r}_i)\right)+\sum_{i<j}U(\mathbf{r}_i,\mathbf{r}_j)\right]\Psi(\mathbf{r}_1,\mathbf{r}_2\ldots,\mathbf{r}_N)=E\Psi(\mathbf{r}_1,\mathbf{r}_2\ldots,\mathbf{r}_N).$$

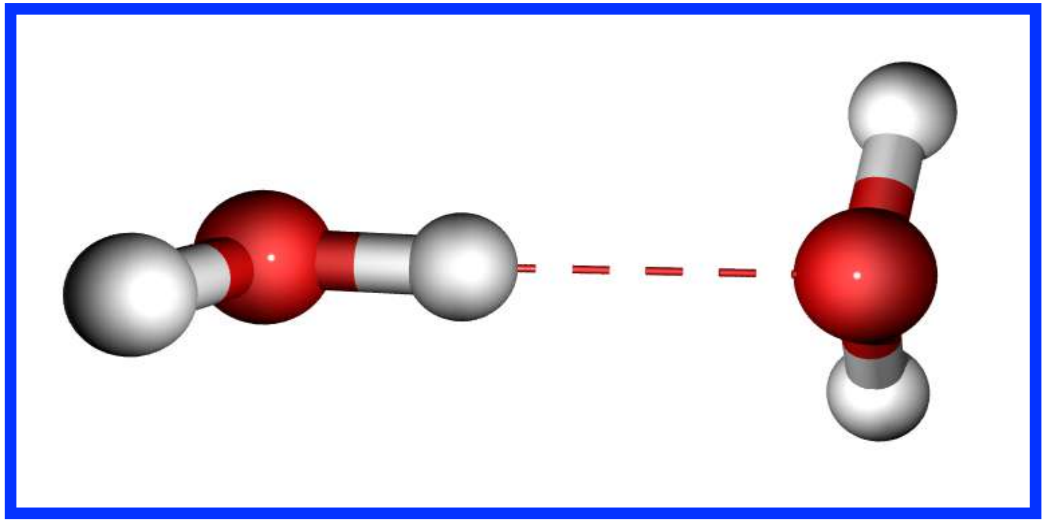




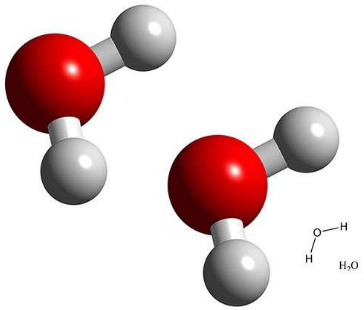



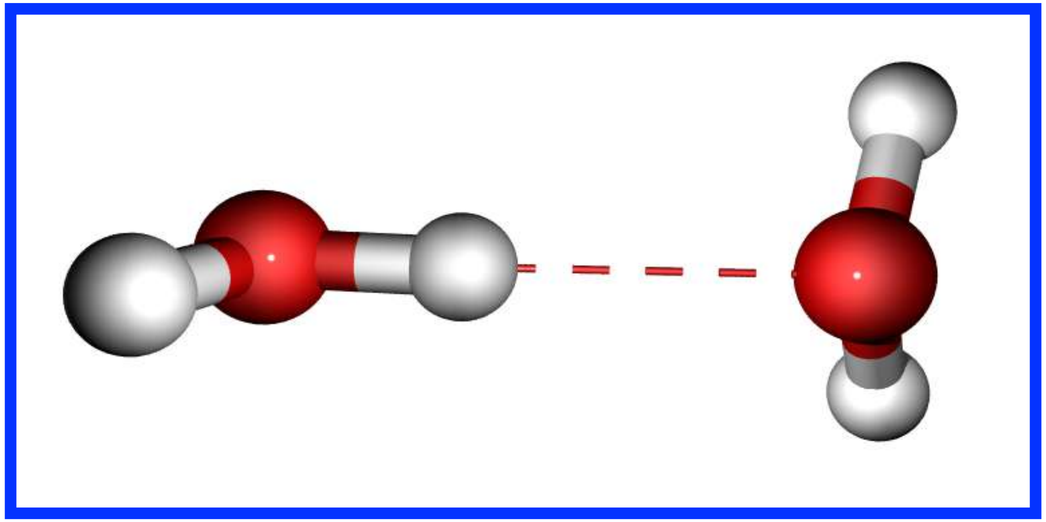
# ESTRUTURA DA ÁGUA: LIGAÇÃO DE HIDROGÊNIO





# ESTRUTURA DA ÁGUA: LIGAÇÃO DE HIDROGÊNIO

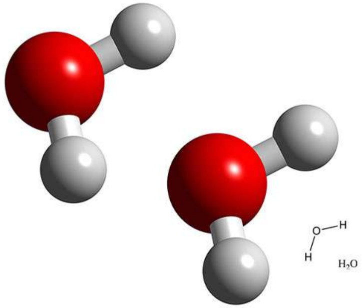


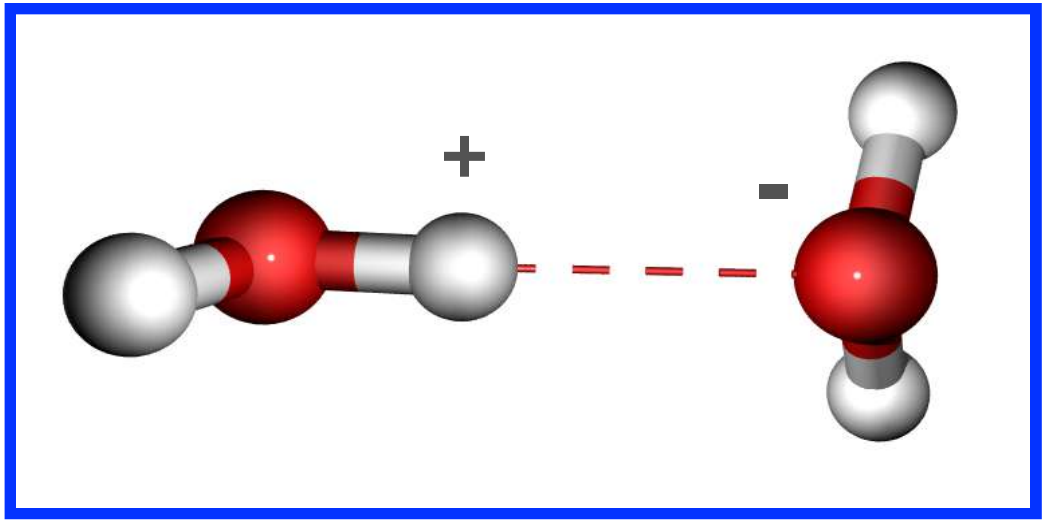


*"It is the hydrogen bond that determines the magnitude and nature of the mutual interaction of water molecules and that is consequently responsible for the striking thermodynamic and spectroscopic properties of this uniquely important substance"*

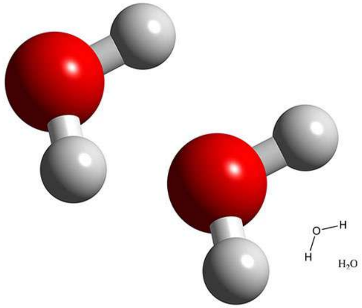
Linus Pauling - "The Nature of Chemical Bond"

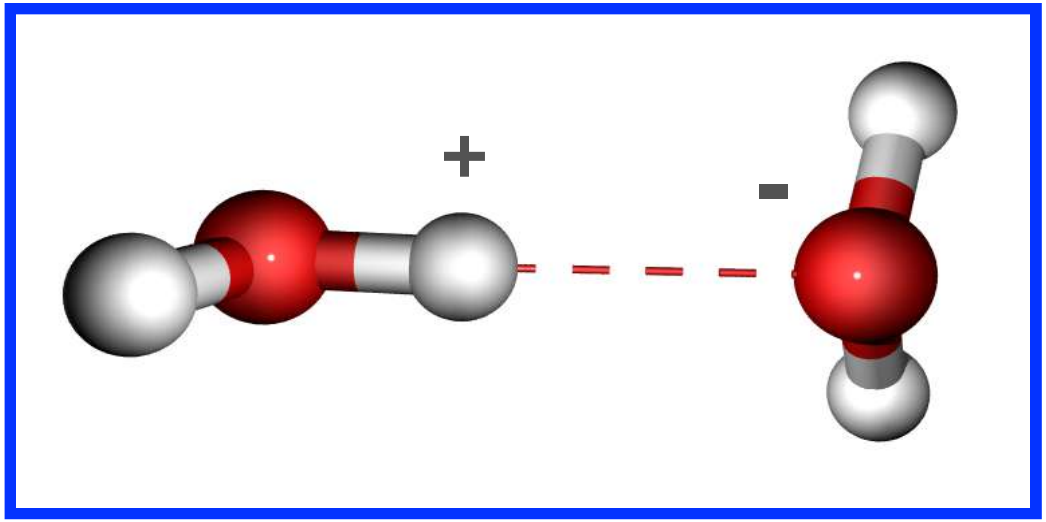
# ESTRUTURA DA ÁGUA: LIGAÇÃO DE HIDROGÊNIO

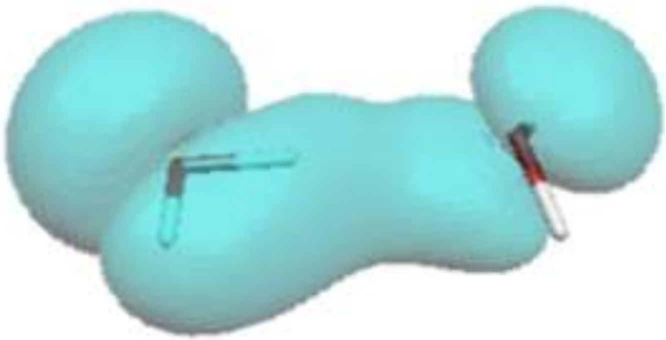


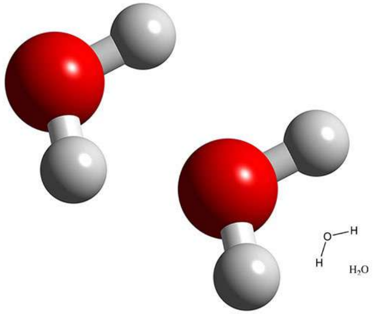
# ESTRUTURA DA ÁGUA: LIGAÇÃO DE HIDROGÊNIO

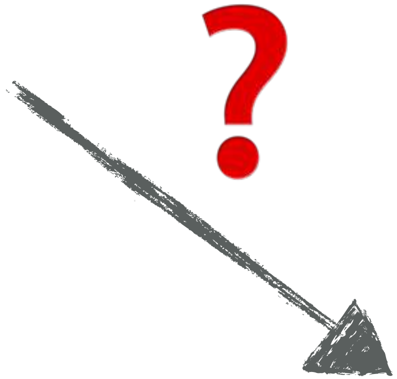


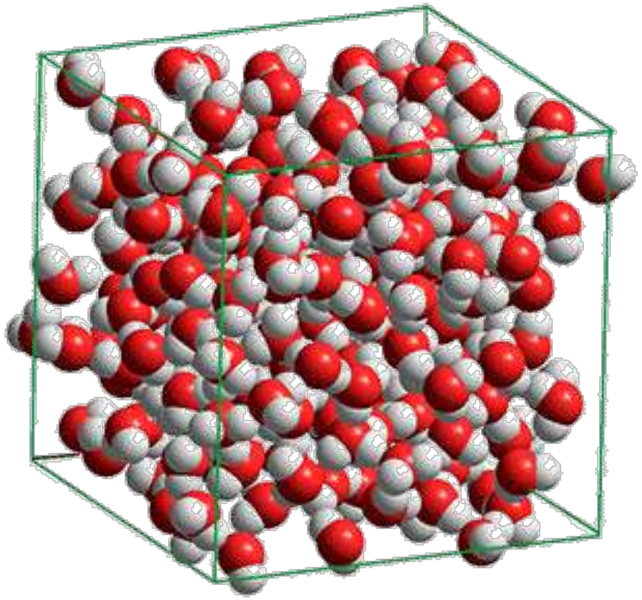



# ESTRUTURA DA ÁGUA







# ESTRUTURA DA ÁGUA

**Science**

www.sciencemag.org
*Science* 1 July 2005:
Vol. 309 no. 5731 pp. 78-102
DOI: 10.1126/science.309.5731.78b

- NEWS

**So Much More to Know …**

**What is the structure of water?**

Researchers continue to tussle over how many bonds each $H_2O$ molecule makes with its nearest neighbors.

# ESTRUTURA DA ÁGUA

**Science**
www.sciencemag.org
*Science* 1 July 2005:
Vol. 309 no. 5731 pp. 78-102
DOI: 10.1126/science.309.5731.78b

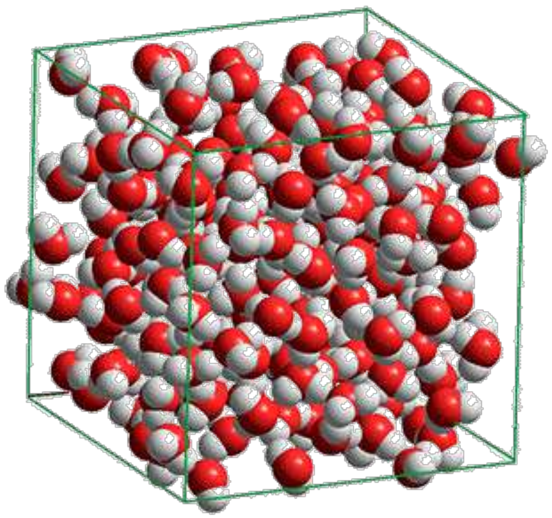
- NEWS

**So Much More to Know ...**

**What is the structure of water?**

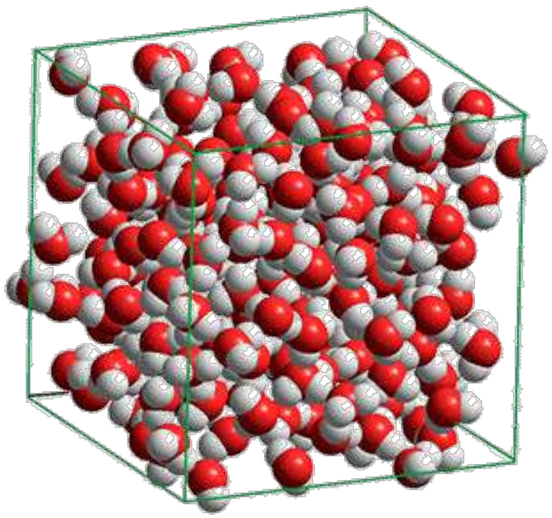
Researchers continue to tussle over how many bonds each $H_2O$ molecule makes with its nearest neighbors.

# MODELOS PARA INTERAÇÕES



$$E_{ab} = \sum_{ij} \frac{q_i q_j e^2}{r_{ij}} + 4\varepsilon_0 \left[ \left( \frac{\sigma_0}{r_{OO}} \right)^{12} - \left( \frac{\sigma_0}{r_{OO}} \right)^{6} \right]$$

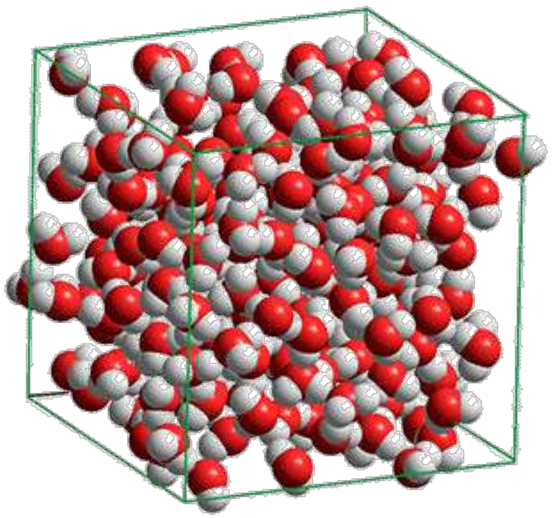
# MODELOS PARA INTERAÇÕES



$$E_{ab} = \sum_{ij} \frac{q_i q_j e^2}{r_{ij}} + 4\varepsilon_0 \left[ \left( \frac{\sigma_0}{r_{OO}} \right)^{12} - \left( \frac{\sigma_0}{r_{OO}} \right)^{6} \right]$$

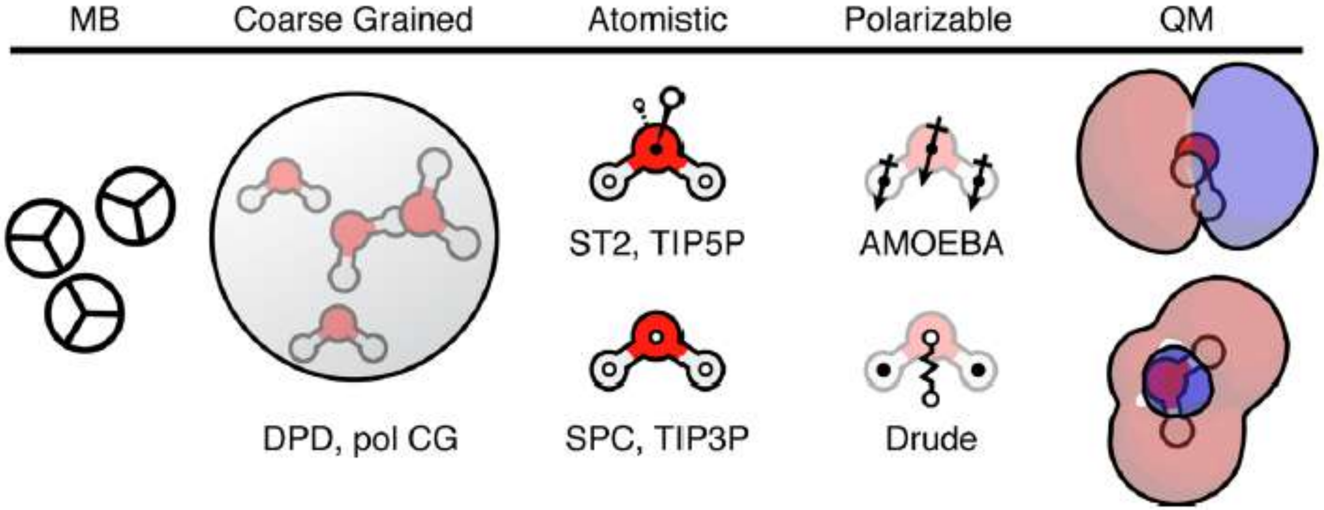
$$\left[ \sum_i^N \left( -\frac{\hbar^2 \nabla_i^2}{2m} + v(\mathbf{r}_i) \right) + \sum_{i<j} U(\mathbf{r}_i, \mathbf{r}_j) \right] \Psi(\mathbf{r}_1, \mathbf{r}_2 \dots, \mathbf{r}_N) = E\Psi(\mathbf{r}_1, \mathbf{r}_2 \dots, \mathbf{r}_N),$$

# MODELOS PARA INTERAÇÕES



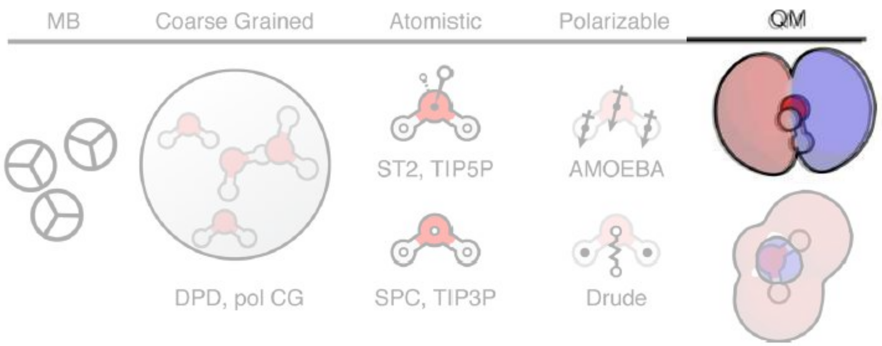
$$E_{ab} = \sum_{ij} \frac{q_i q_j e^2}{r_{ij}} + 4\varepsilon_0 \left[ \left( \frac{\sigma_0}{r_{OO}} \right)^{12} - \left( \frac{\sigma_0}{r_{OO}} \right)^{6} \right]$$

$$\left[ \sum_i^N \left( -\frac{\hbar^2 \nabla_i^2}{2m} + v(\mathbf{r}_i) \right) + \sum_{i<j} U(\mathbf{r}_i, \mathbf{r}_j) \right] \Psi(\mathbf{r}_1, \mathbf{r}_2 \ldots, \mathbf{r}_N) = E \Psi(\mathbf{r}_1, \mathbf{r}_2 \ldots, \mathbf{r}_N).$$

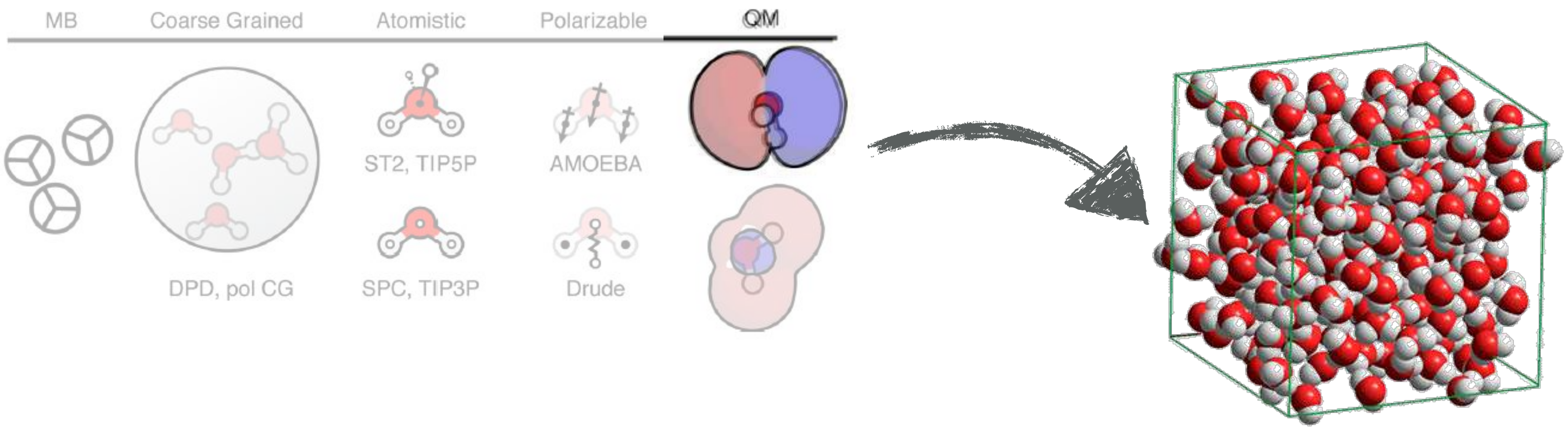



E. Brini *et al*, Chem. Rev. 2017, 117, 12385−12414

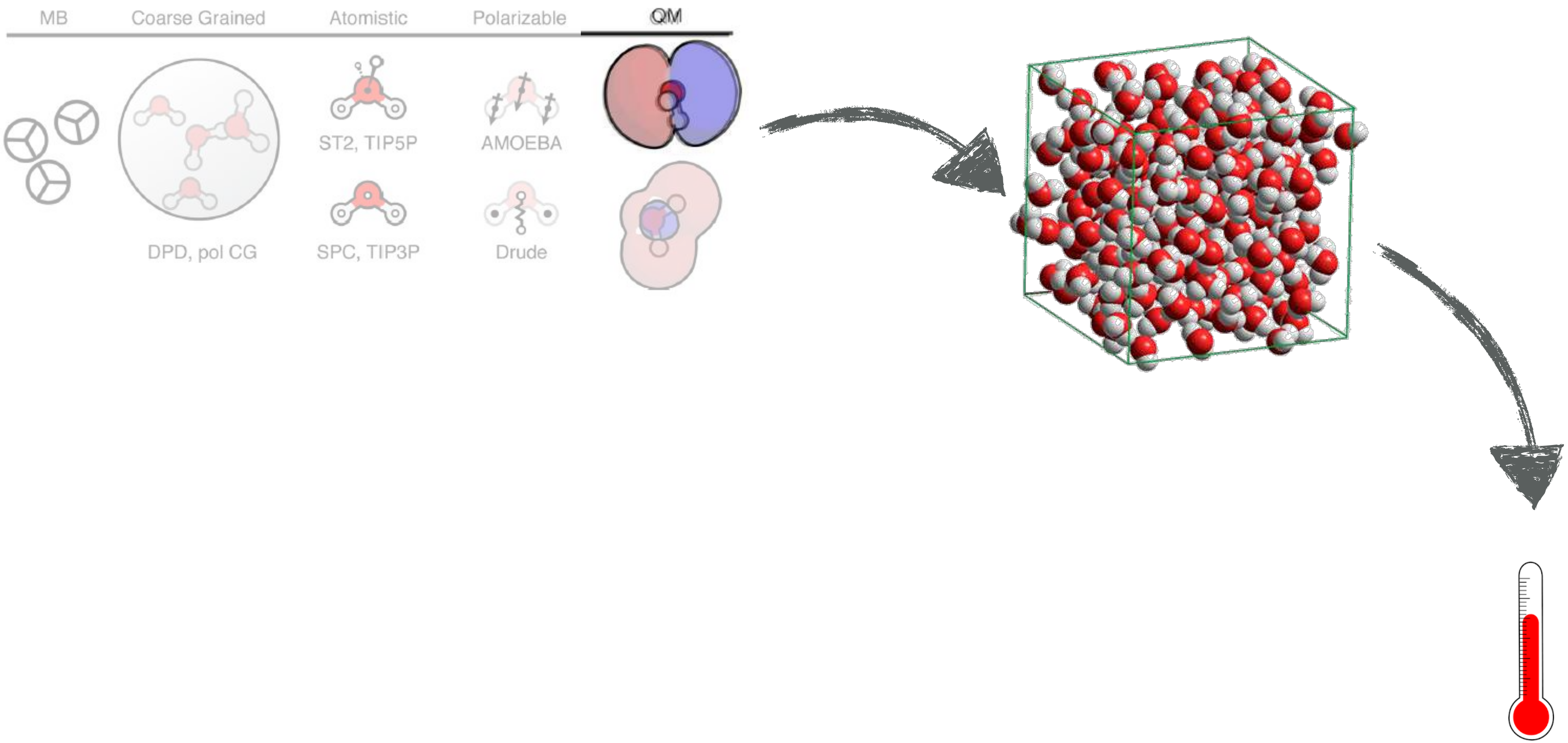
# SIMULAÇÕES COMPUTACIONAIS



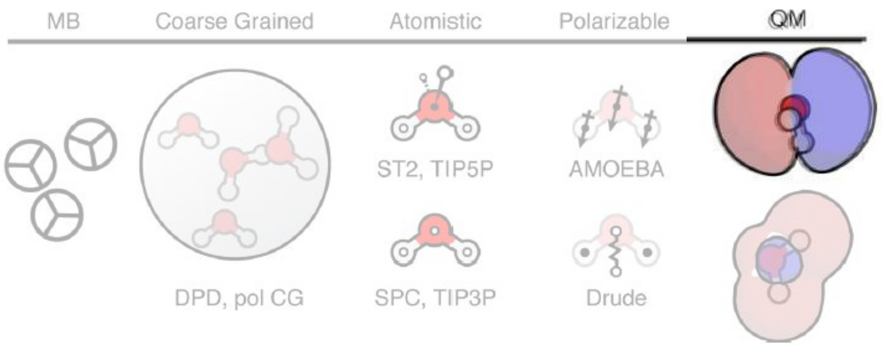
# SIMULAÇÕES COMPUTACIONAIS

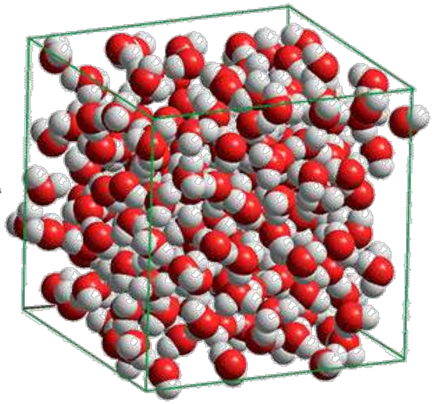


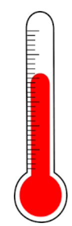
# SIMULAÇÕES COMPUTACIONAIS



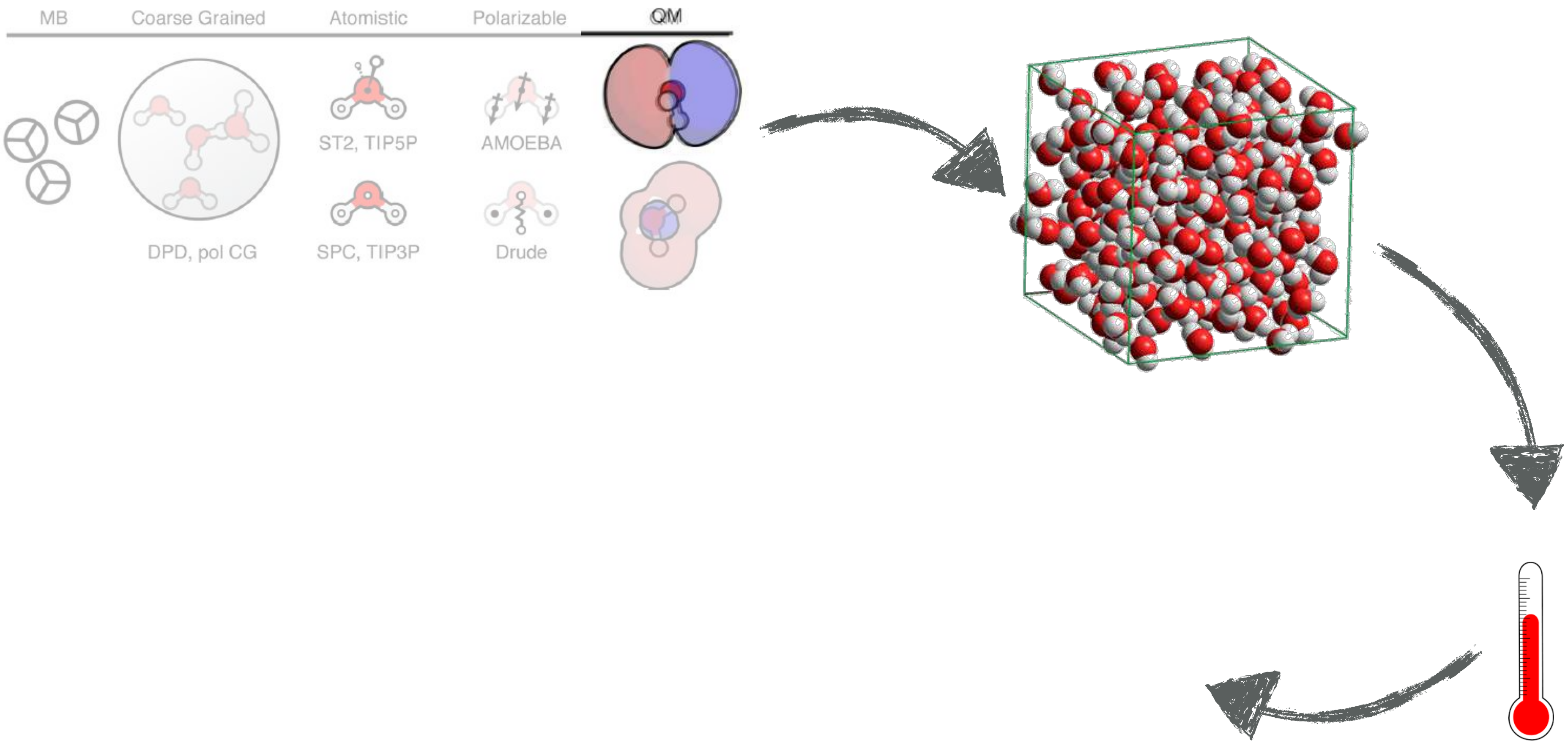
# SIMULAÇÕES COMPUTACIONAIS



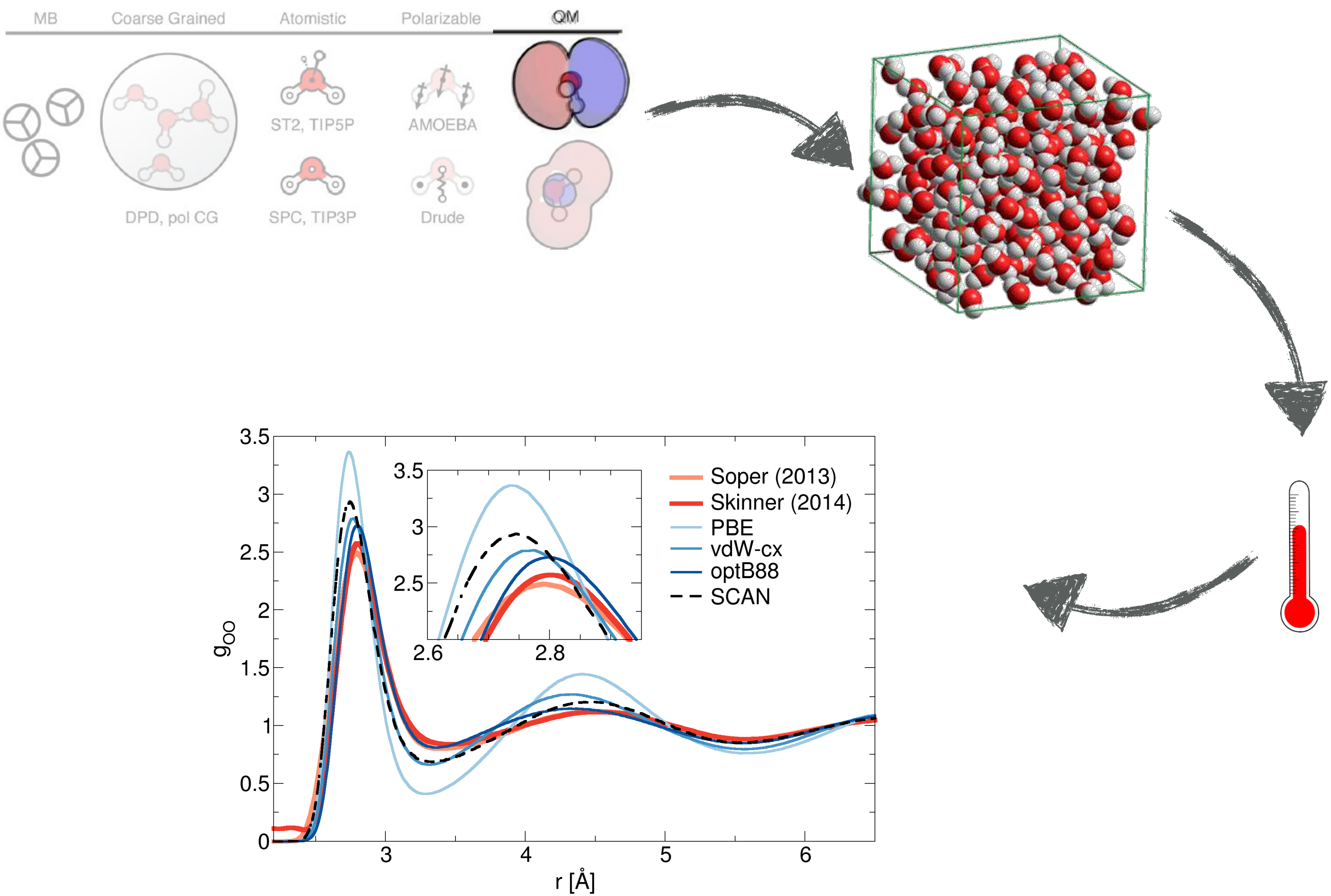





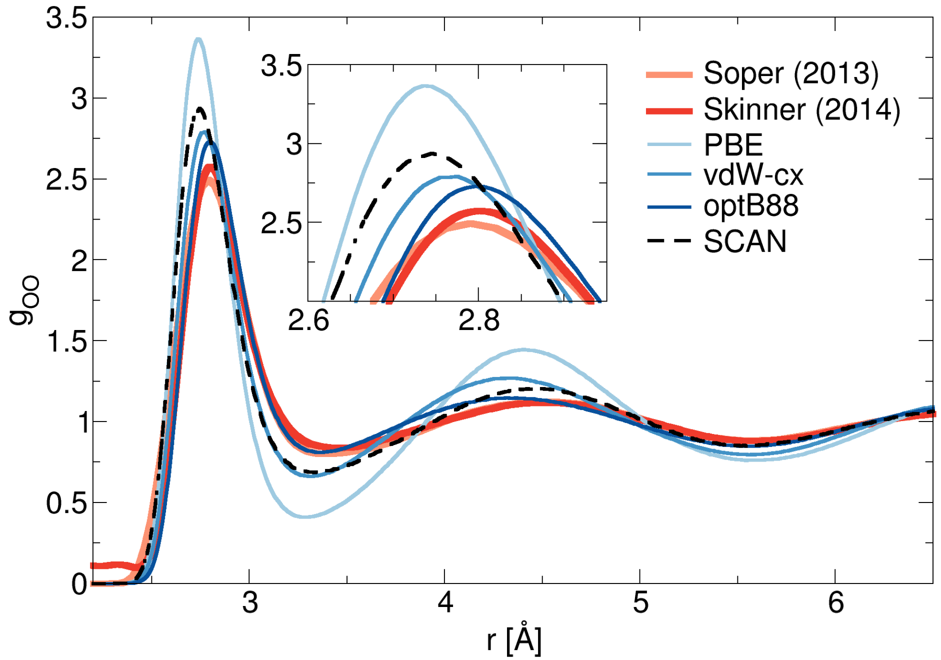
# SIMULAÇÕES COMPUTACIONAIS

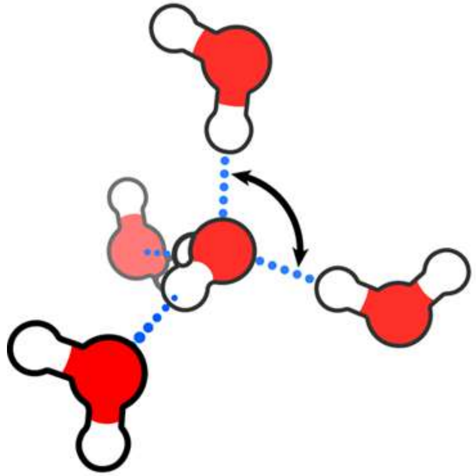


# SIMULAÇÕES COMPUTACIONAIS



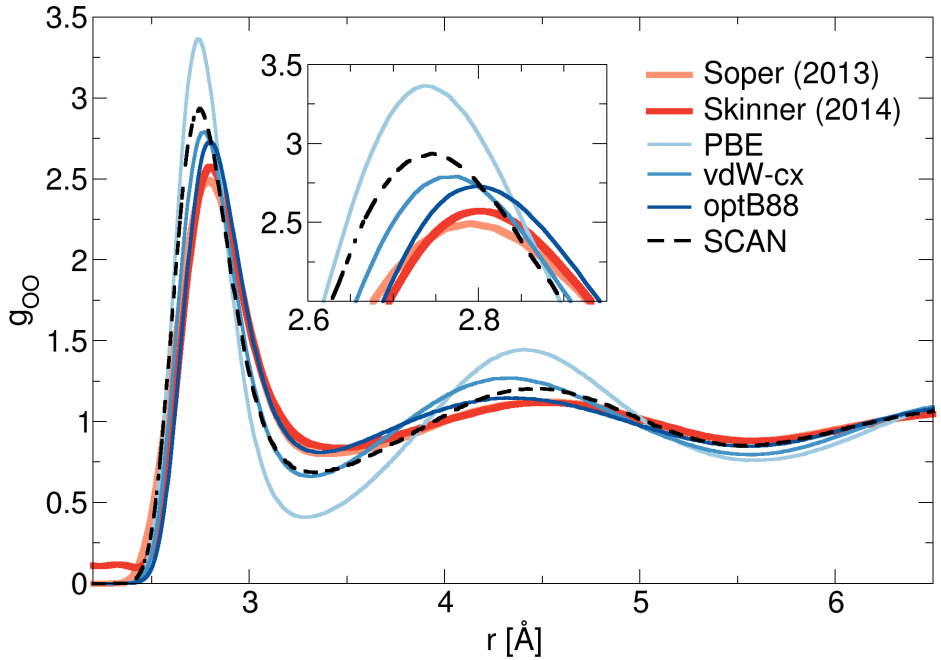
# ESTRUTURA DA ÁGUA: LIGAÇÃO DE HIDROGÊNIO

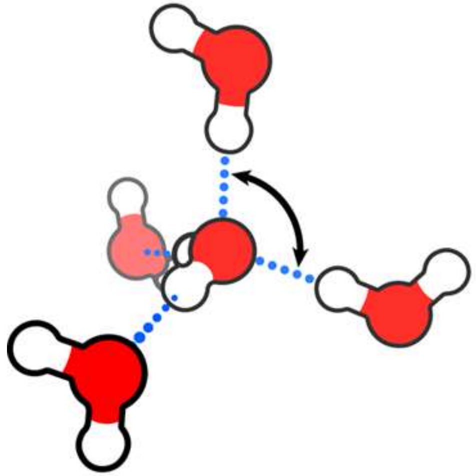


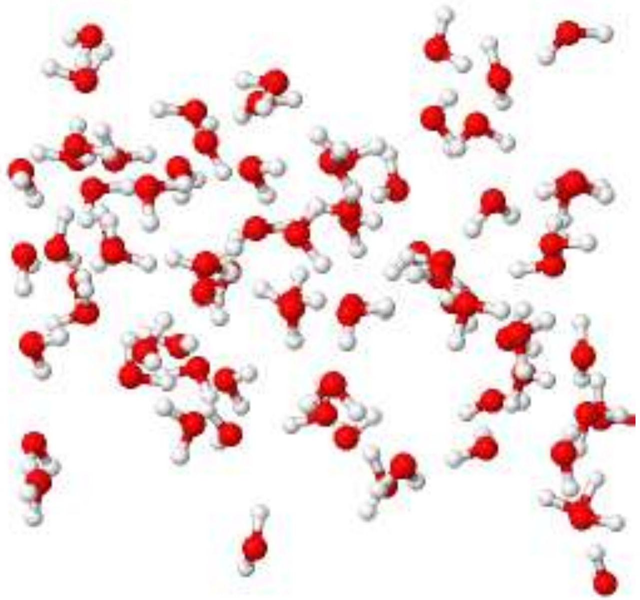
Estrutura tetraédrica

# ESTRUTURA DA ÁGUA: LIGAÇÃO DE HIDROGÊNIO



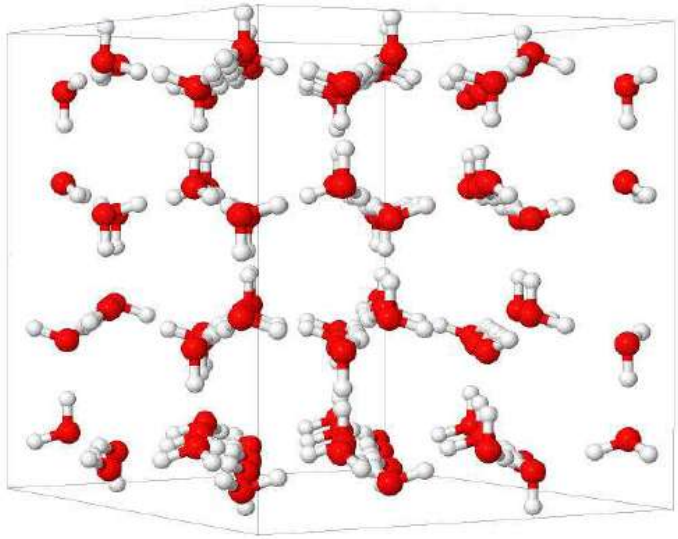



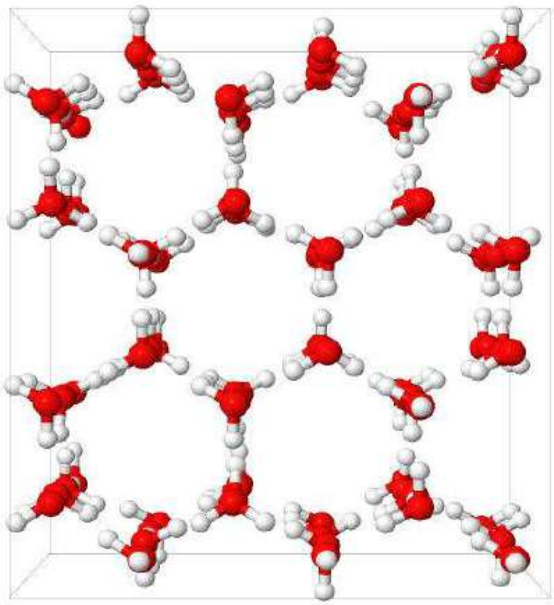
Estrutura tetraédrica



# ESTRUTURA DA ÁGUA: GELO

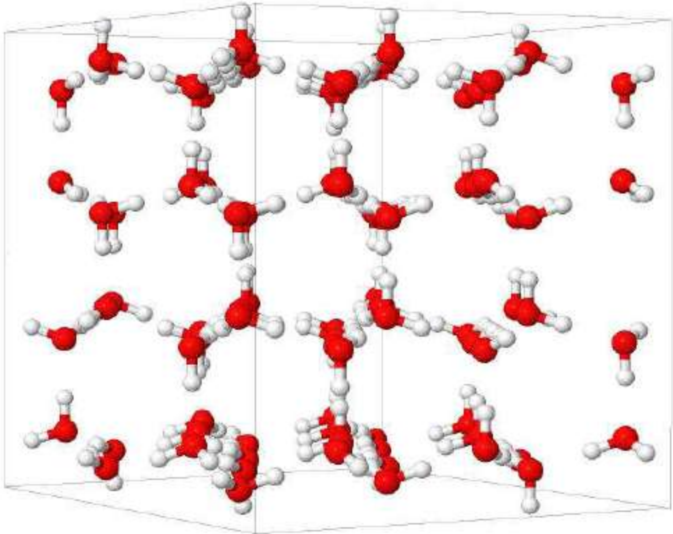
Gelo Ih

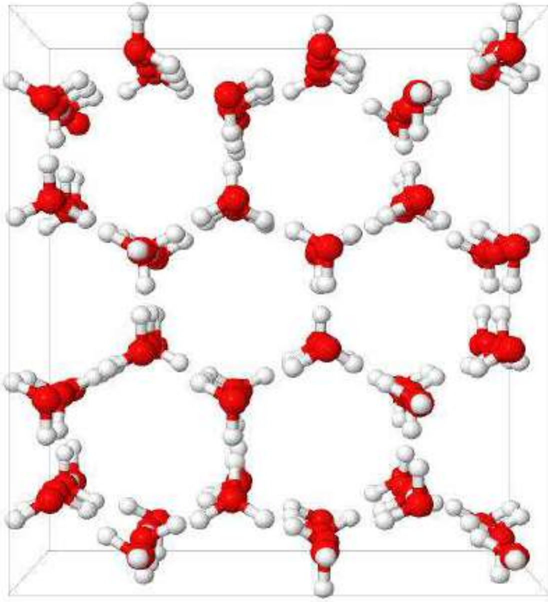


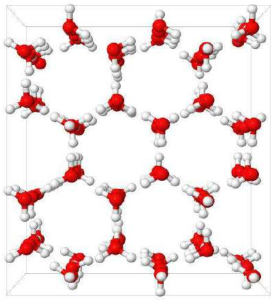


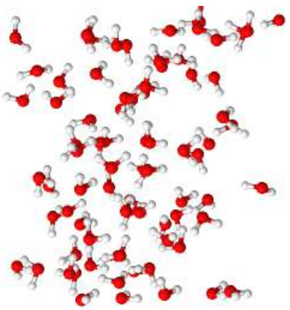
# ESTRUTURA DA ÁGUA: GELO

Gelo Ih



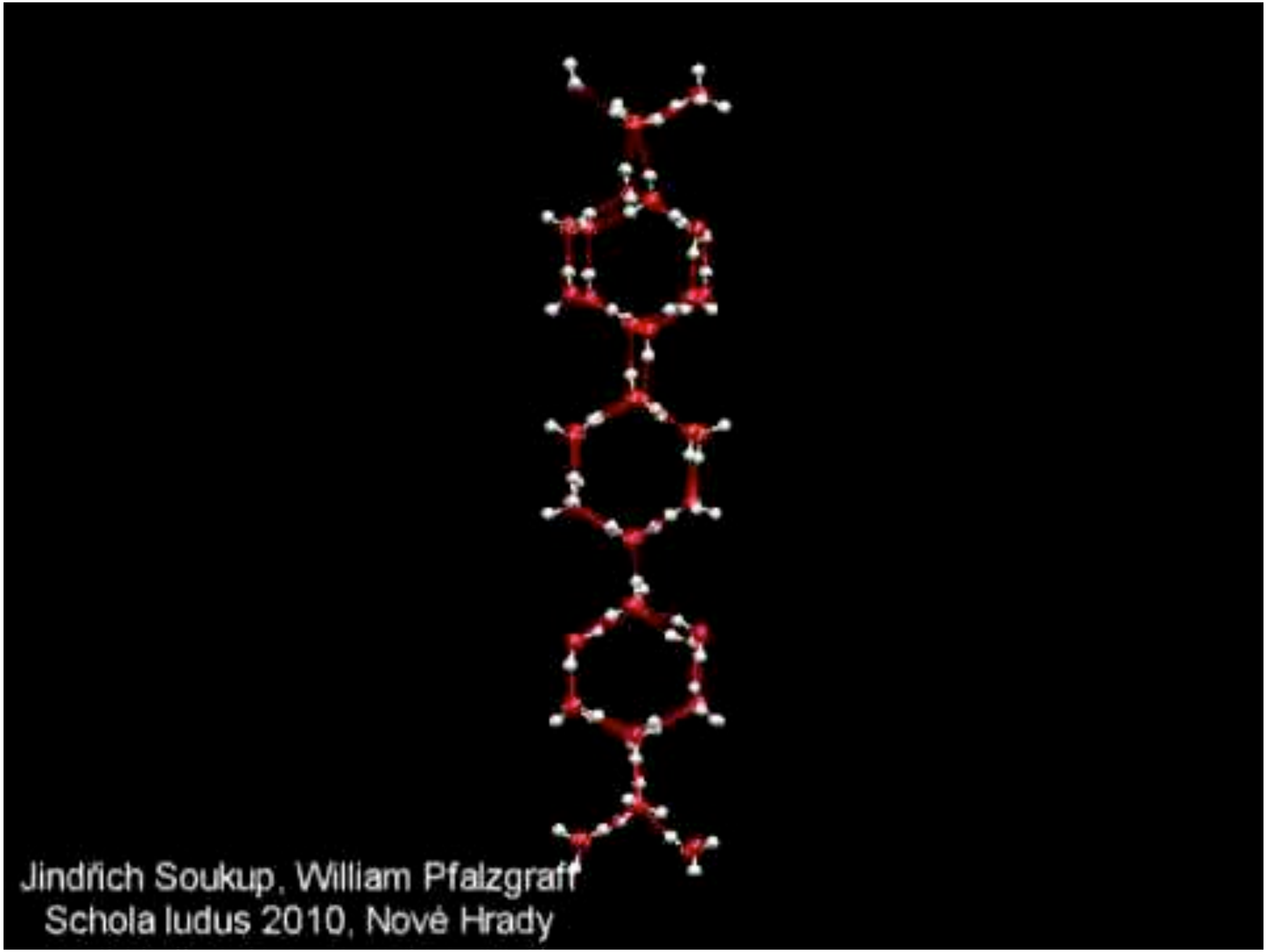




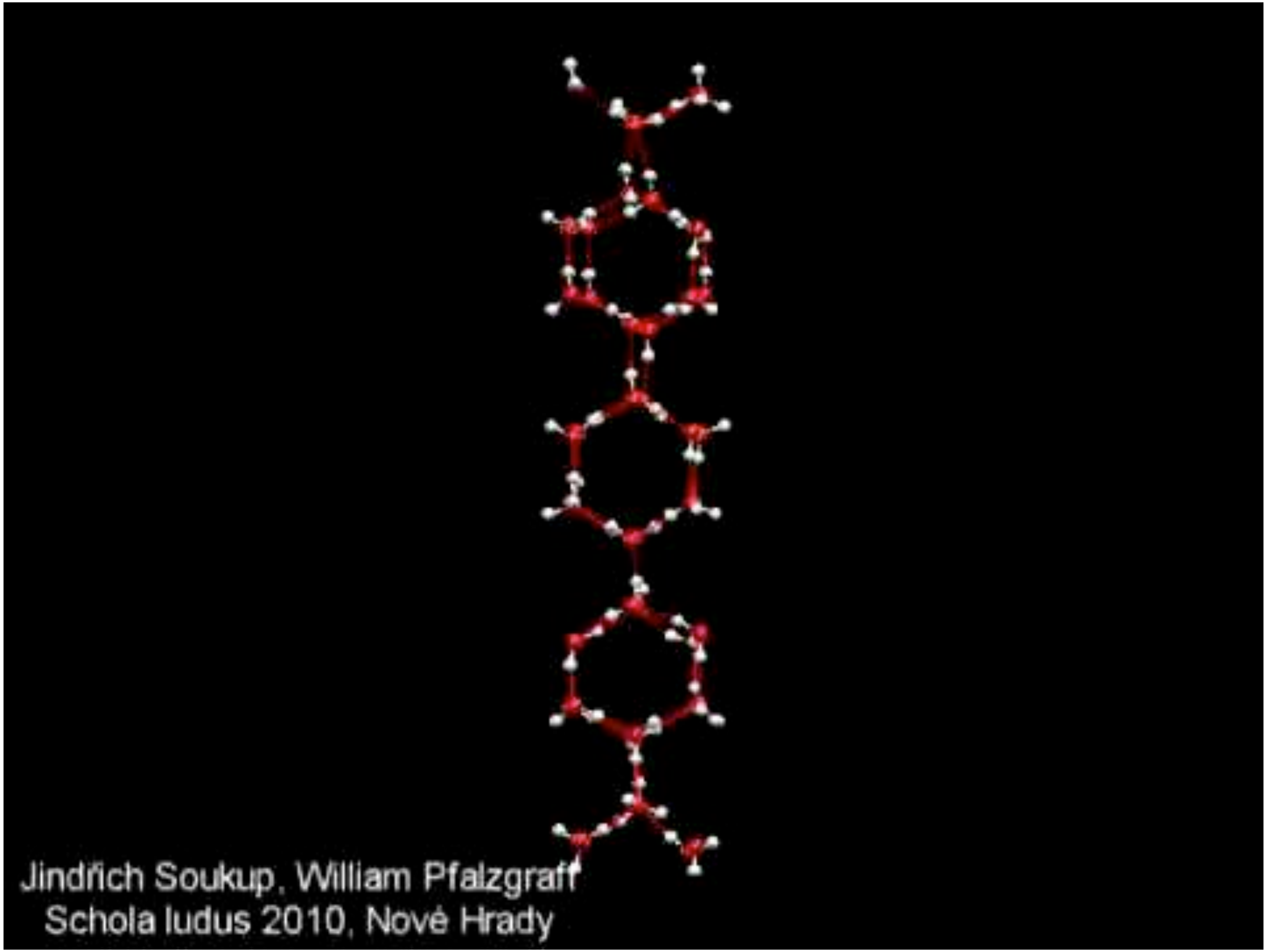


Gelo é menos denso que a água líquida

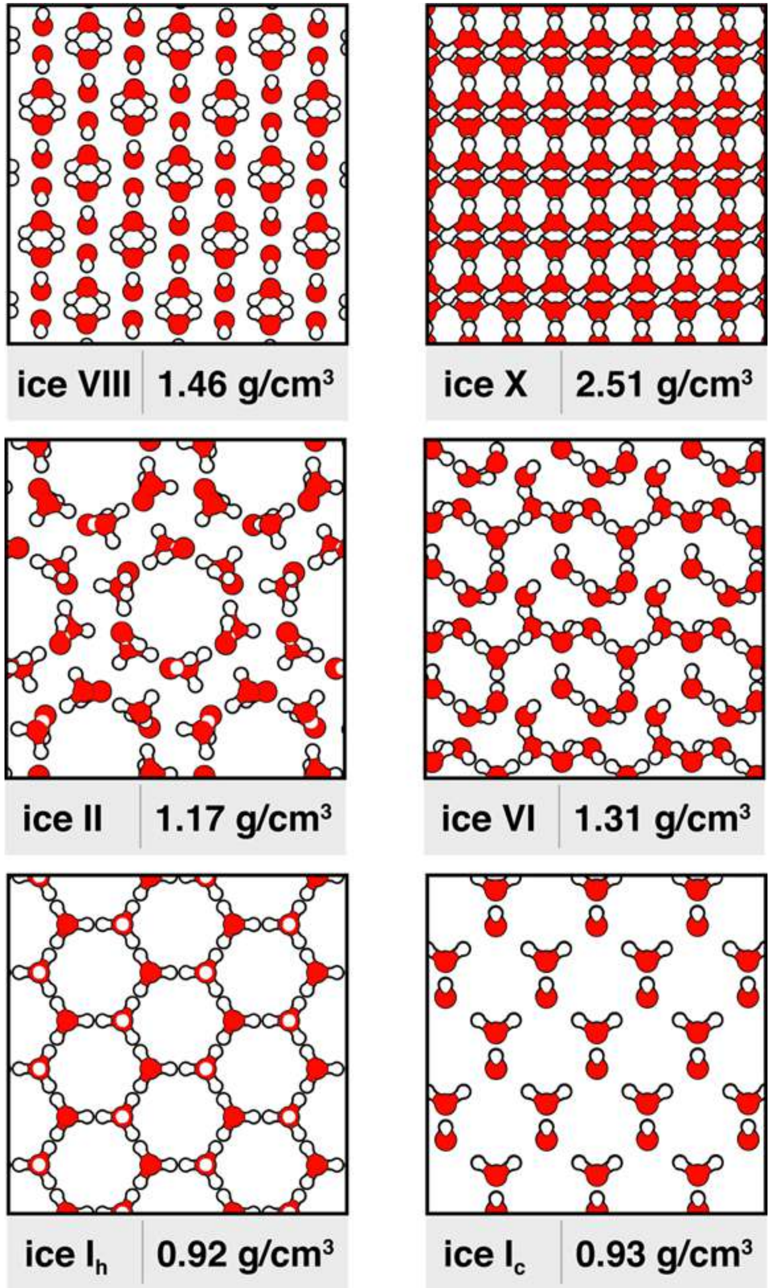
# ESTRUTURA DA ÁGUA-GELO

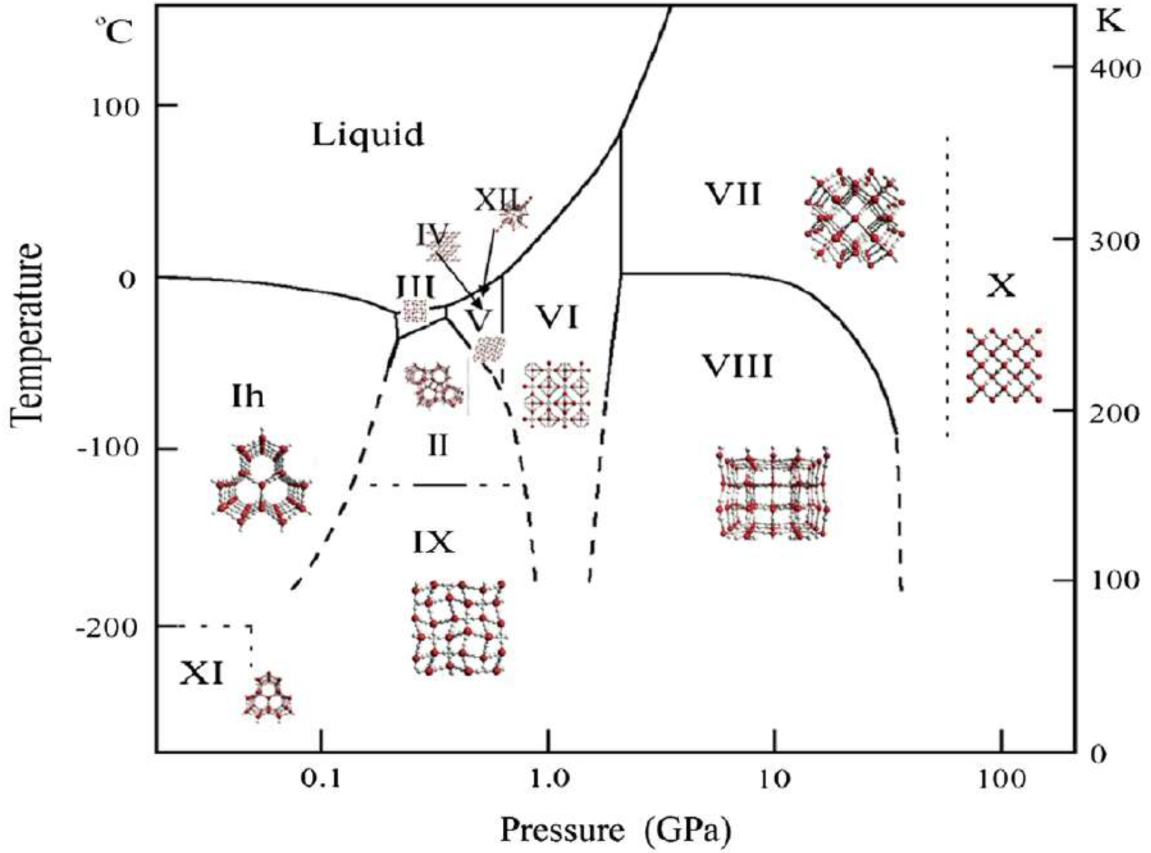


# ESTRUTURA DA ÁGUA-GELO



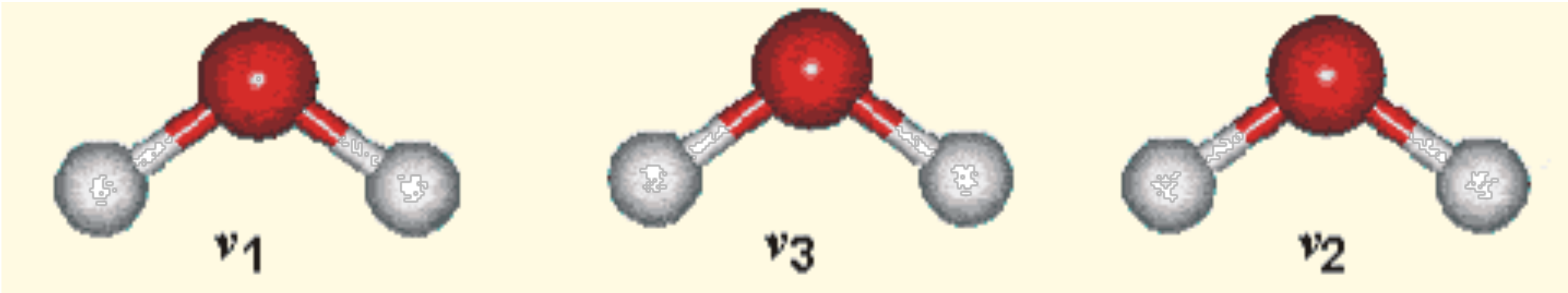
# ESTRUTURA DA ÁGUA: GELO (S)



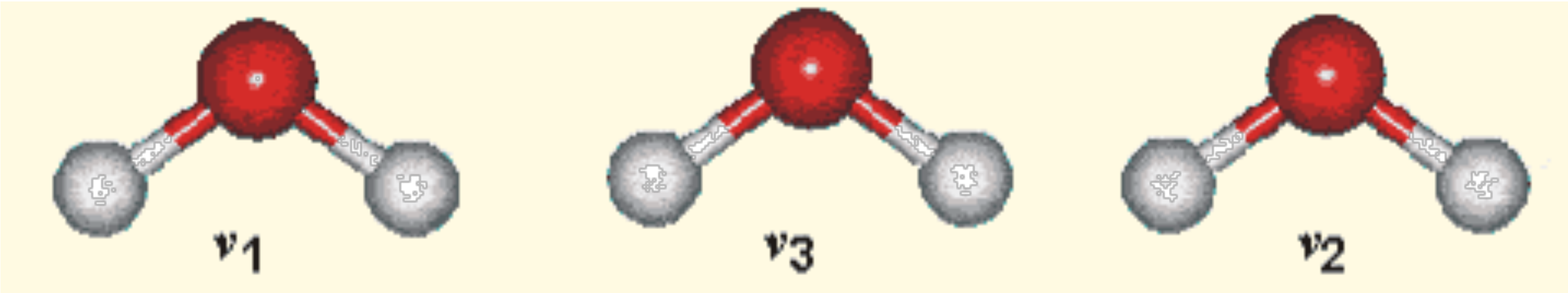
# COR DA ÁGUA

# MODOS NORMAIS DE VIBRAÇÃO



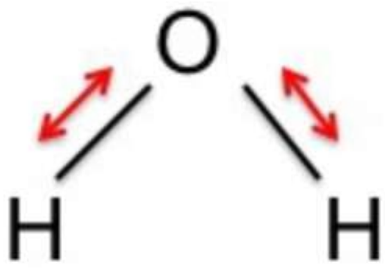

http://www1.lsbu.ac.uk/water/water_vibrational_spectrum.html

# MODOS NORMAIS DE VIBRAÇÃO



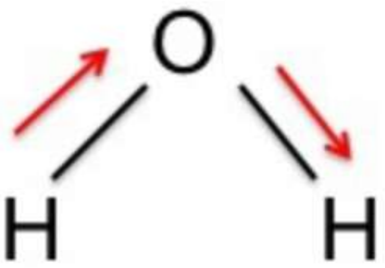

http://www1.lsbu.ac.uk/water/water_vibrational_spectrum.html

# MODOS NORMAIS DE VIBRAÇÃO



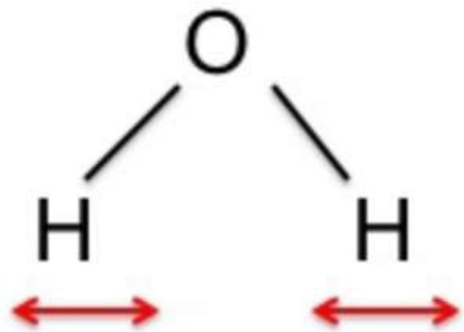

estiramento
simétrico

~3657 $cm^{-1}$




estiramento
assimétrico

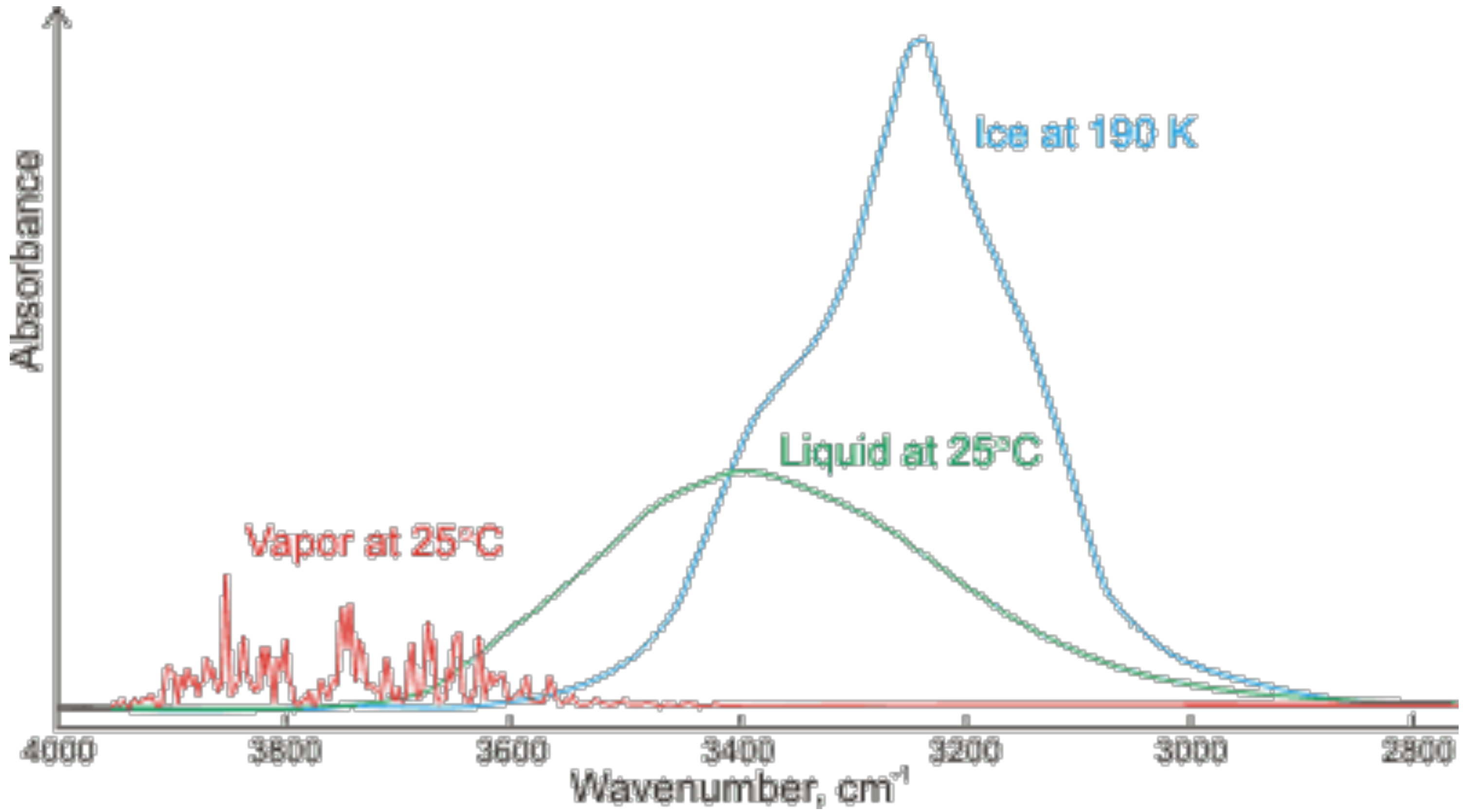
~3700 $cm^{-1}$




deformação
angular

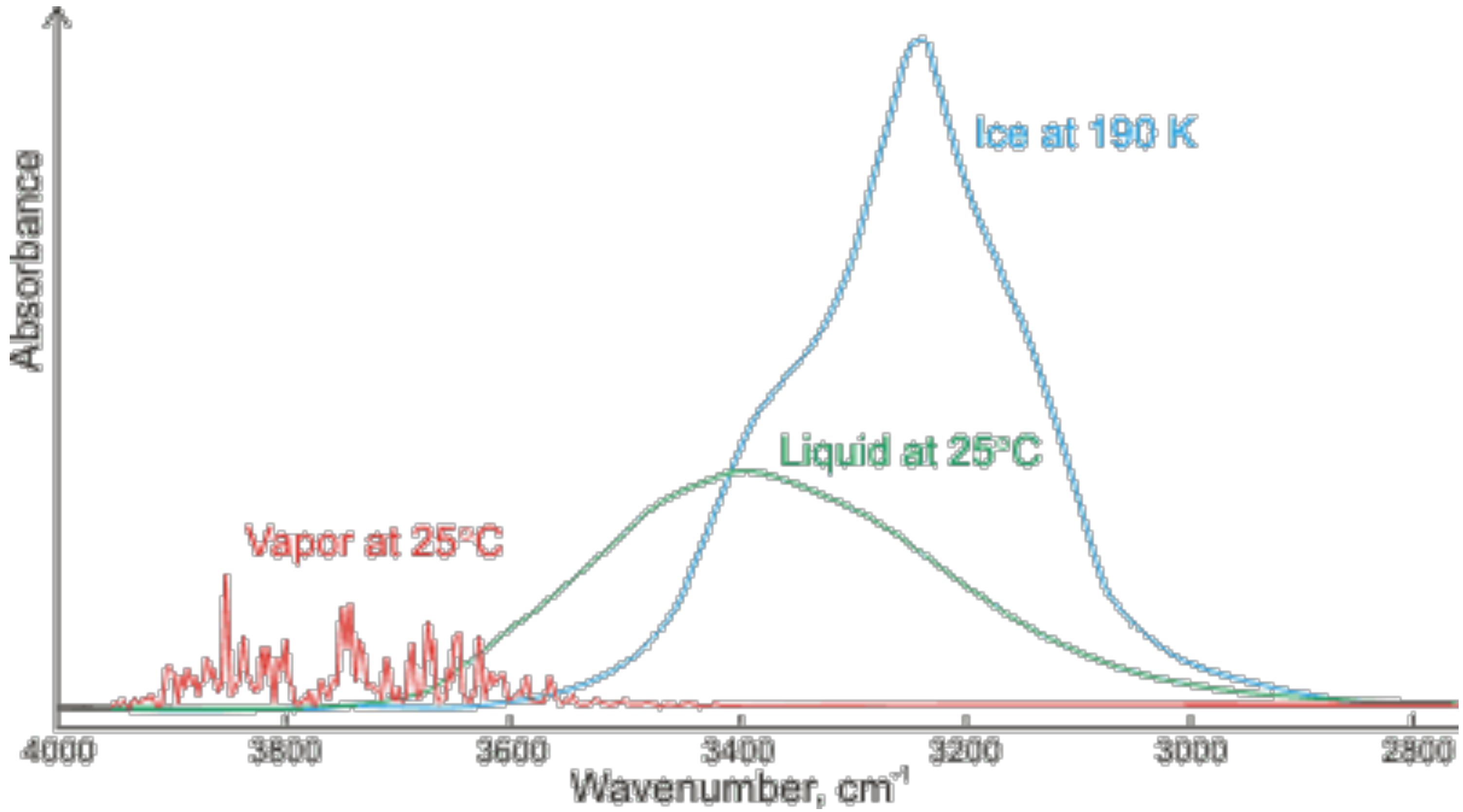
~1600 $cm^{-1}$

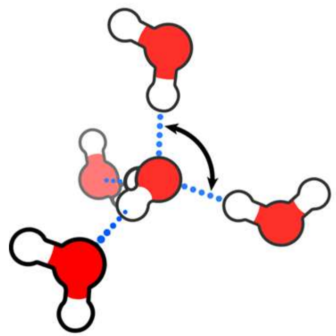
# ESPECTRO VIBRACIONAL




http://www1.lsbu.ac.uk/water/water_vibrational_spectrum.html

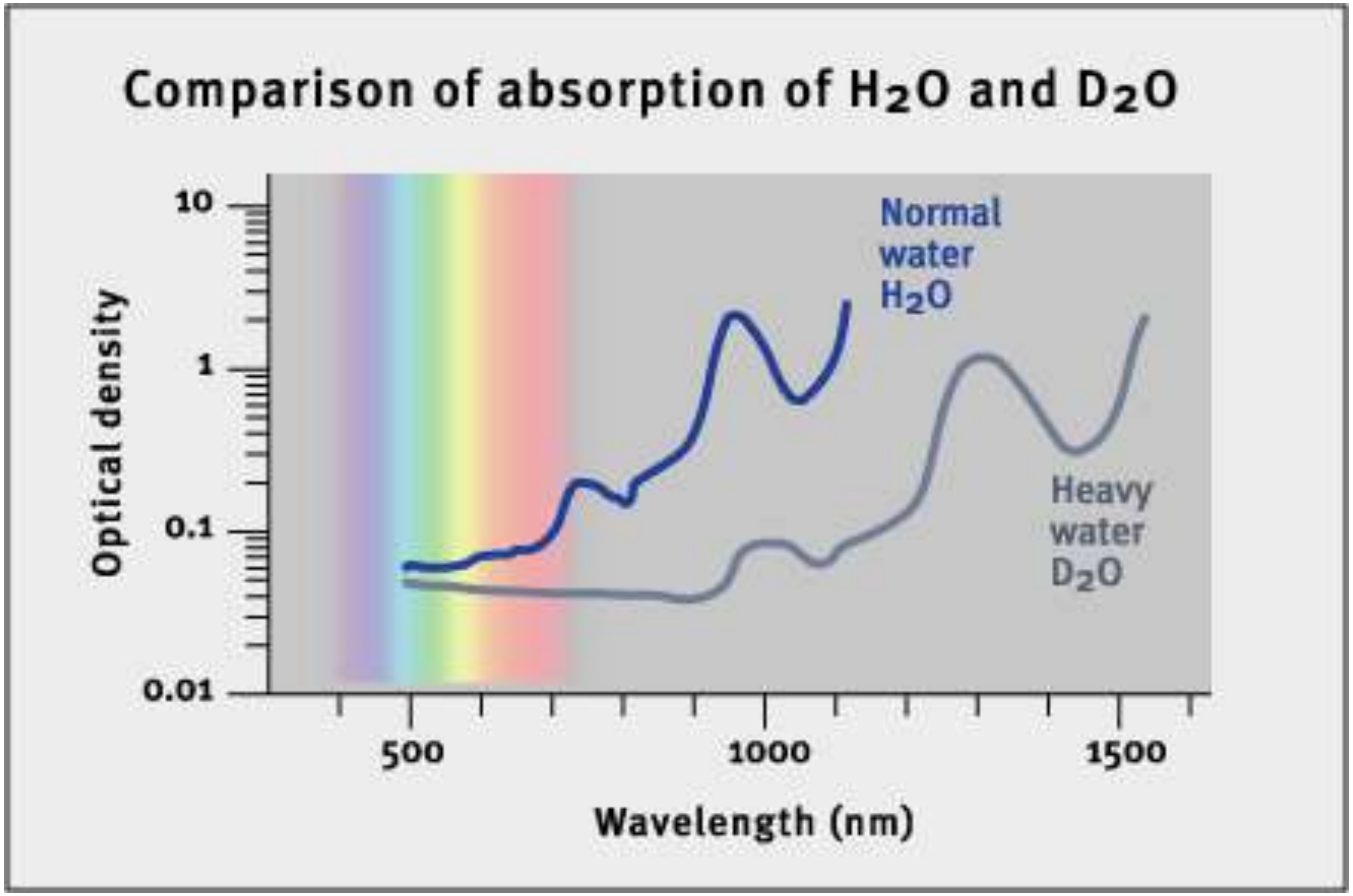
# ESPECTRO VIBRACIONAL



http://www1.lsbu.ac.uk/water/water_vibrational_spectrum.html

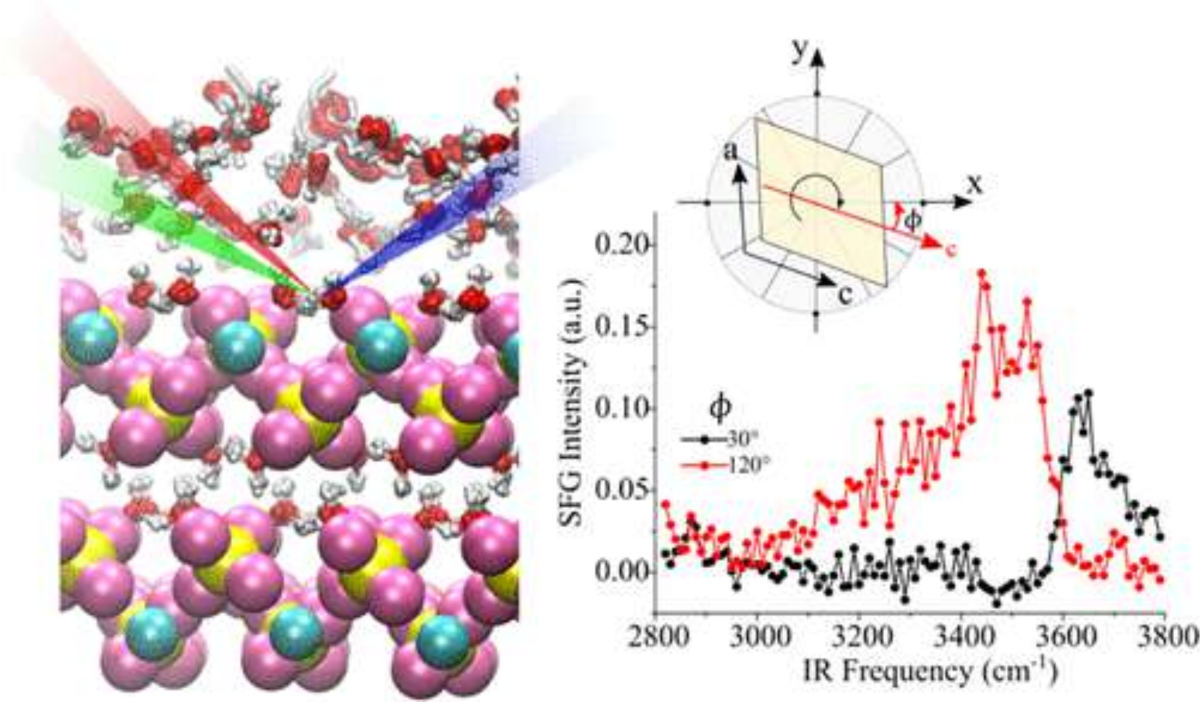
# COR DA ÁGUA




http://www.webexhibits.org/causesofcolor/5B.html

# INTERFACES SÓLIDO-ÁGUA

# INTERFACES SÓLIDO-ÁGUA

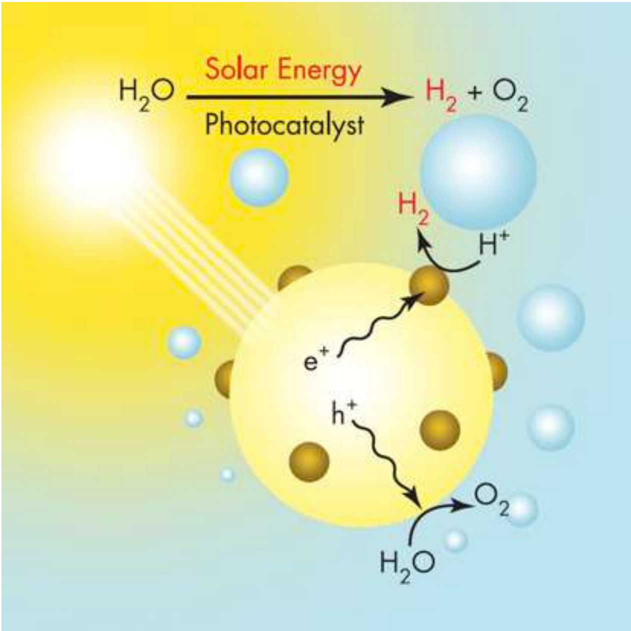



J. C. C. S., *et al*, JACS 140, 17141 (2018)

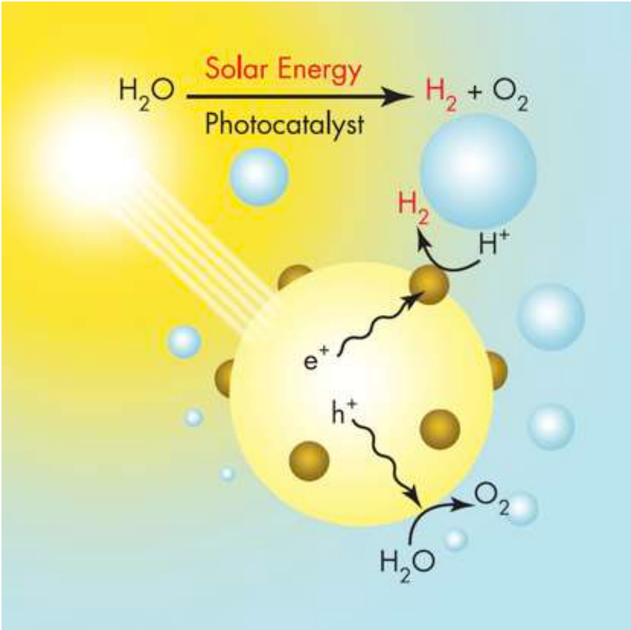
# INTERFACES SÓLIDO-ÁGUA

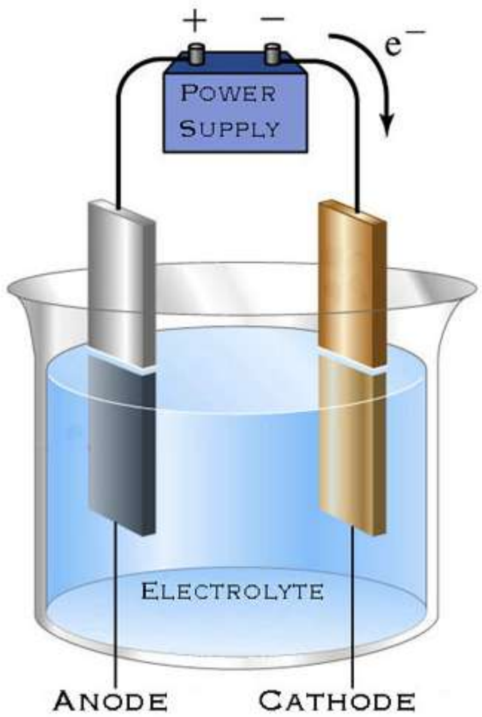
# INTERFACES SÓLIDO-ÁGUA

# INTERFACES SÓLIDO-ÁGUA

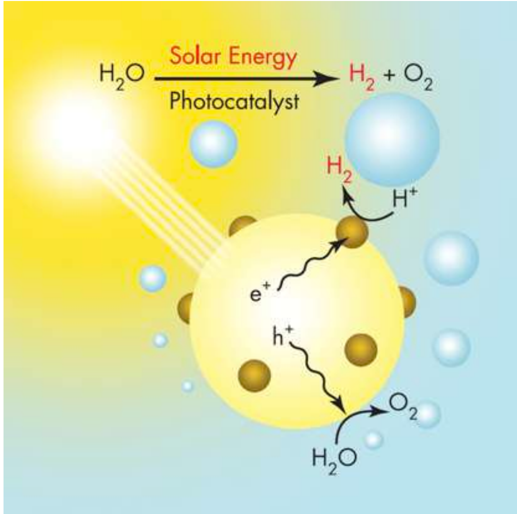


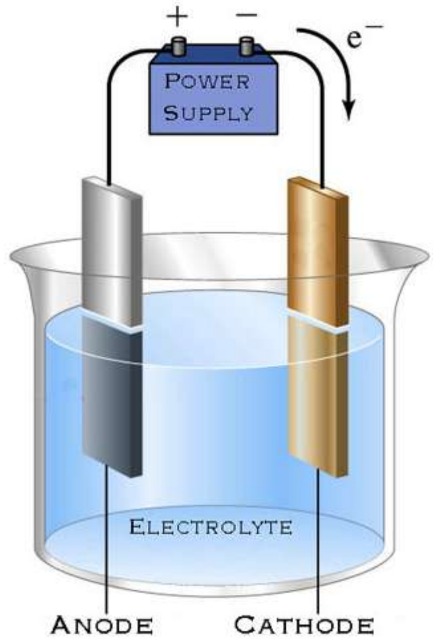
# INTERFACES SÓLIDO-ÁGUA

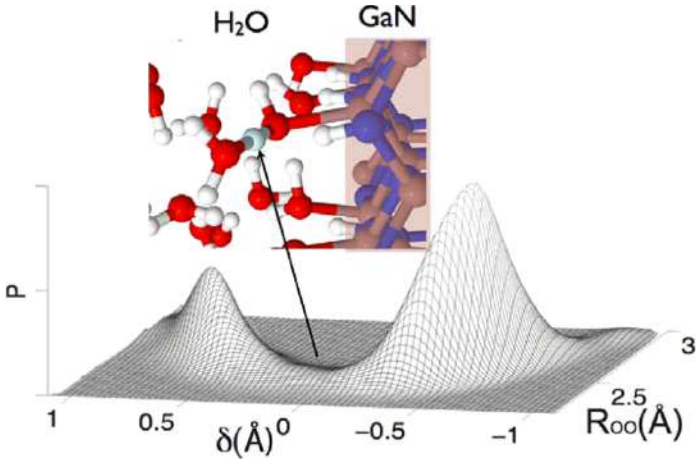


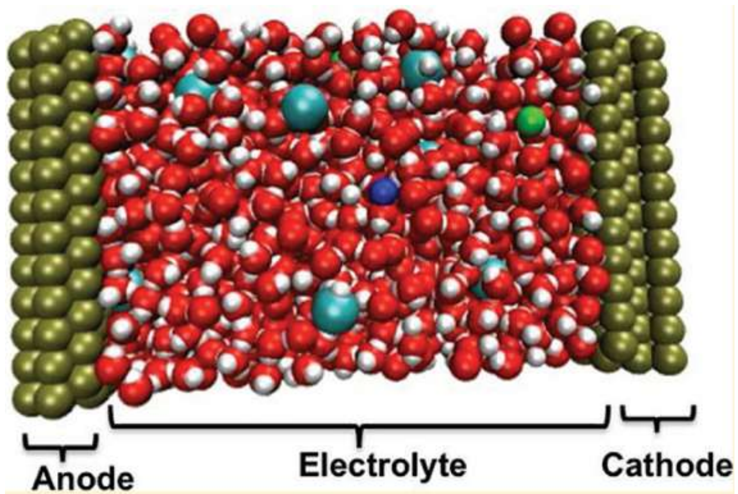
# INTERFACES SÓLIDO-ÁGUA




J. Wang *et al*,
J. Phys. Chem. C, 116, 14382 (2012)



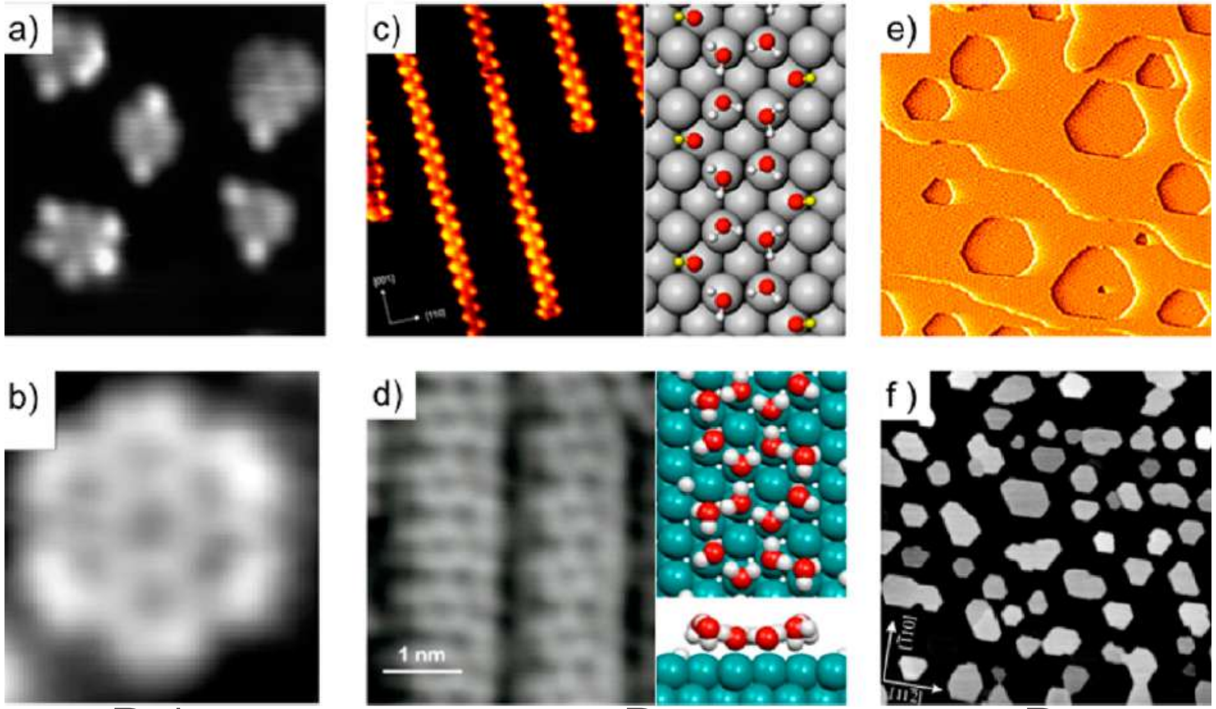

M. K. Petersen *et al*,
J. Phys. Chem. C, 116, 4903 (2012)

# METAL-ÁGUA

## METAL-ÁGUA (MONOCAMADA)

- Diferentes estruturas de água

Ru 130 K | Cu 150 K | Pt 140 K



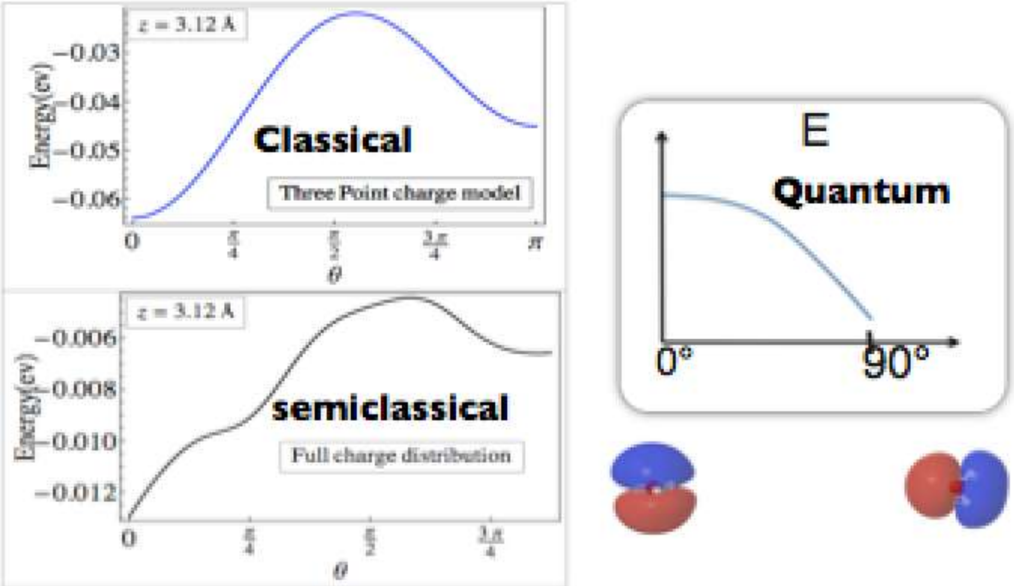

Pd 100 K | Ru 145 K | Pt 140 K

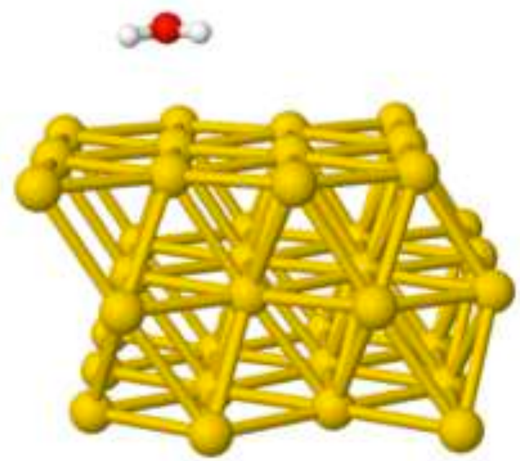
O. Björneholm *et al*, Chem. Rev., 116, 7698 (2016)

# METAL-ÁGUA

METAL-ÁGUA (1 $H_2O$)

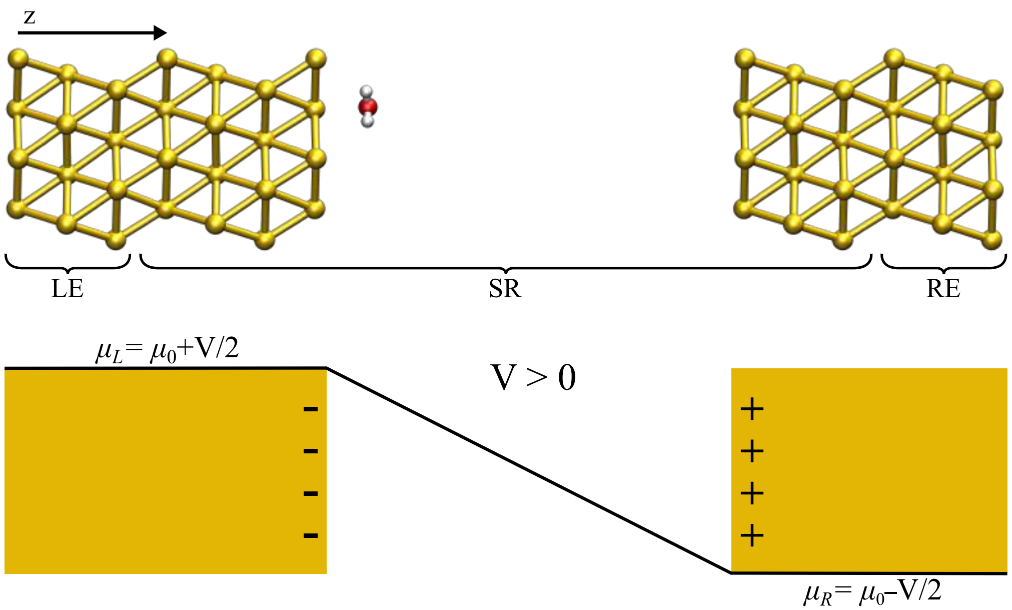
- Descrição quântica

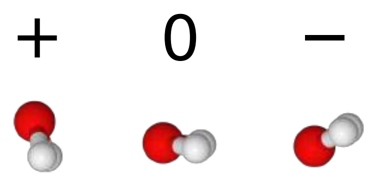


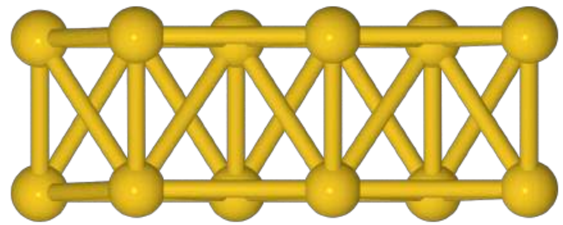



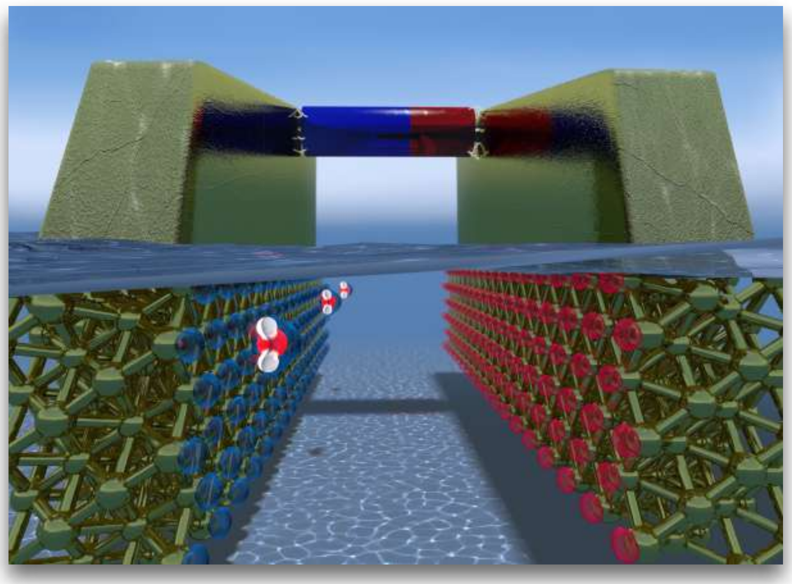
A. Poissier *et al*,
Phys. Chem. Chem. Phys., 13, 3375 (2011)

# SÓLIDO-ÁGUA





LSP *et al*, Chem. Science, 142, 034706 (2017)

Mecânica quântica

$$\left[\sum_{i}^{N}\left(-\frac{\hbar^2\nabla_i^2}{2m}+v(\mathbf{r}_i)\right)+\sum_{i<j}U\left(\mathbf{r}_i,\mathbf{r}_j\right)\right]\Psi=E\Psi$$

Mecânica quântica

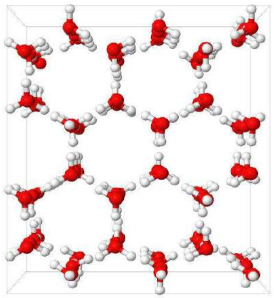
$$\left[\sum_{i}^{N}\left(-\frac{\hbar^2\nabla_i^2}{2m}+v(\mathbf{r}_i)\right)+\sum_{i<j}U\left(\mathbf{r}_i,\mathbf{r}_j\right)\right]\Psi=E\Psi$$

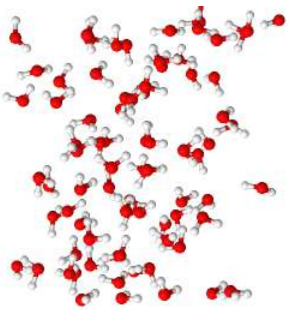
Computação alto desempenho

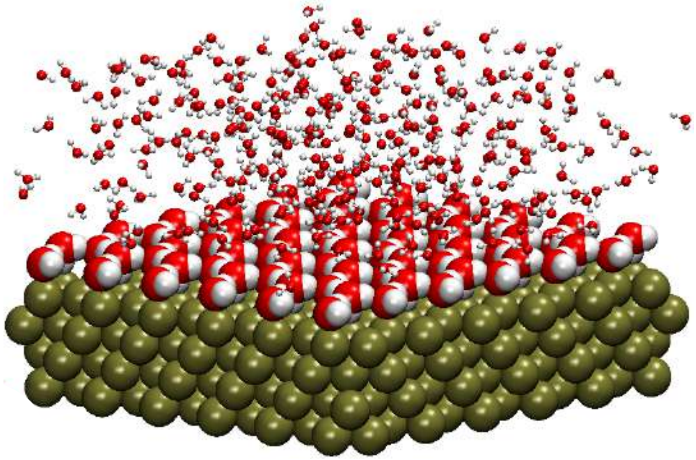
Mecânica quântica

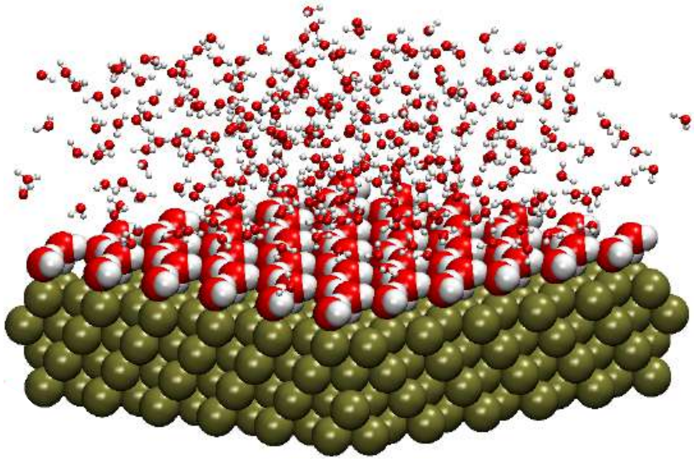
$$\left[\sum_{i}^{N}\left(-\frac{\hbar^2\nabla_i^2}{2m}+v(\mathbf{r}_i)\right)+\sum_{i<j}U\left(\mathbf{r}_i,\mathbf{r}_j\right)\right]\Psi=E\Psi$$

Computação alto desempenho



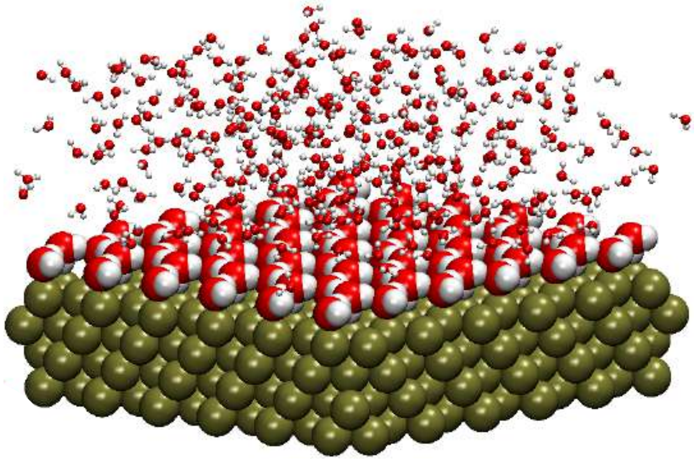






Mecânica quântica

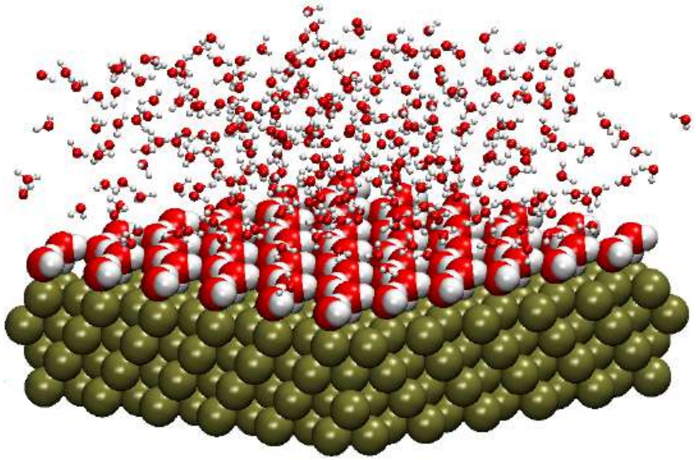
$$\left[\sum_{i}^{N}\left(-\frac{\hbar^2\nabla_i^2}{2m}+v(\mathbf{r}_i)\right)+\sum_{i<j}U\left(\mathbf{r}_i,\mathbf{r}_j\right)\right]\Psi=E\Psi$$



Mecânica quântica

$$\left[\sum_{i}^{N}\left(-\frac{\hbar^2\nabla_i^2}{2m}+v(\mathbf{r}_i)\right)+\sum_{i<j}U\left(\mathbf{r}_i,\mathbf{r}_j\right)\right]\Psi=E\Psi$$

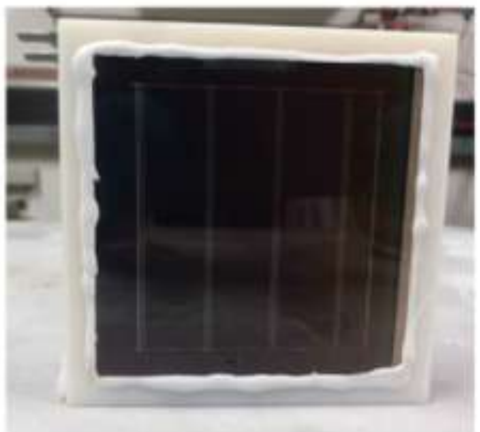
Computação alto desempenho



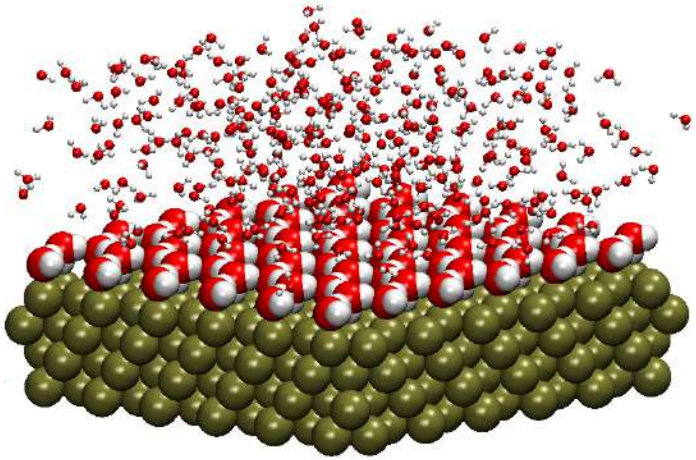
Mecânica quântica

$$\left[\sum_{i}^{N}\left(-\frac{\hbar^2\nabla_i^2}{2m}+v(\mathbf{r}_i)\right)+\sum_{i<j}U\left(\mathbf{r}_i,\mathbf{r}_j\right)\right]\Psi=E\Psi$$

Computação alto desempenho



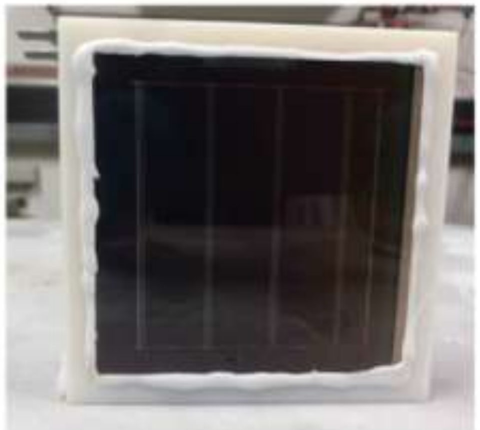
Adv. Sustainable Syst. 4, 2000070 (2020)



Mecânica quântica

$$\left[\sum_{i}^{N}\left(-\frac{\hbar^2\nabla_i^2}{2m}+v(\mathbf{r}_i)\right)+\sum_{i<j}U\left(\mathbf{r}_i,\mathbf{r}_j\right)\right]\Psi=E\Psi$$

Computação alto desempenho



Adv. Sustainable Syst. 4, 2000070 (2020)

# Obrigada!