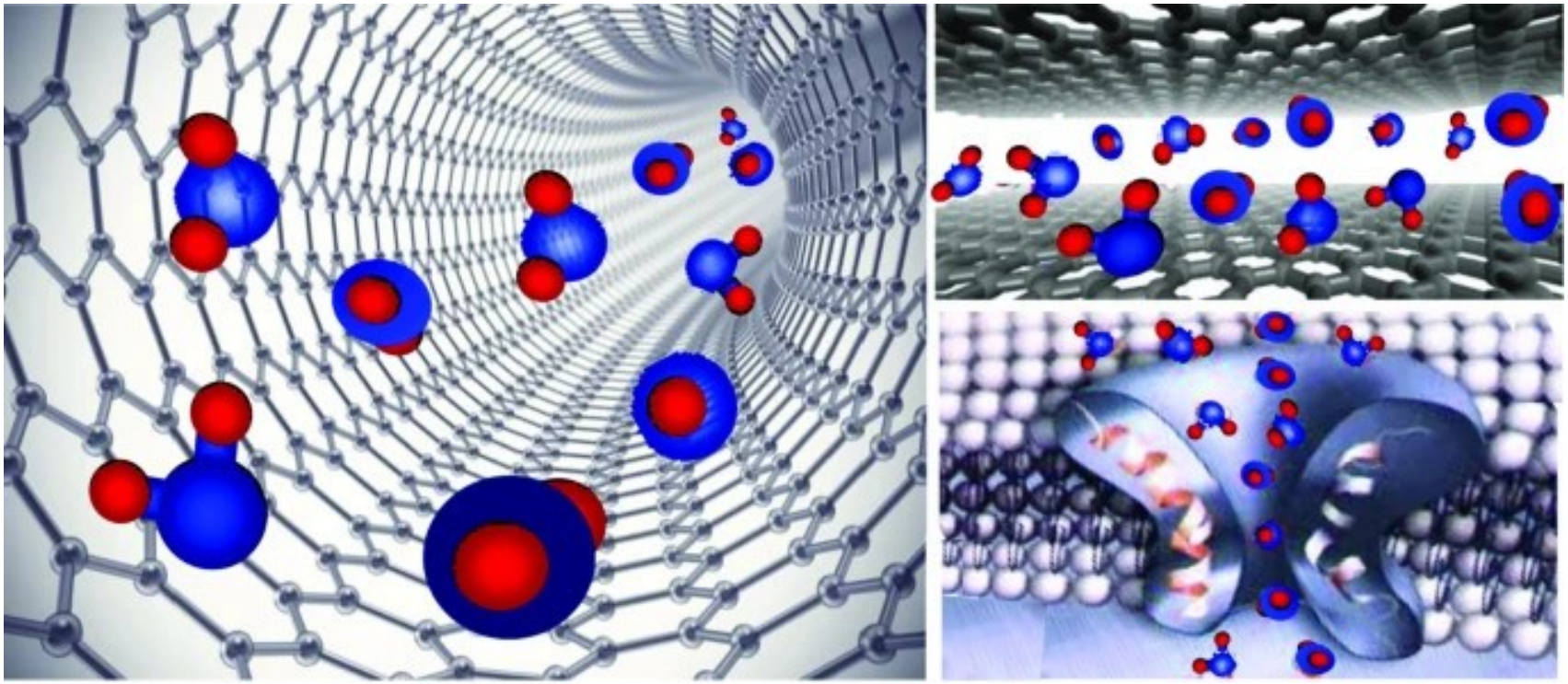
# Nanoconfined Water



https://link.springer.com/article/10.1140/epje/s10189-021-00136-4

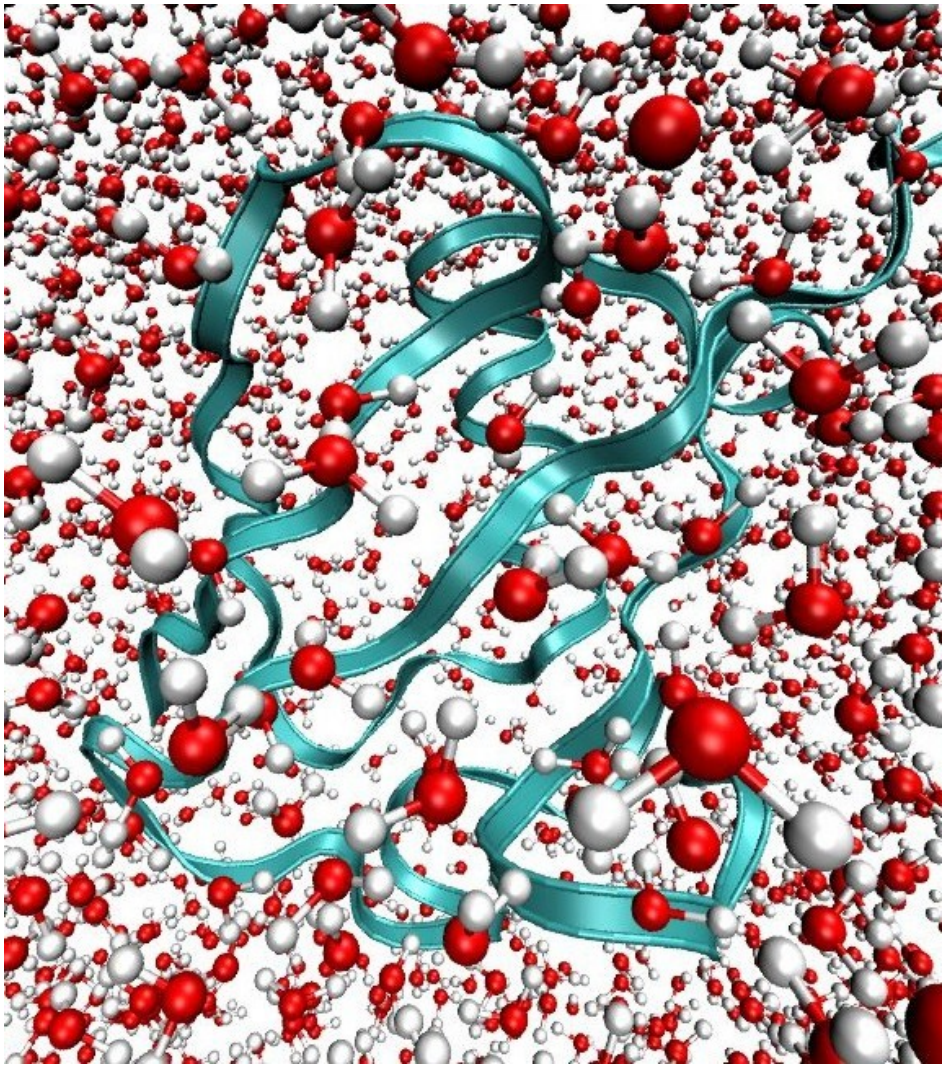
# Summary

**Phase Transitions-**
**Water Anomalies**

**Nanoconfined Water in**
**Solid State Materials**

**Nanoconfined Water in**
**Biology**

# Bio – Nanoconfined Water



https://web.mit.edu/tokmakofflab/ResearchProtein.htm

# Review

# Diffusion

$$< \Delta^2 r(t) >= \frac{1}{N} \sum_{i=1}^{N} < [\underline{R}_i(t) - \underline{R}_i(0)]^2 >$$

$$< \Delta^2 r(t) > \sim 6Dt$$

$$C(\mathbf{e}) = \langle \mathbf{e}(t) \cdot \mathbf{e}(0) \rangle$$

# Diffusion

$$\eta = \frac{V}{k_B T}\int_0^\infty \mathrm{d}t \left\langle P_{\alpha\beta}(t) P_{\alpha\beta}(0) \right\rangle,$$

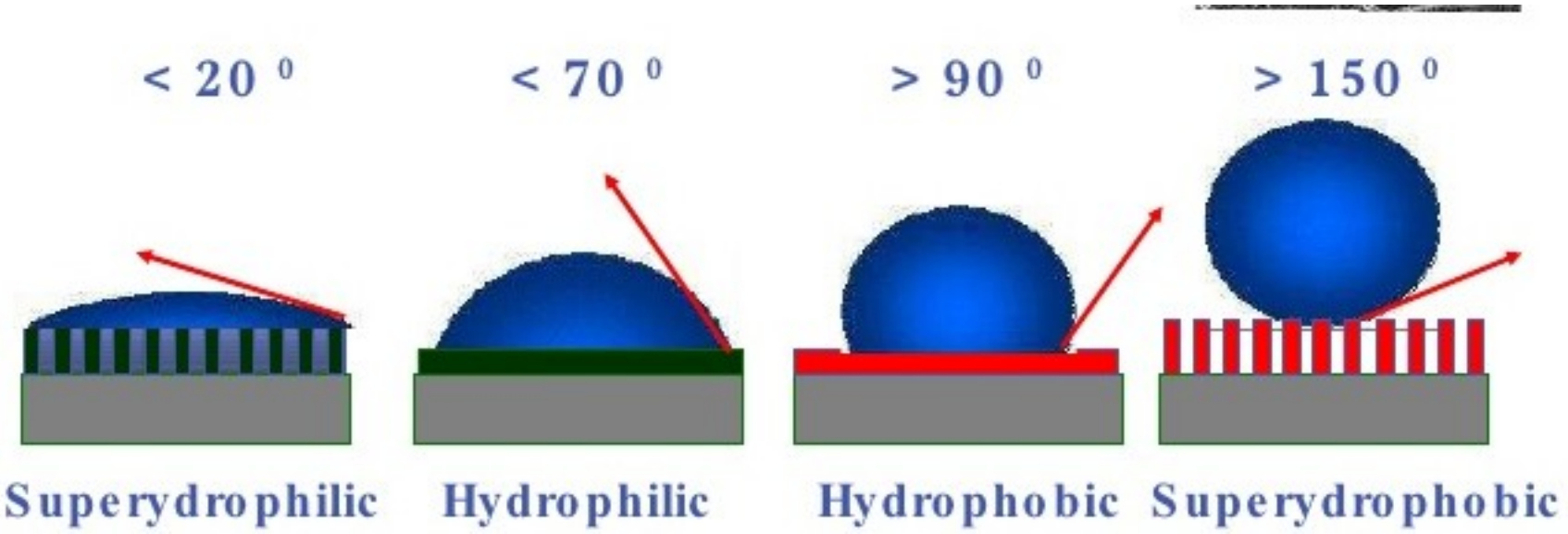
$$P_{\alpha\beta} = \frac{1}{V}\left(\sum_{i=1}^{N} \frac{p_{i\alpha} p_{i\beta}}{m} + \sum_{i=1}^{N}\sum_{j>i}^{N} r_{ij\alpha} f_{ij\beta}\right), \qquad (2)$$

where $P_{\alpha\beta}$ is the stress tensor, $r_{ij} = |\vec{r}_i - \vec{r}_j|$, $f_{ij} = -\partial U(r_{ij})/\partial r_{ij}$ and $\alpha, \beta \in (x,y,z)$ denotes Cartesian components.

$$D = \frac{k_B T}{6\pi\eta\sigma^3};$$

$$\langle \Delta^2 r(t) \rangle \sim 6Dt$$

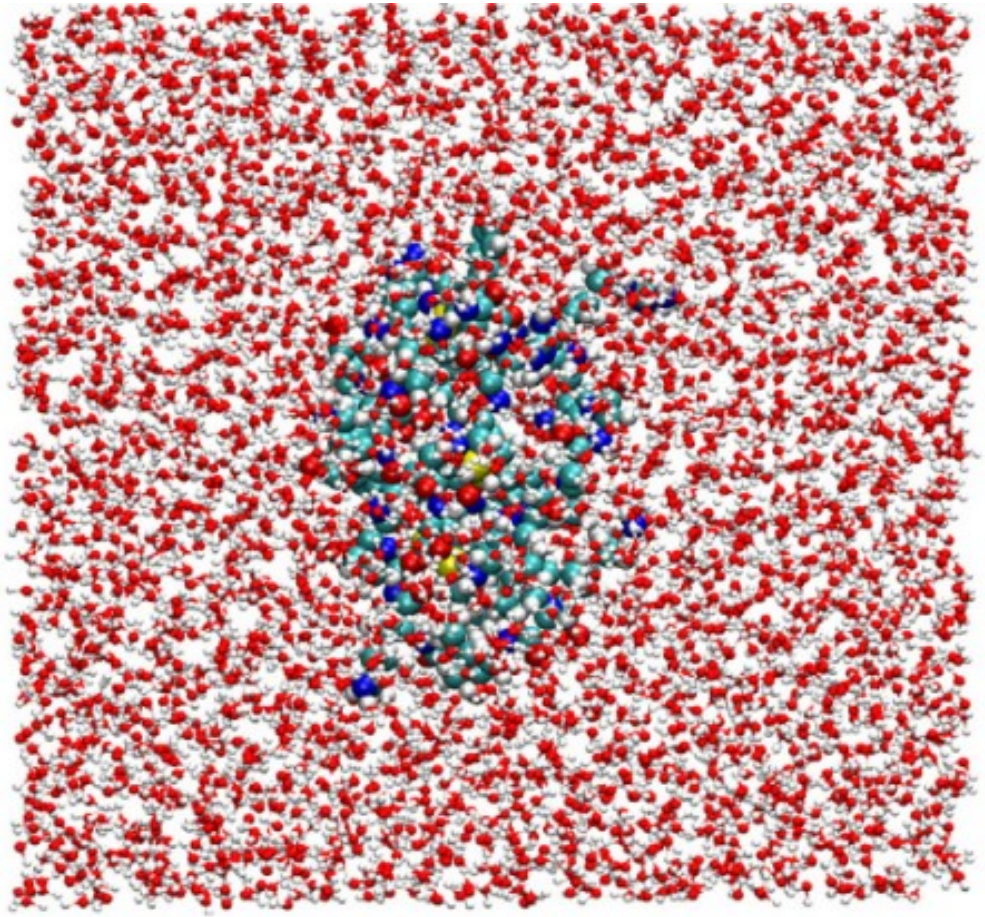
# Hydrophobic and Hydrophilic

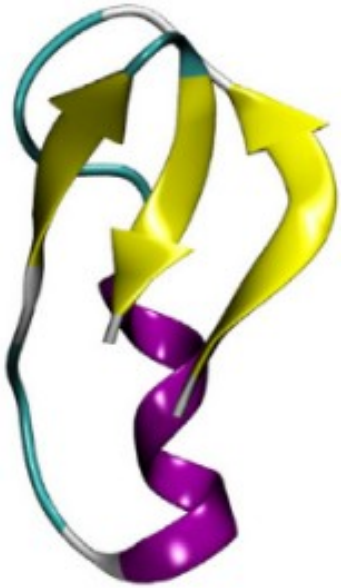


# Water in Proteins

# Water in Protein Surface

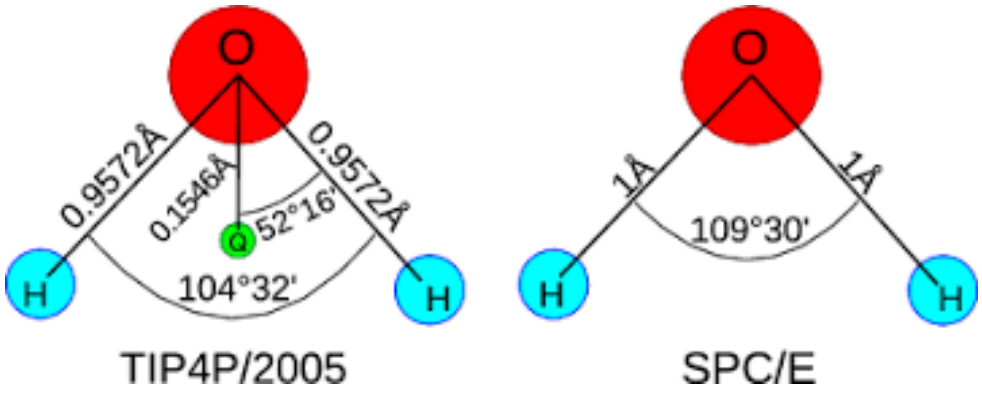
**R. Barbosa and MCB, Physica A 439 48 (2015).**





# Water in Protein Surface

**R. Barbosa and MCB, Physica A 439 48 (2015).**

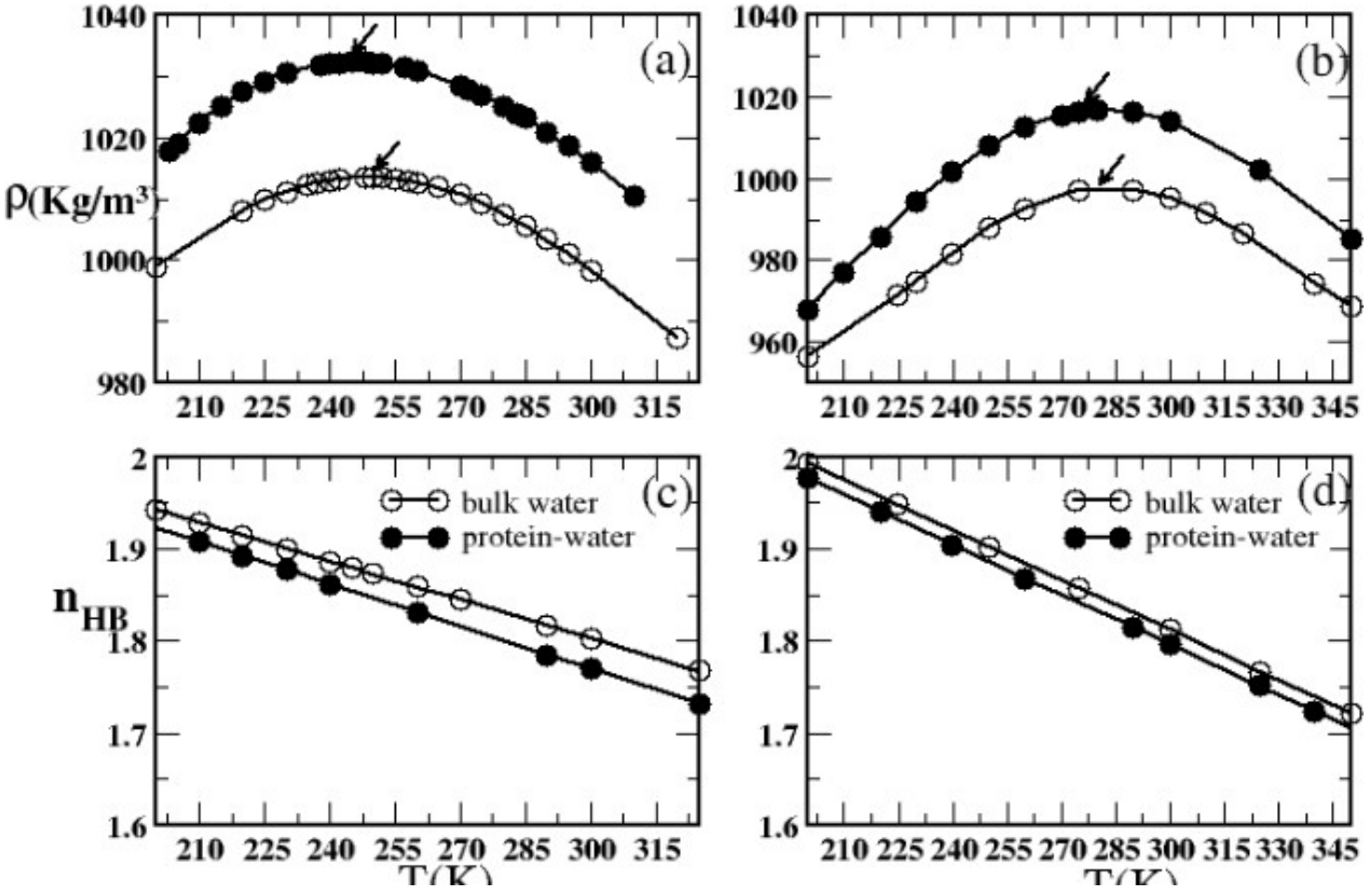



| Hydrophilic | Hydrophobic |
|---|---|
| Lysine | Valine |
| Arginine | Alanine |
| Aspartic Acid | Proline |
| Glycine | Leucine |
| Serine | Isoleucine |
| Threonine | - |
| Tyrosine | - |
| Asparagine | - |
| Glutamine | - |

3946 SPC/E water molecules
3916 TIP4P-2005 water molecules
Box 5.5 nm of length

# Density Anomaly

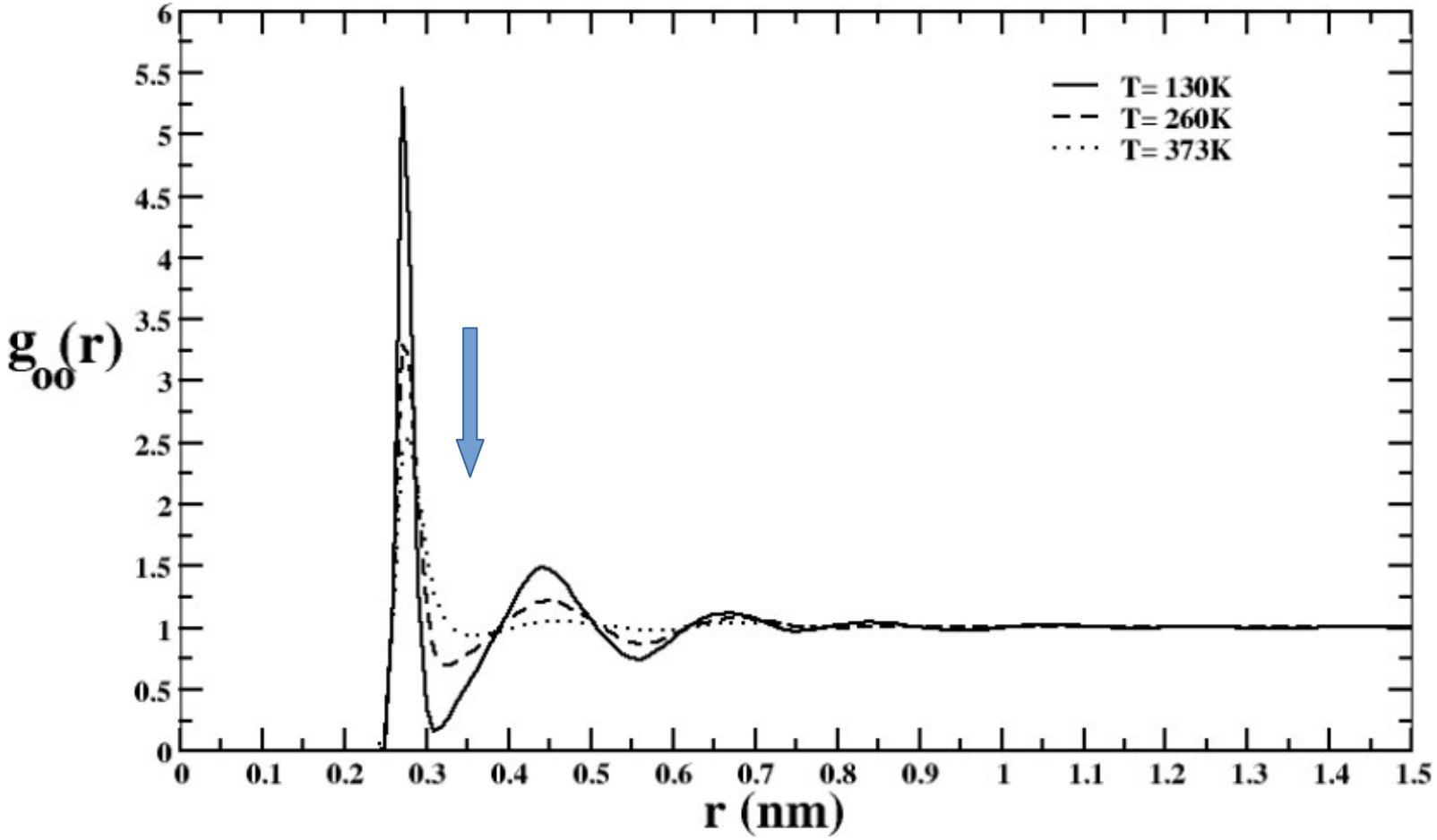
**R. Barbosa and MCB, Physica A 439 48 (2015).**




**SPC/E** **Tip4p/2005**

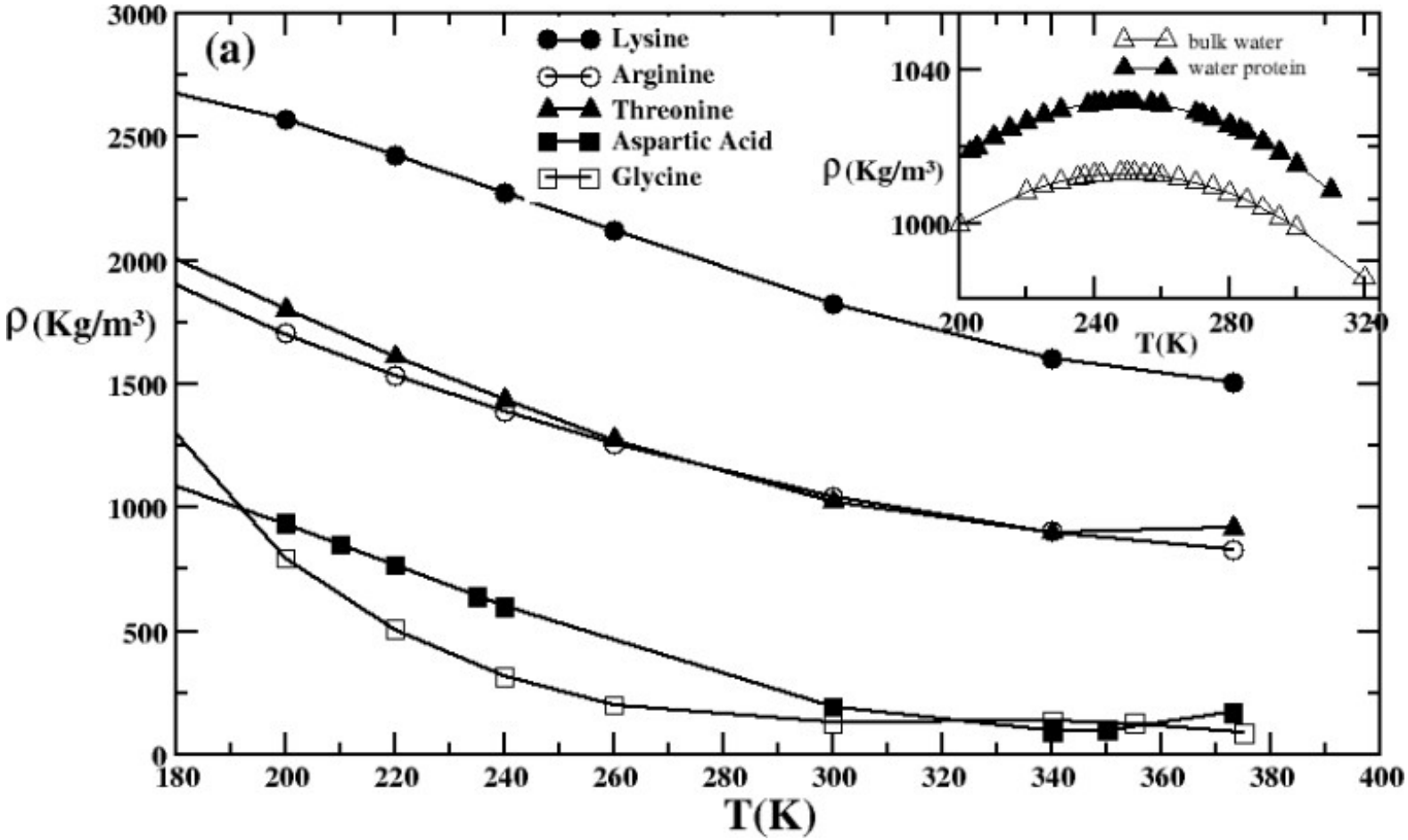
# Radial Distribution Function

R. Barbosa and MCB, Physica A 439 48 (2015).



# Density at Hydrophilic

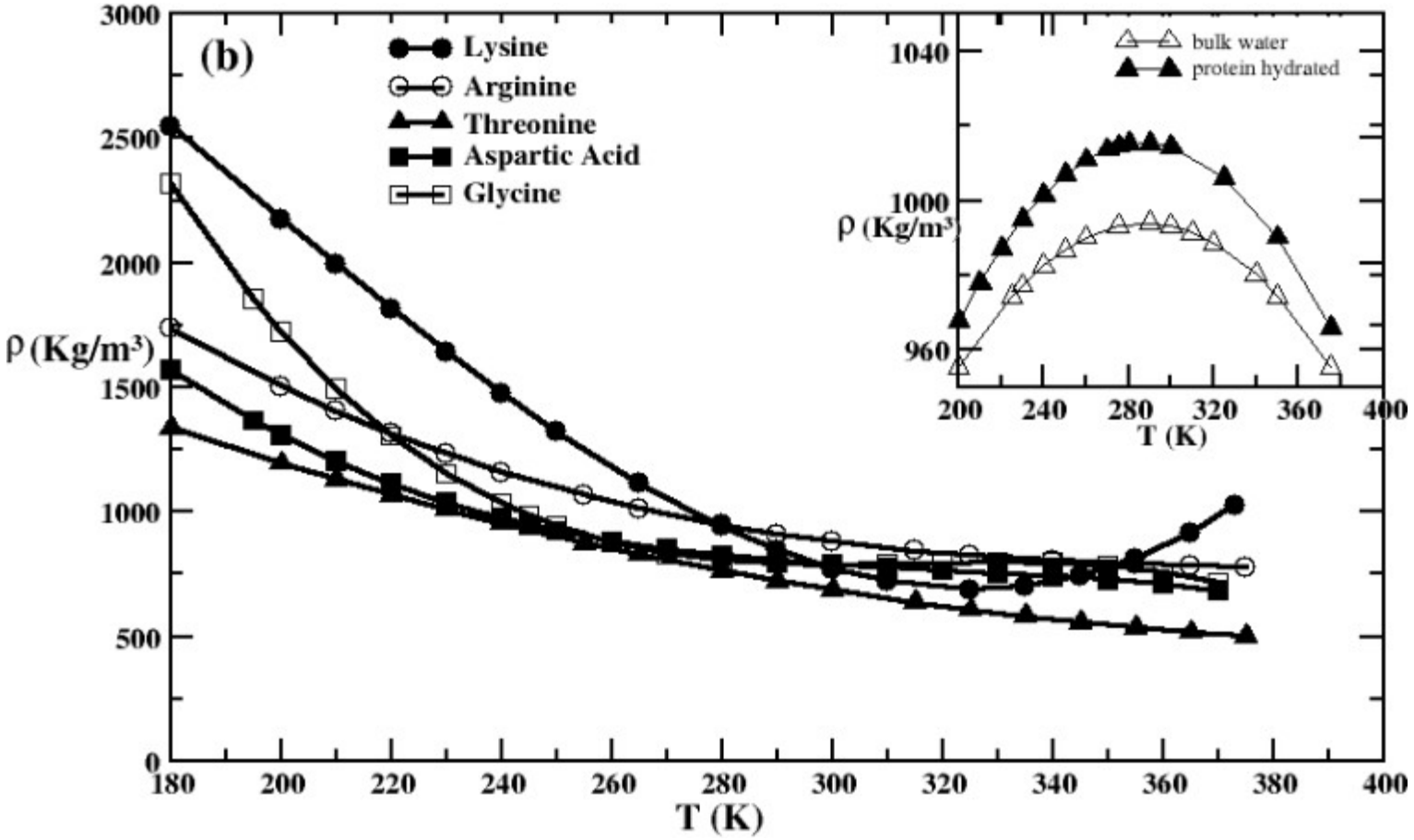
**R. Barbosa and MCB, Physica A 439 48 (2015).**




**SPC/E**

# Density at Hydrophilic

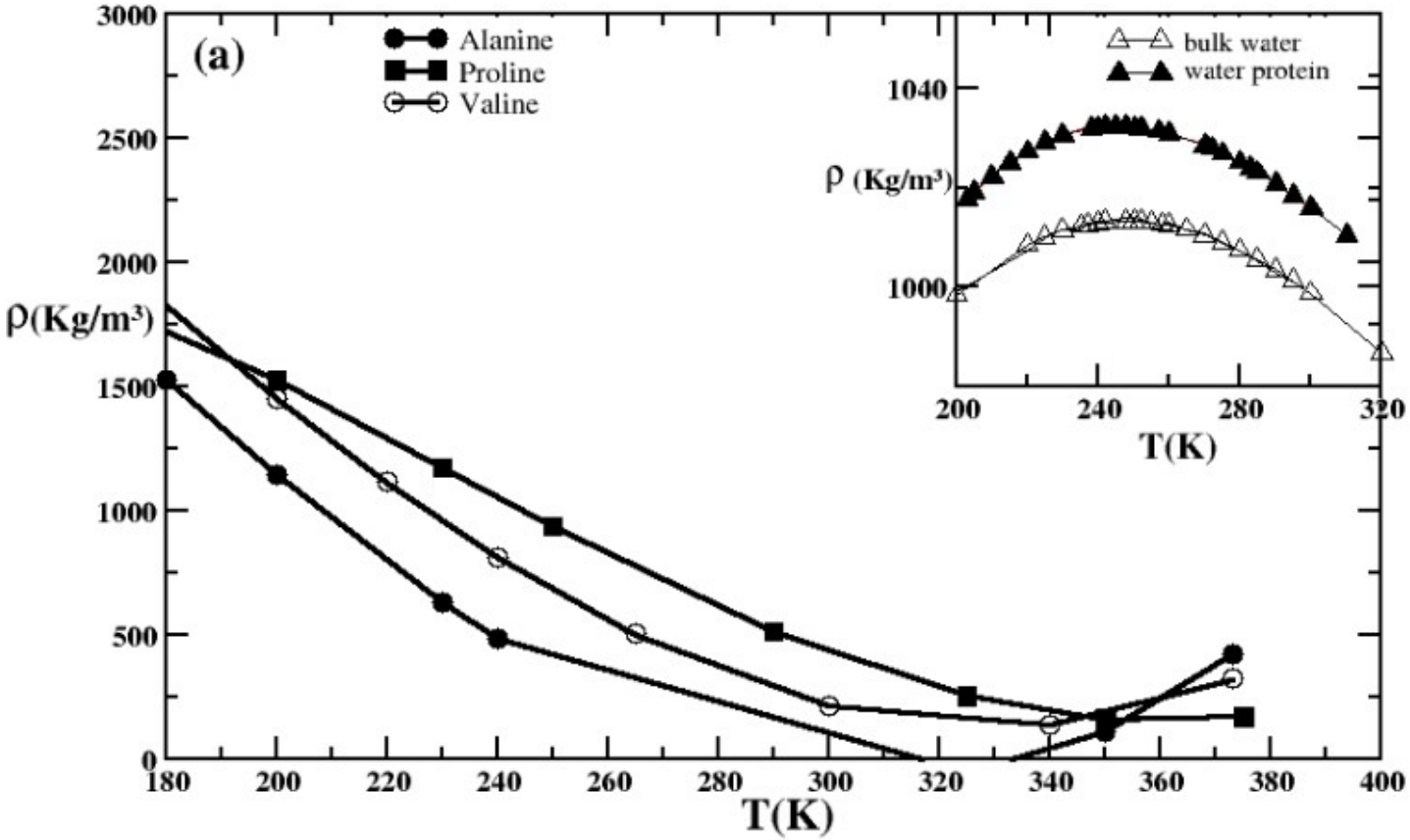
**R. Barbosa and MCB, Physica A 439 48 (2015).**




**Tip4p/2005**

# Density at Hydrophobic

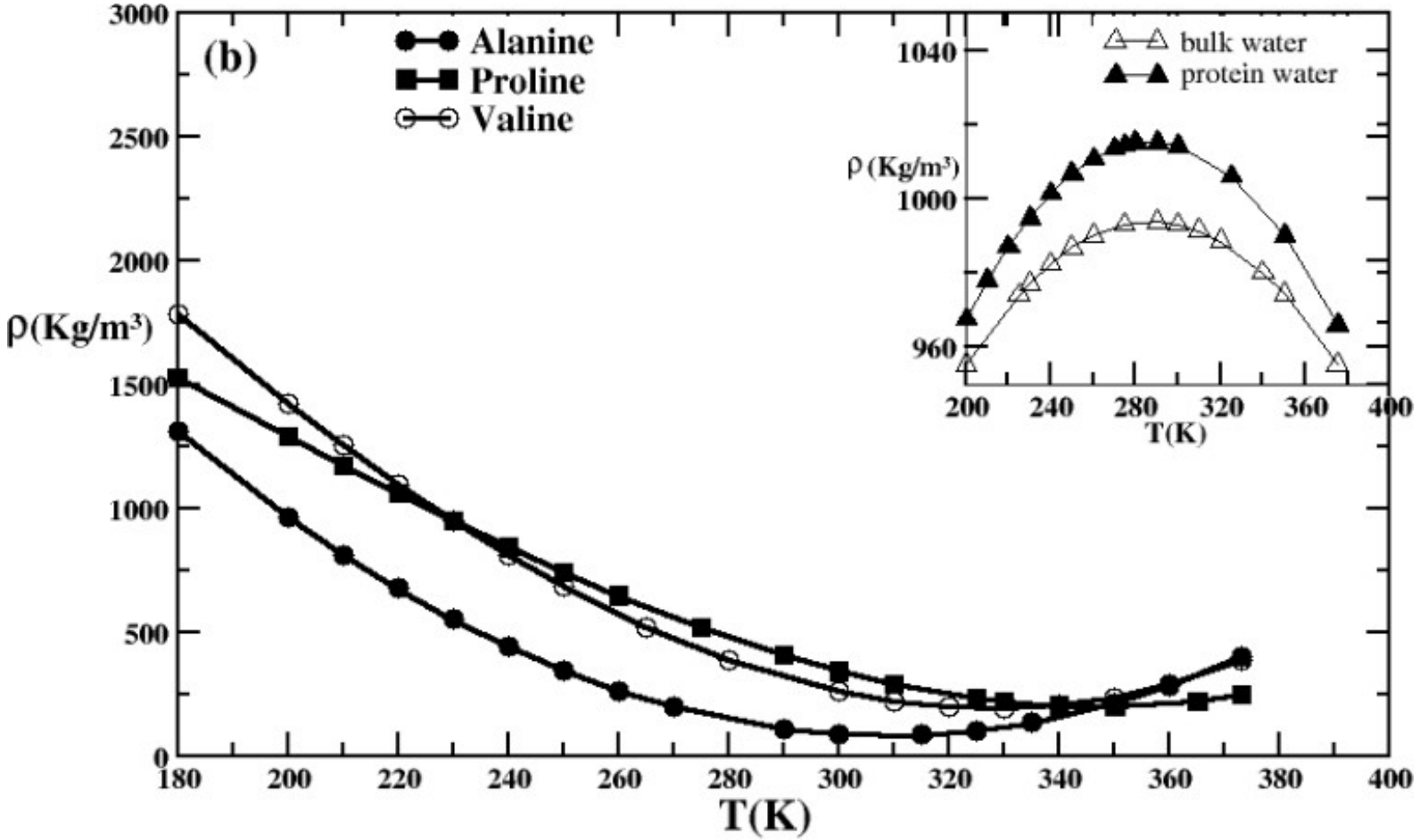
**R. Barbosa and MCB, Physica A 439 48 (2015).**




**SPC/E**

# Density at Hydrophobic

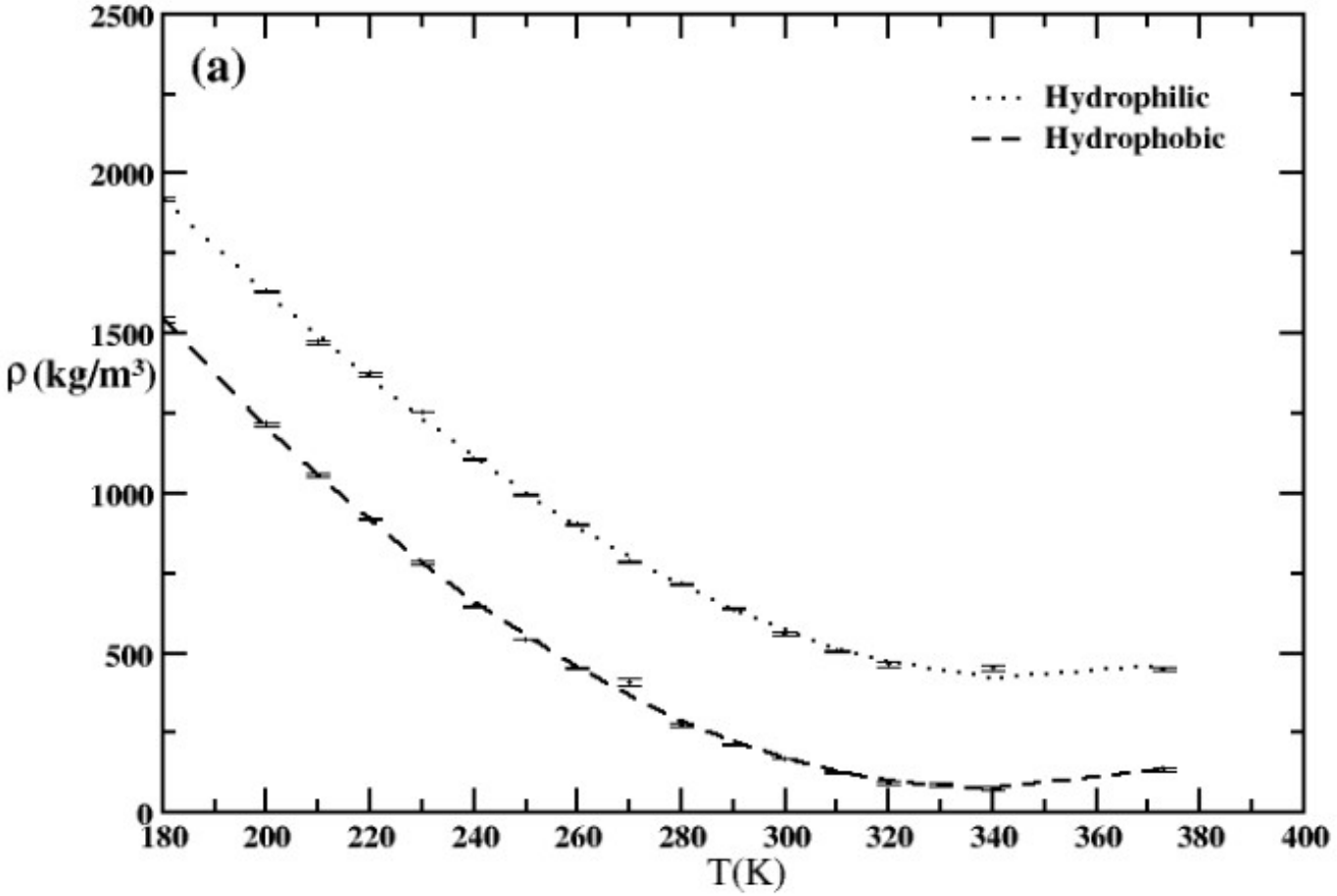
**R. Barbosa and MCB, Physica A 439 48 (2015).**




**Tip4p/2005**

# Density at Phobic/Philic

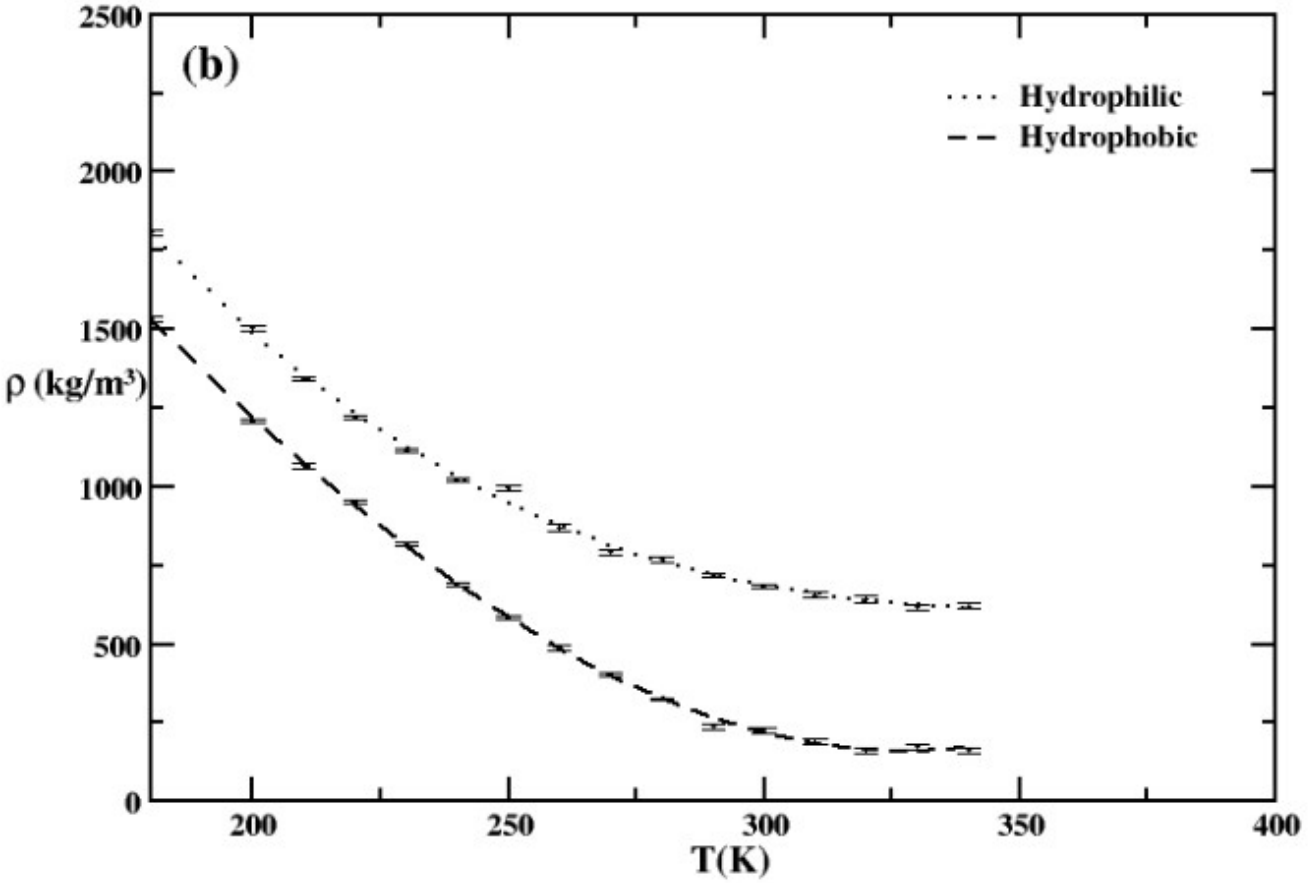
**R. Barbosa and MCB, Physica A 439 48 (2015).**




**SPC/E**

# Water in Protein Surface

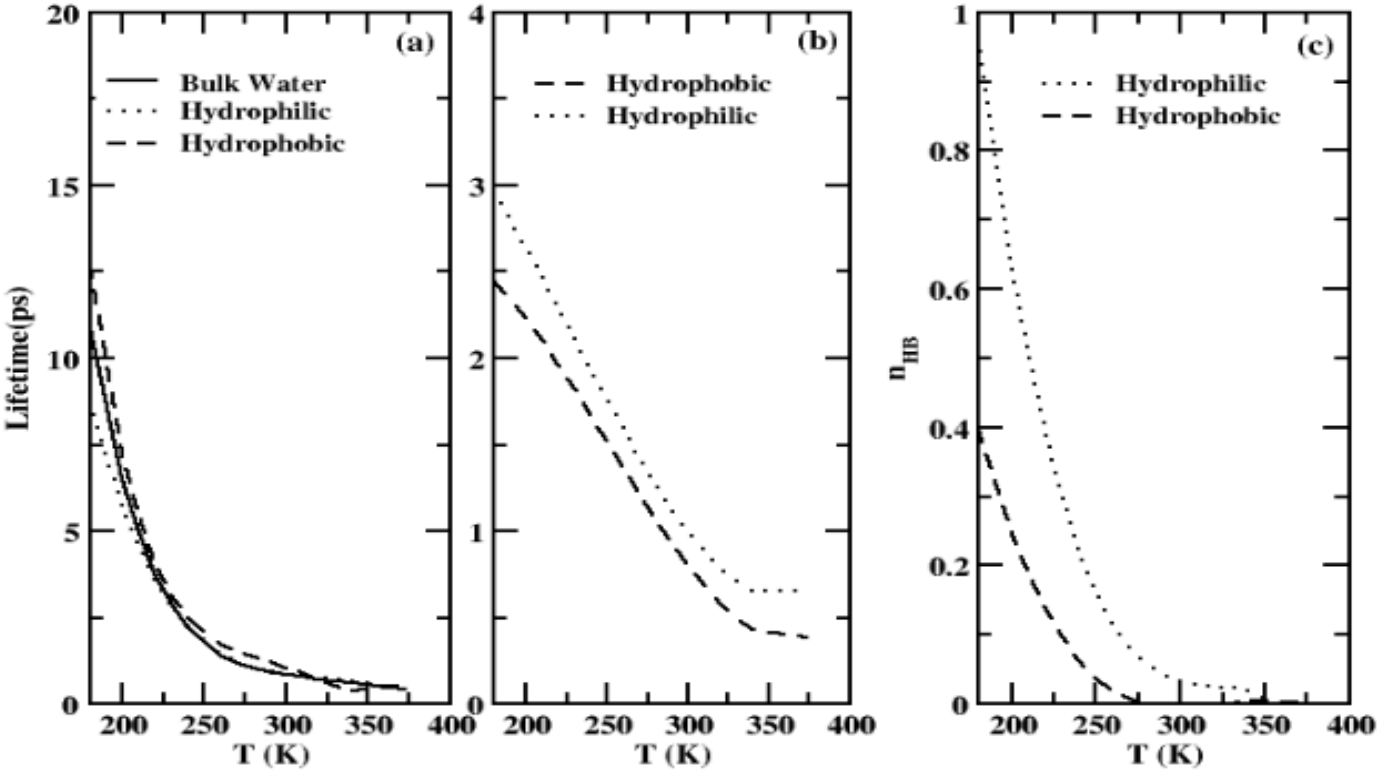
**R. Barbosa and MCB, Physica A 439 48 (2015).**




**Tip4p/2005**

# Hydrogen Bond

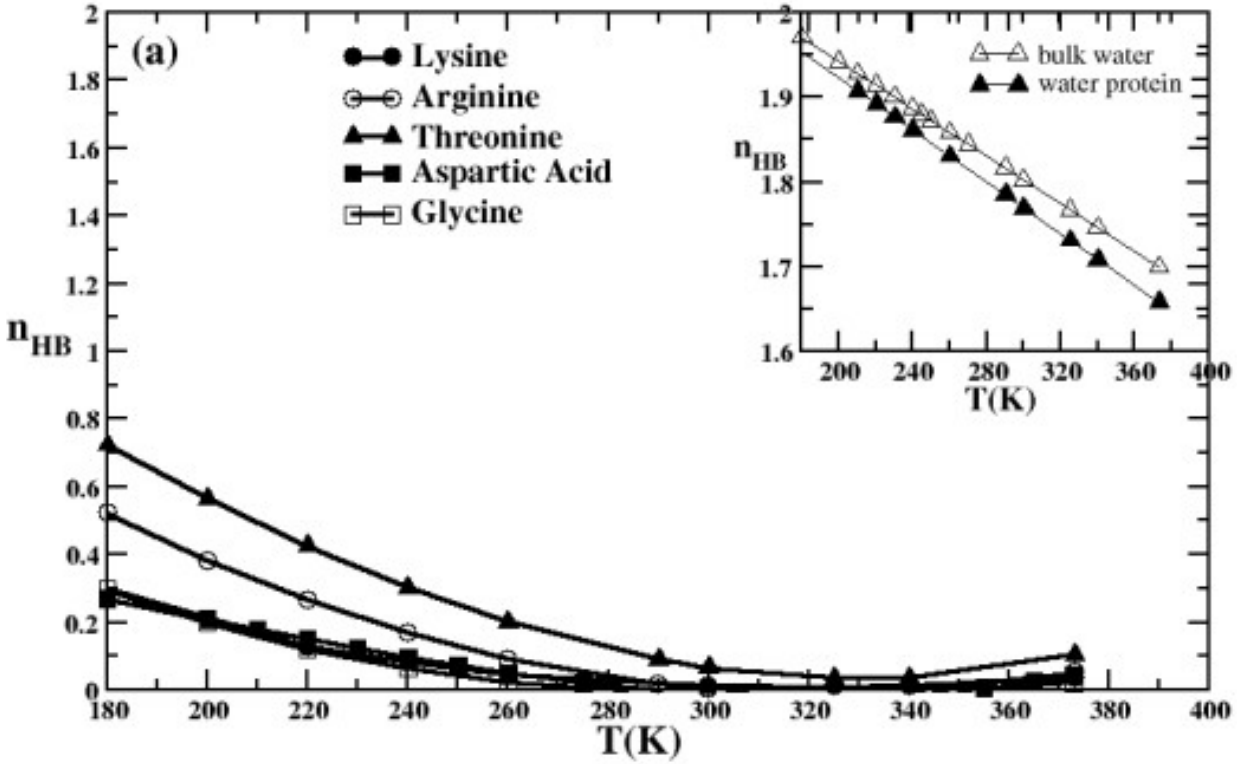
**R. Barbosa and MCB, Physica A 439 48 (2015).**




(a) Lifetime of the water-water H-bonds at the bulk (solid line), near the hydrophobic (dashed line) and hydrophilic (dotted line) sites of the protein. (b) Lifetime of the H-bonds of water and hydrophilic and water-hydrophobic sites of the protein (c) Number of the H-bonds between the water and the hydrophobic add the hydrophilic sites of the protein. All the quantities were computed for the SPC/E water model.

# Hydrogen Bonds - Philic

**R. Barbosa and MCB, Physica A 439 48 (2015).**




: Number of water-water Hydrogen bonds per water molecule *versus* temperature for the SPC/E water model around the hydrophilic amino acids. The inset represents the H-bonds between water molecules for bulk system (open triangles) and protein hydrated system (filled triangles).

# Hydrogen Bonds - Philic

**R. Barbosa and MCB, Physica A 439 48 (2015).**

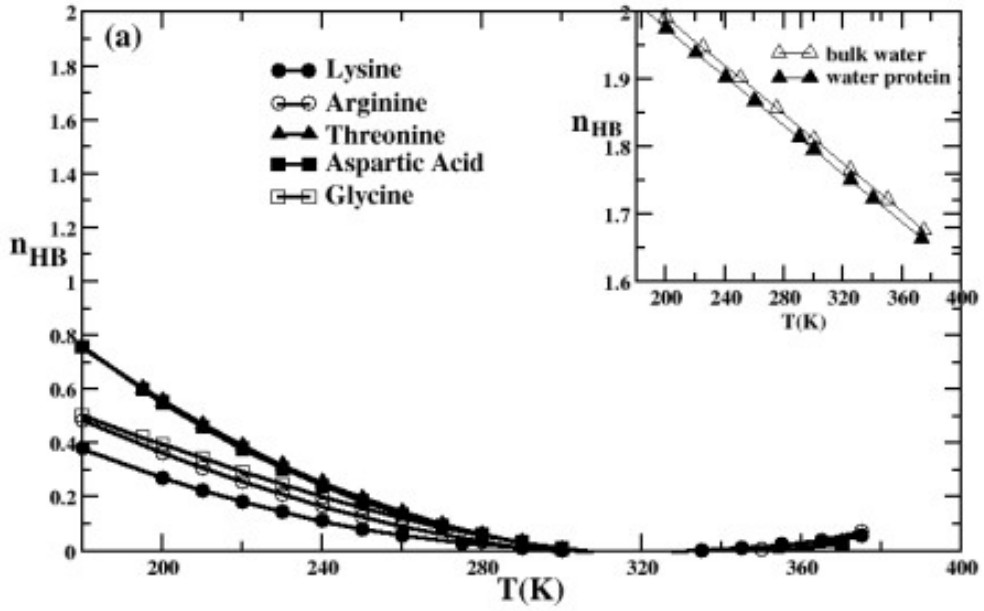



Figure 10: Number of water-water Hydrogen bonds per water molecule *versus* temperature for the TIP4P-2005 water model around the hydrophilic amino acids. The inset represents the H-bonds between water molecules for bulk system (open triangles) and protein hydrated system (filled triangles).

# Hydrogen Bond - Phobic

**R. Barbosa and MCB, Physica A 439 48 (2015).**

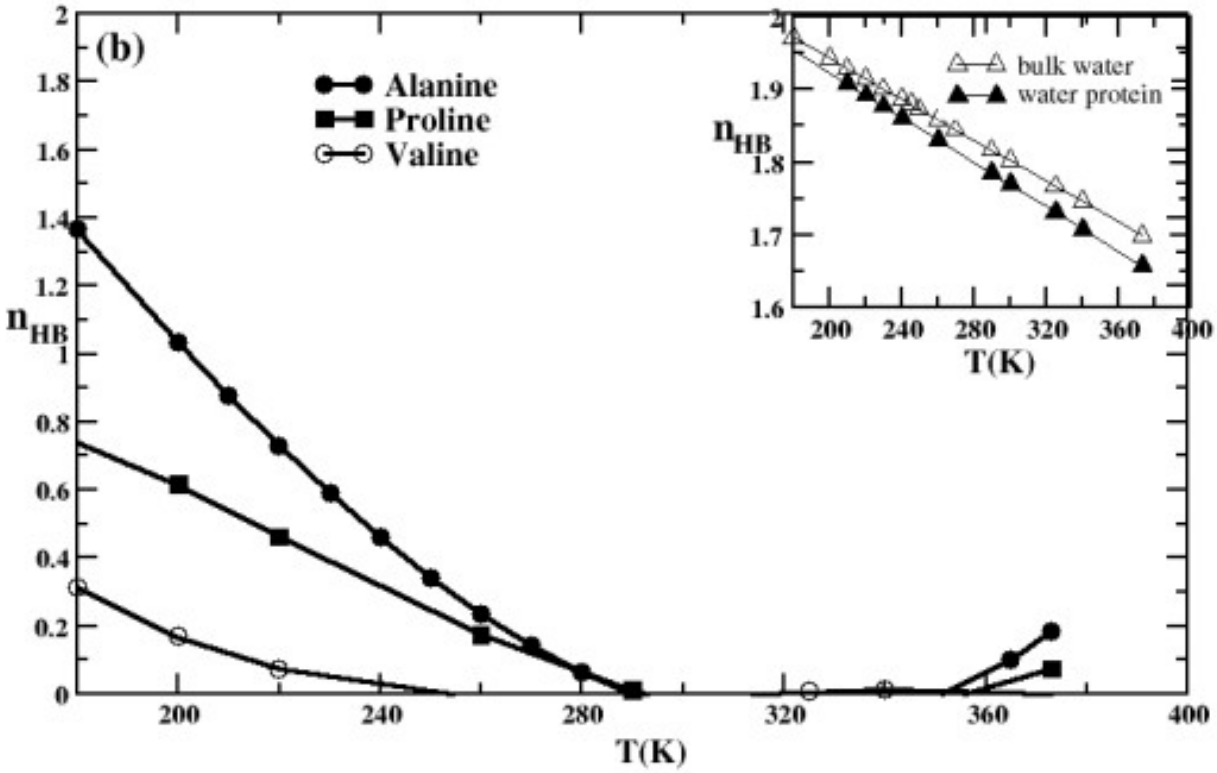



Figure 8: Number of water-water Hydrogen bonds per water molecule *versus* temperature for the SPC/E water model around the hydrophobic amino acids. The inset represents the H-bonds between water molecules for bulk system (open triangles) and protein hydrated system (filled triangles).

# Hydrogen Bond - Phobic

**R. Barbosa and MCB, Physica A 439 48 (2015).**

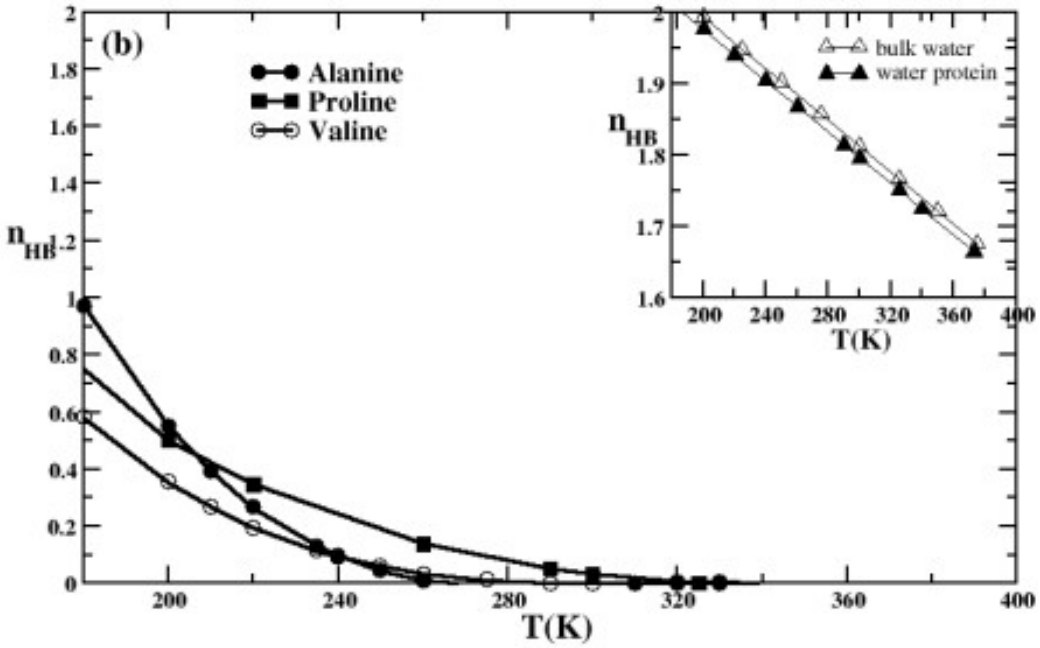



Figure 11: Number of water-water Hydrogen bonds per water molecule *versus* temperature for the TIP4P-2005 water model around the hydrophobic amino acids. The inset represents the H-bonds between water molecules for bulk system (open triangles) and protein hydrated system (filled triangles).

# Hydrogen Bond - Phobic

**R. Barbosa and MCB, Physica A 439 48 (2015).**

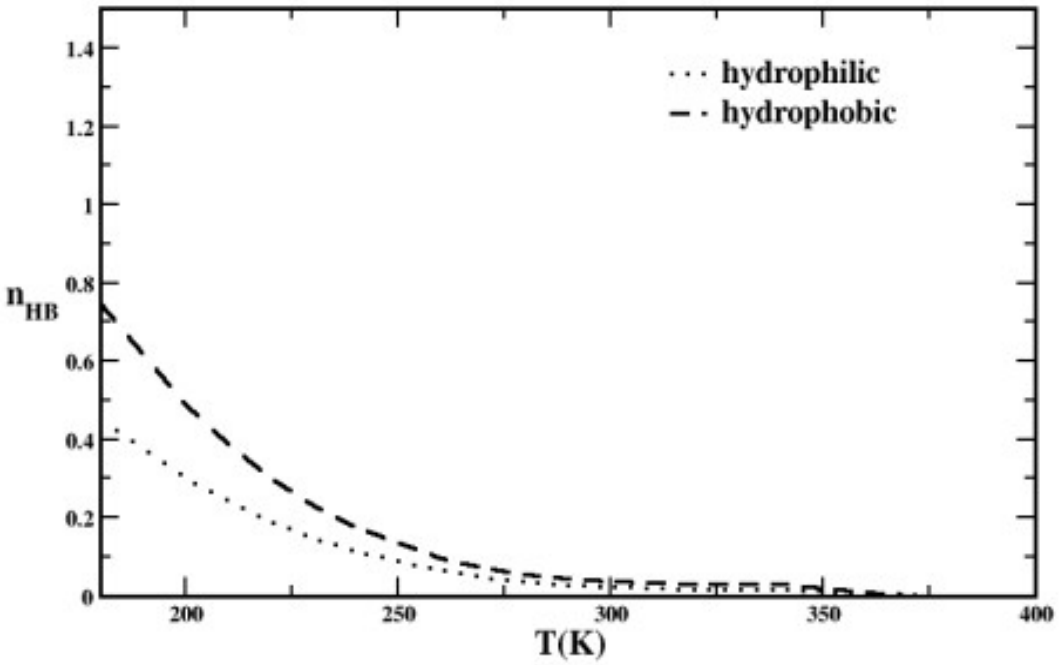



Figure 9: Average number of water-water Hydrogen bonds per water molecule *versus* temperature for the SPC/E water model averaged over the hydrophilic (dotted line) and the hydrophobic (dashed line) amino acids.

# Hydrogen Bond - Phobic

**R. Barbosa and MCB, Physica A 439 48 (2015).**

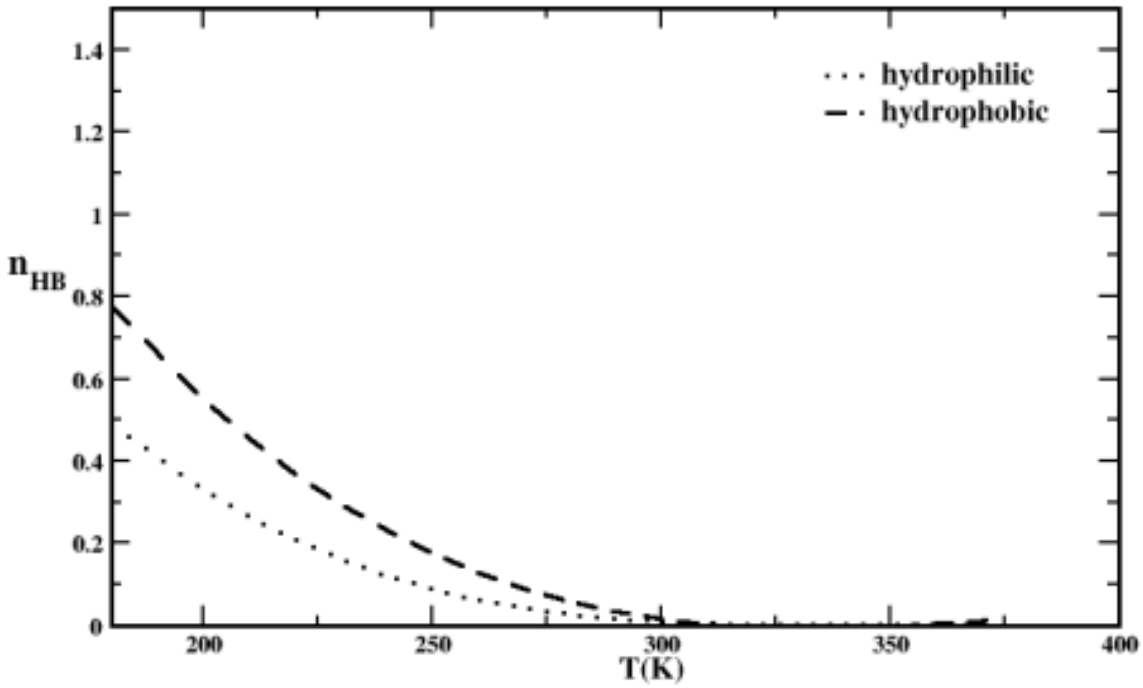



Figure 12: Average number of water-water Hydrogen bonds per water molecule *versus* temperature for the TIP4P-2005 water model averaged over the hydrophilic (dotted line) and the hydrophobic (dashed line) amino acids.

# Diffusion

**M Kohler, R Barbosa, L da Silva, MCB, Physica A 468 733 (2017)**

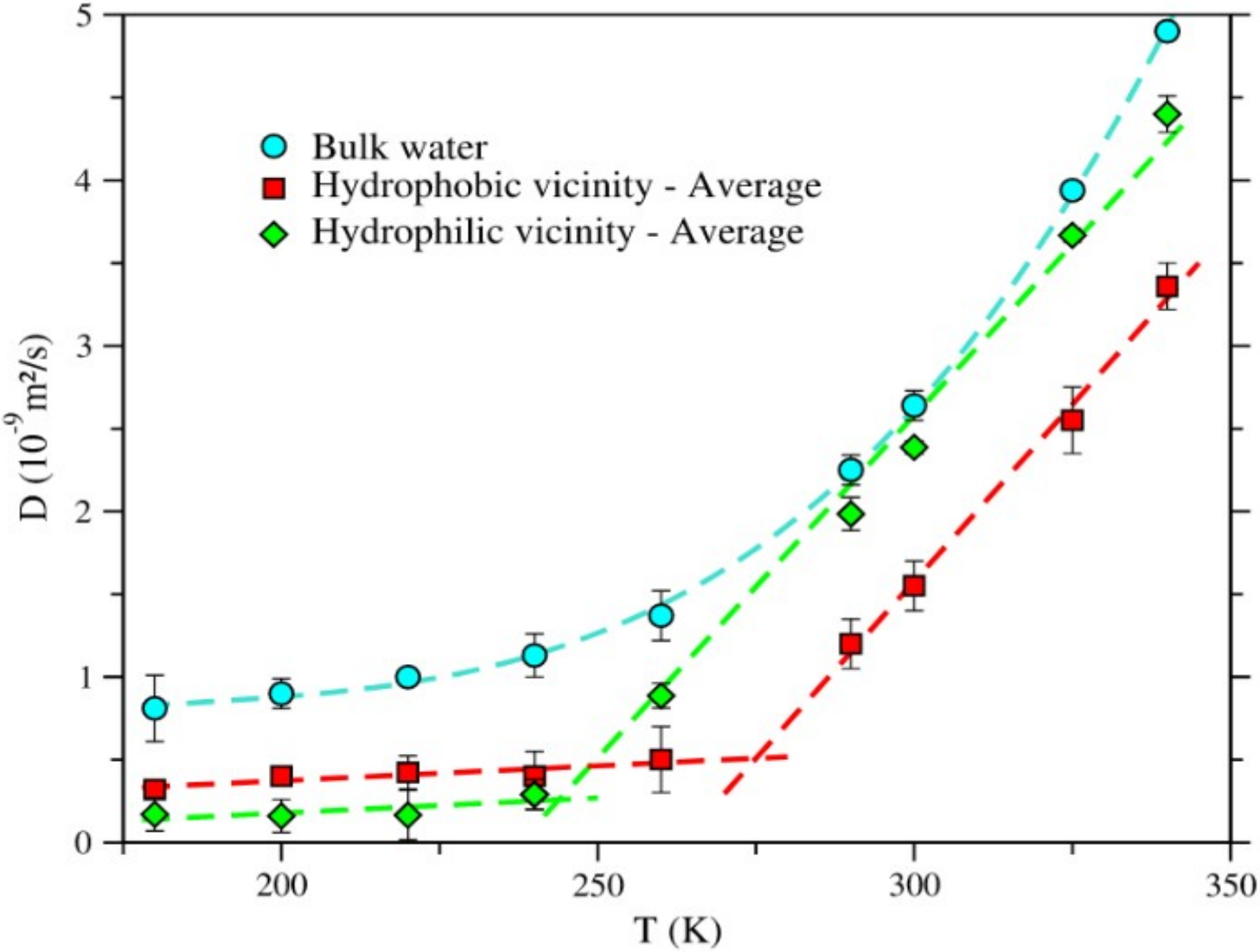
$$C(t) = 1 - \int_0^t P(\tau)d\tau.$$

$$\tau = \int C(t)dt.$$

$$D = \lim_{t\to\infty} \frac{\left\langle \left|\vec{r}(t) - \vec{r}(0)\right|^2 \right\rangle}{2dt}$$

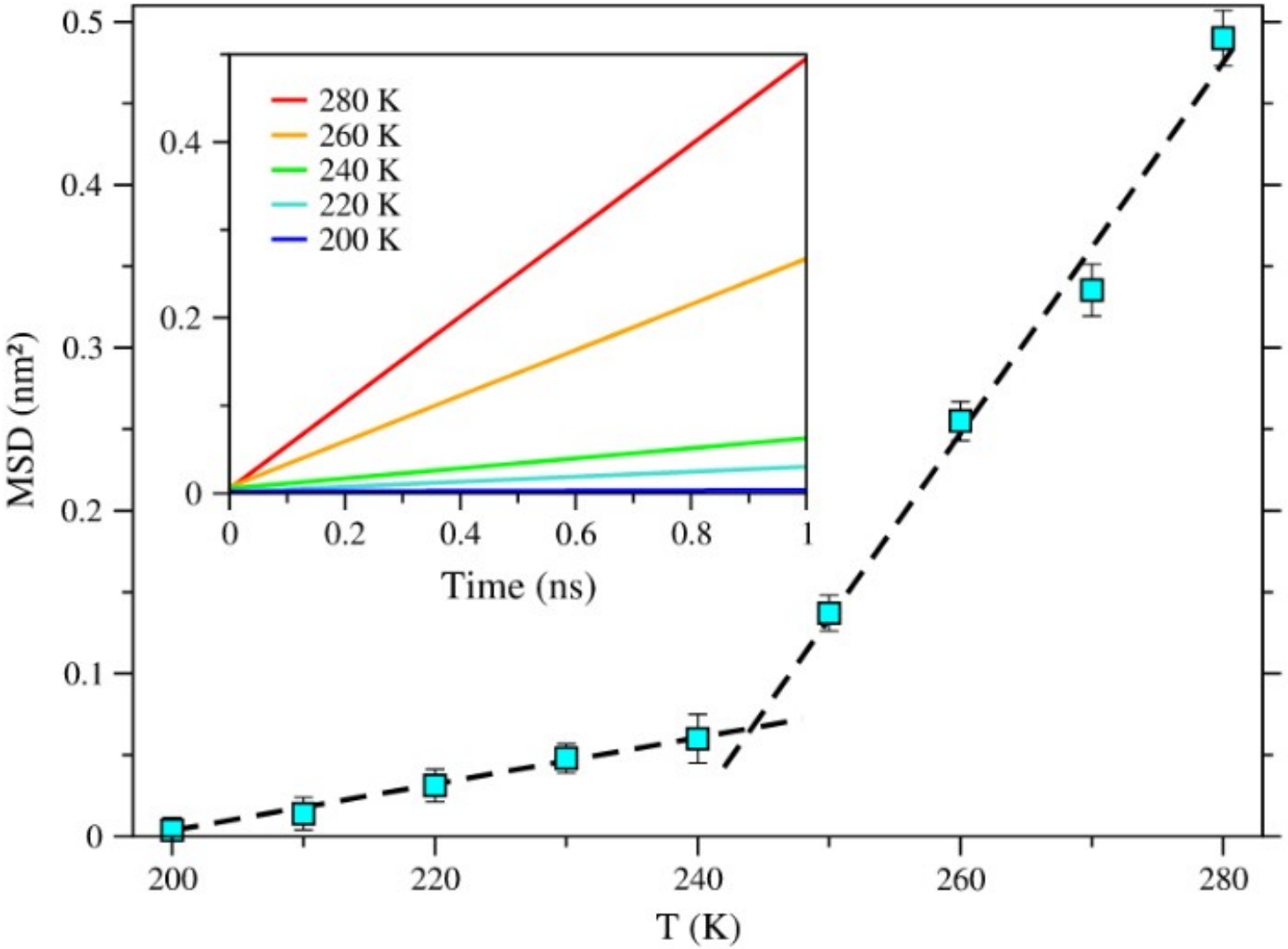
# Water Diffusion

**M Kohler, R Barbosa, L da Silva, MCB, Physica A 468 733 (2017)**



# Protein Mobility

**M Kohler, R Barbosa, L da Silva, MCB, Physica A 468 733 (2017)**



# Water in DNA

# DNA minor and major grooves

**https://quizlet.com/512518859/by511-lecture-5-dna-major-and-minor-grooves-of-a-b-dna-and-their-importance-flash-cards/**

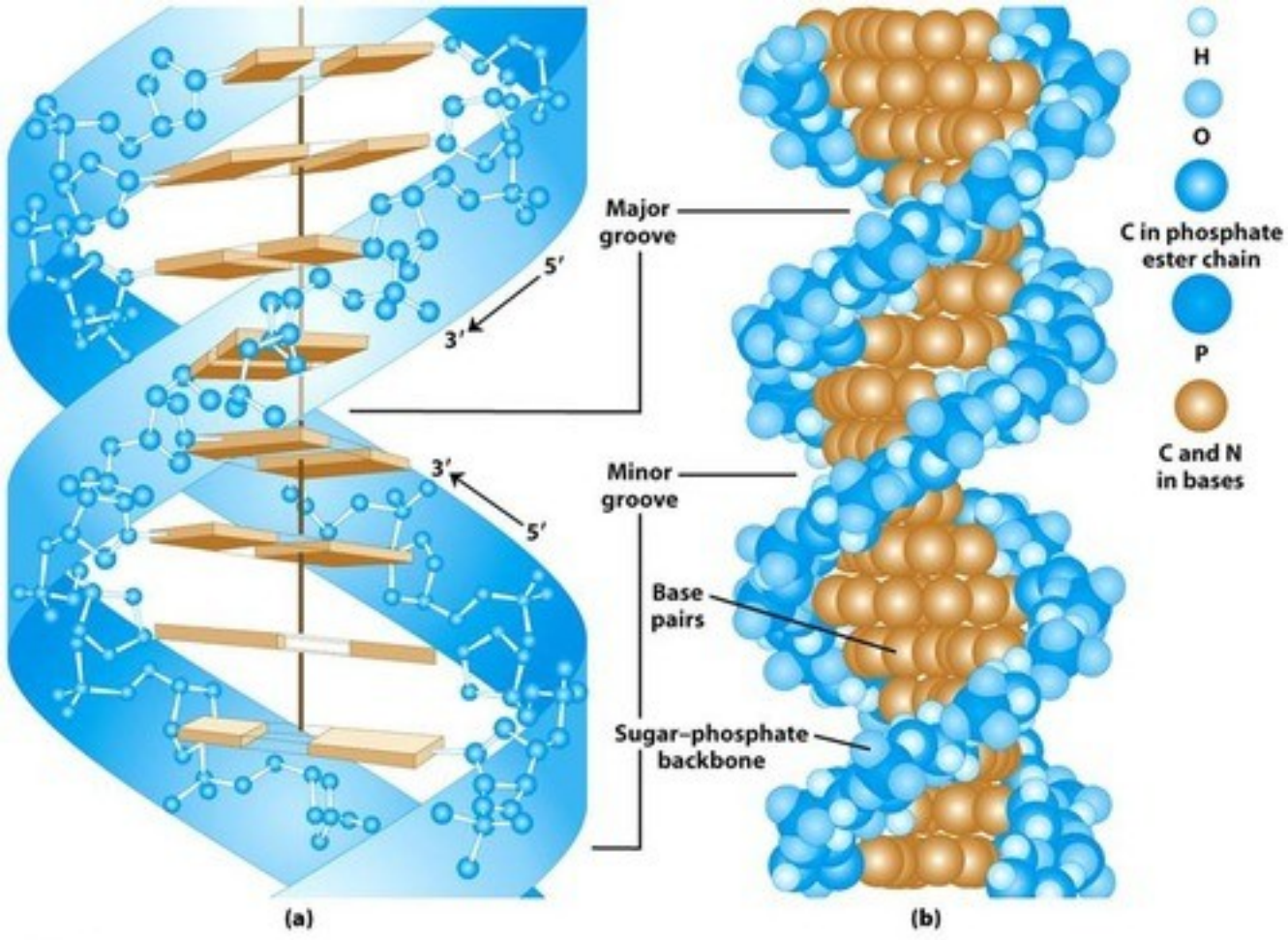
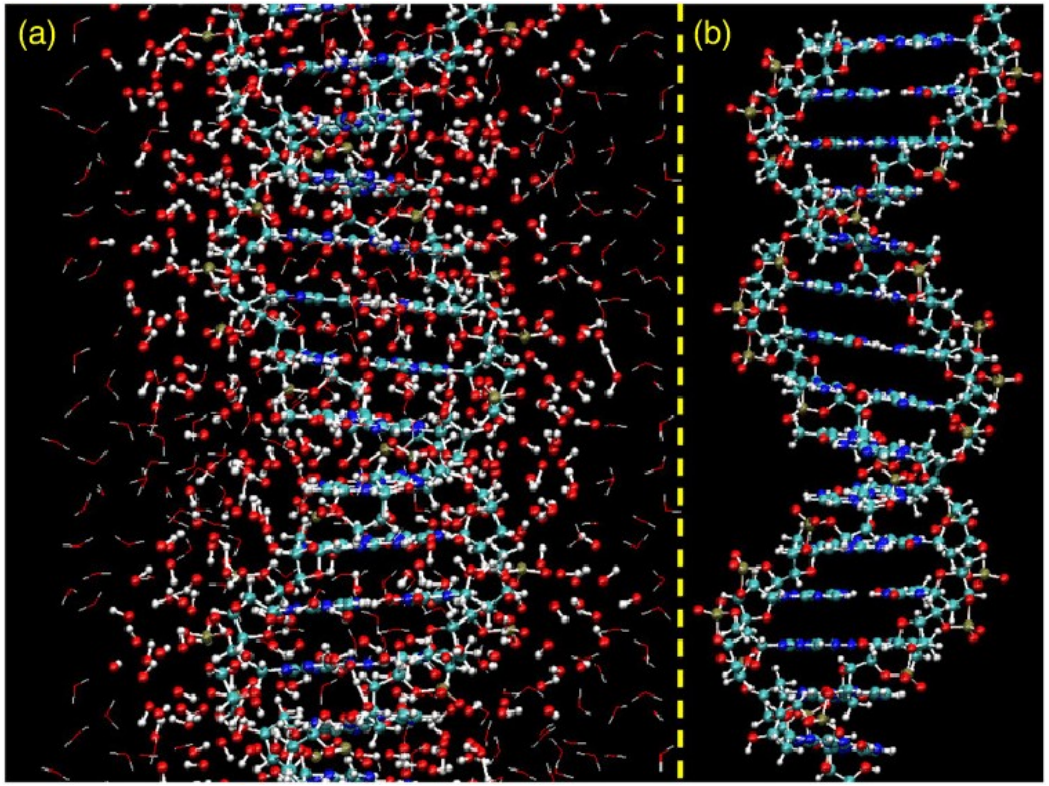



Figure 7-9
*Introduction to Genetic Analysis*, Tenth Edition
© 2012 W. H. Freeman and Company

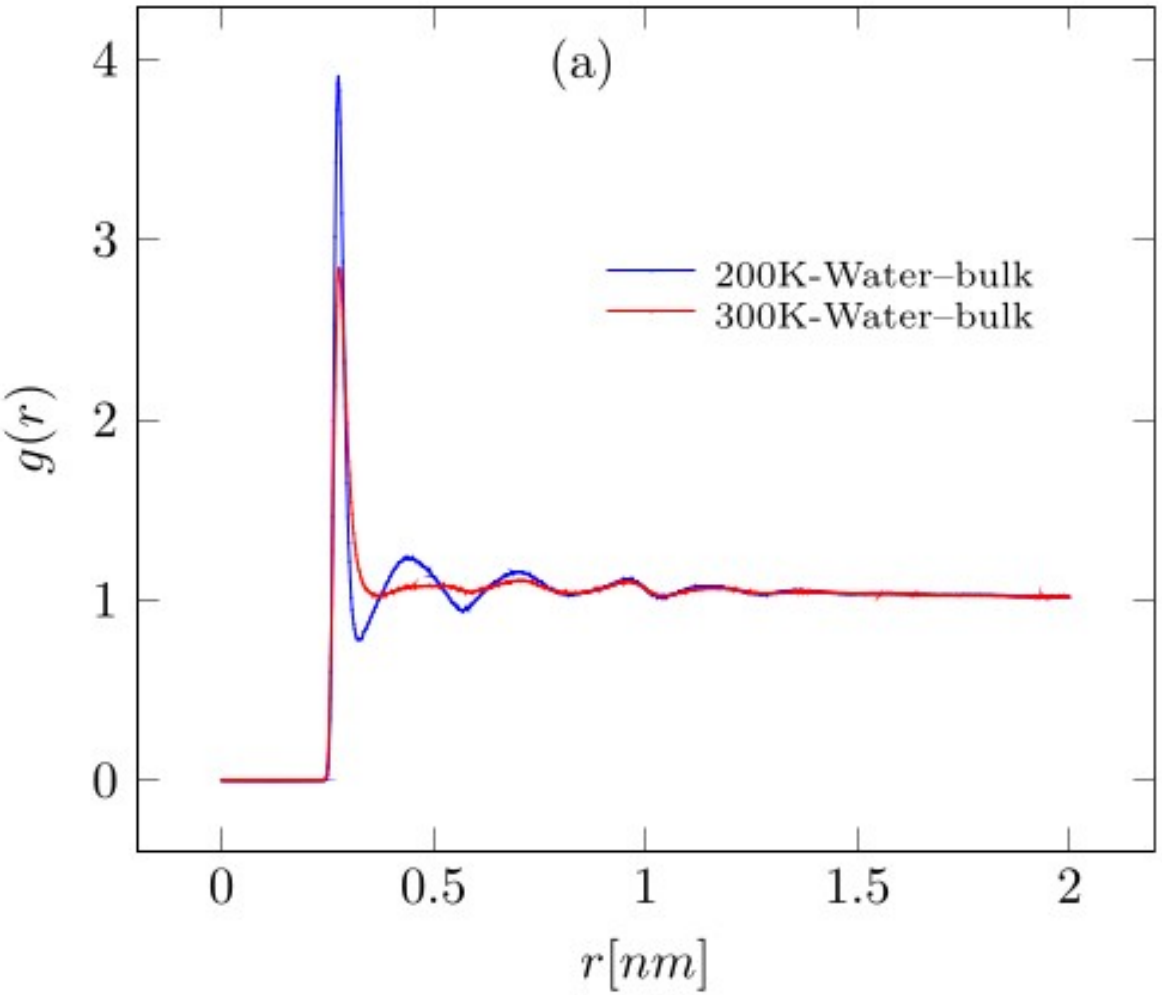
# DNA in water




2.7 × 10 4 TIP3P water
molecules 52 in a cubic box of side 6.4 nm

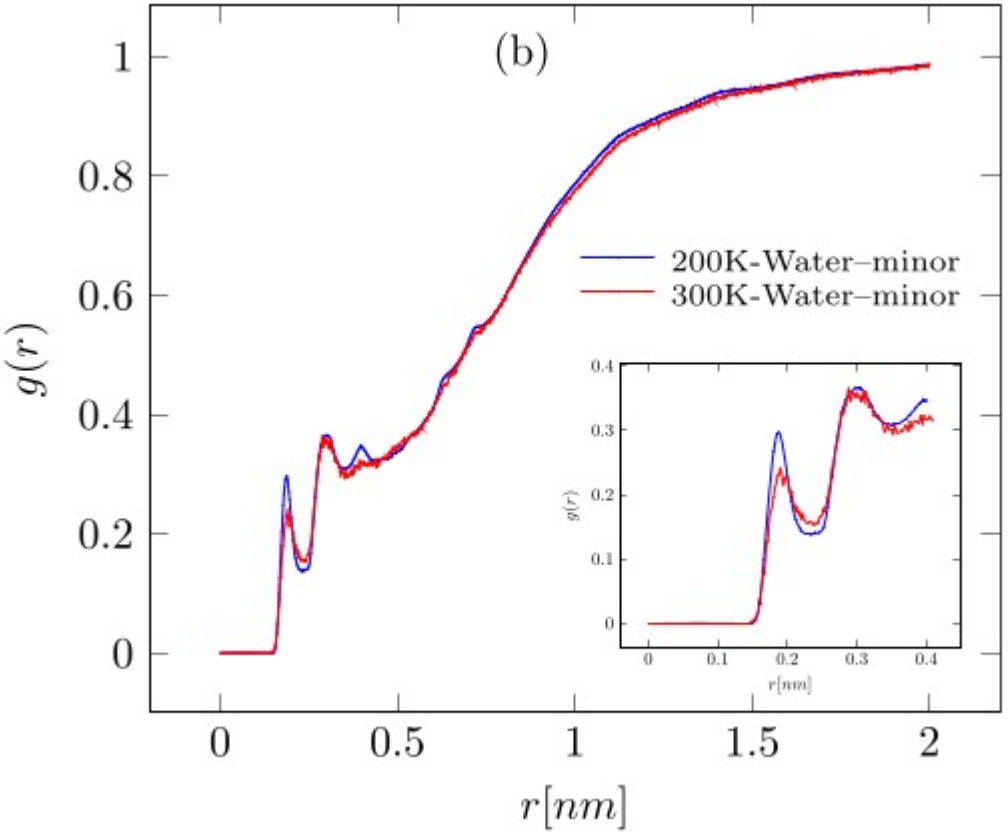
# DNA in water - G(r)

**M. A. F. dos Santos, M. A. Habitzreuter, M. H. Schwade, R. Borrasca, M. Antonacci, G. K. Gonzatti, P. A. Netz, and MCB**
**Journal of Chemical Physics 150 235101 (2019).**



# G(r) minor groove

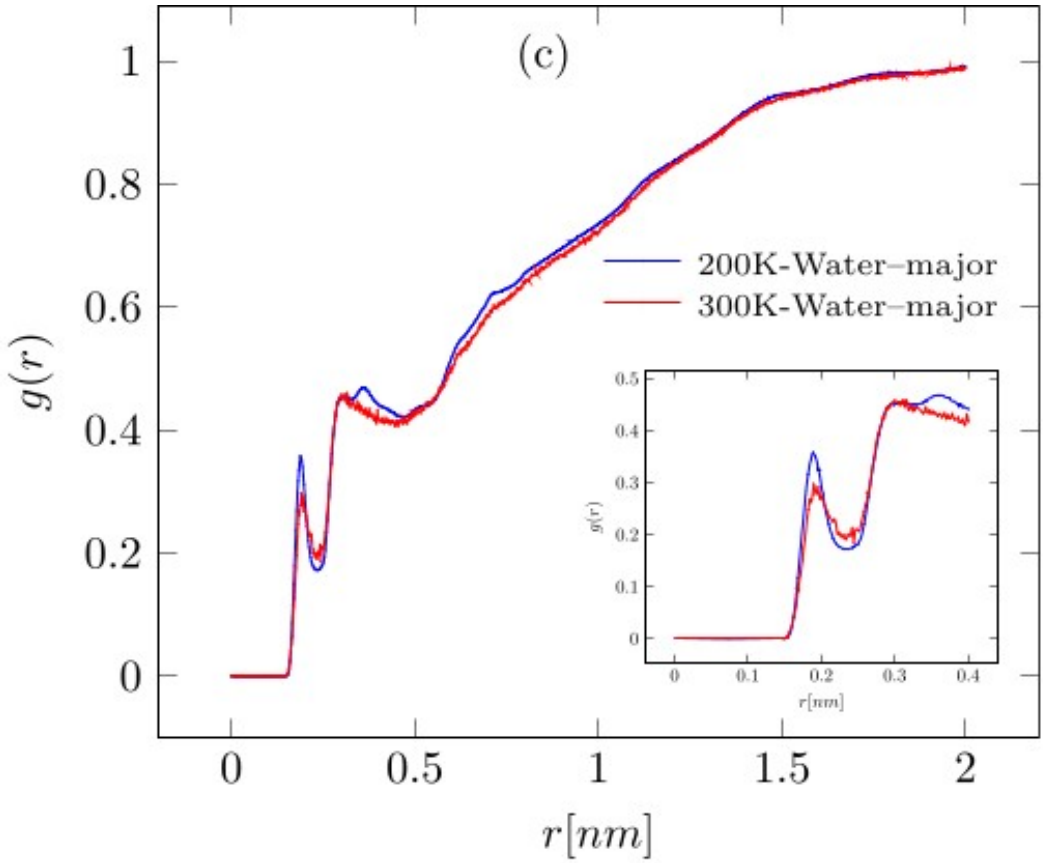
**M. A. F. dos Santos, M. A. Habitzreuter, M. H. Schwade, R. Borrasca, M. Antonacci, G. K. Gonzatti, P. A. Netz, and MCB**
**Journal of Chemical Physics 150 235101 (2019).**



# G(r) major groove

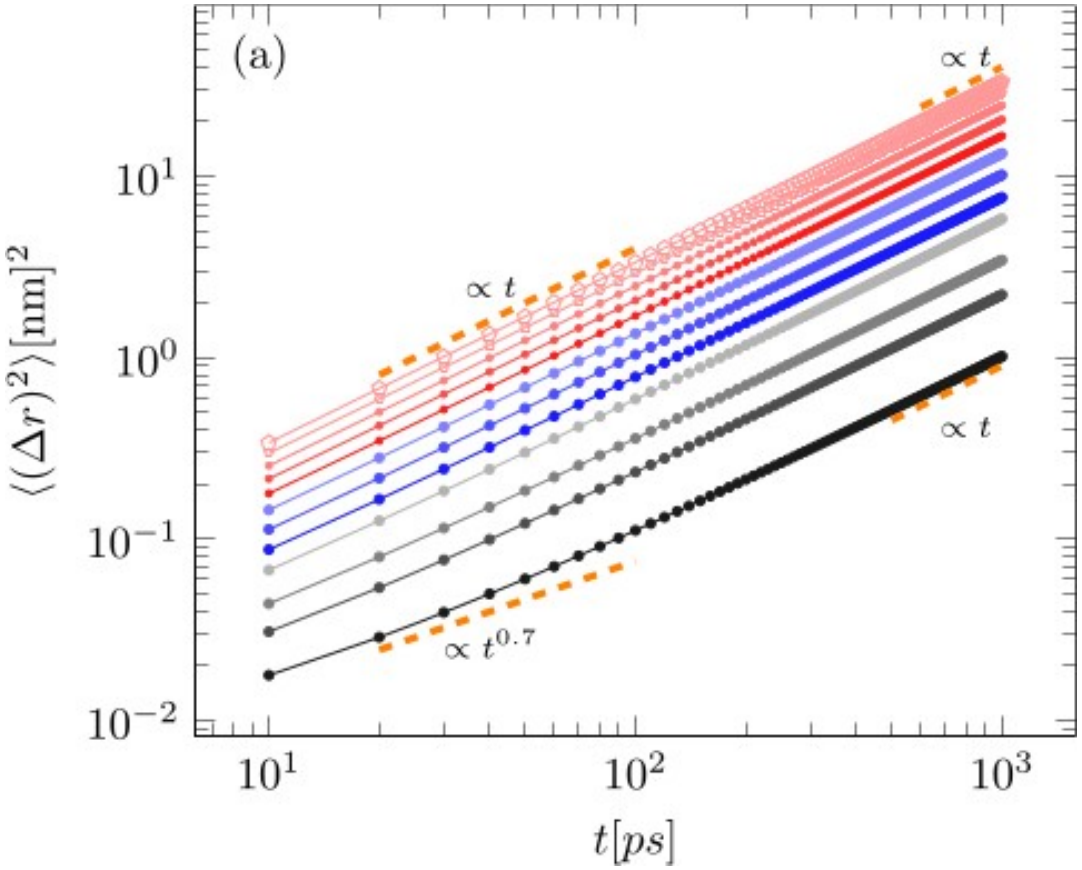
**M. A. F. dos Santos, M. A. Habitzreuter, M. H. Schwade, R. Borrasca, M. Antonacci, G. K. Gonzatti, P. A. Netz, and MCB**

**Journal of Chemical Physics 150 235101 (2019).**



# RDF bulk water

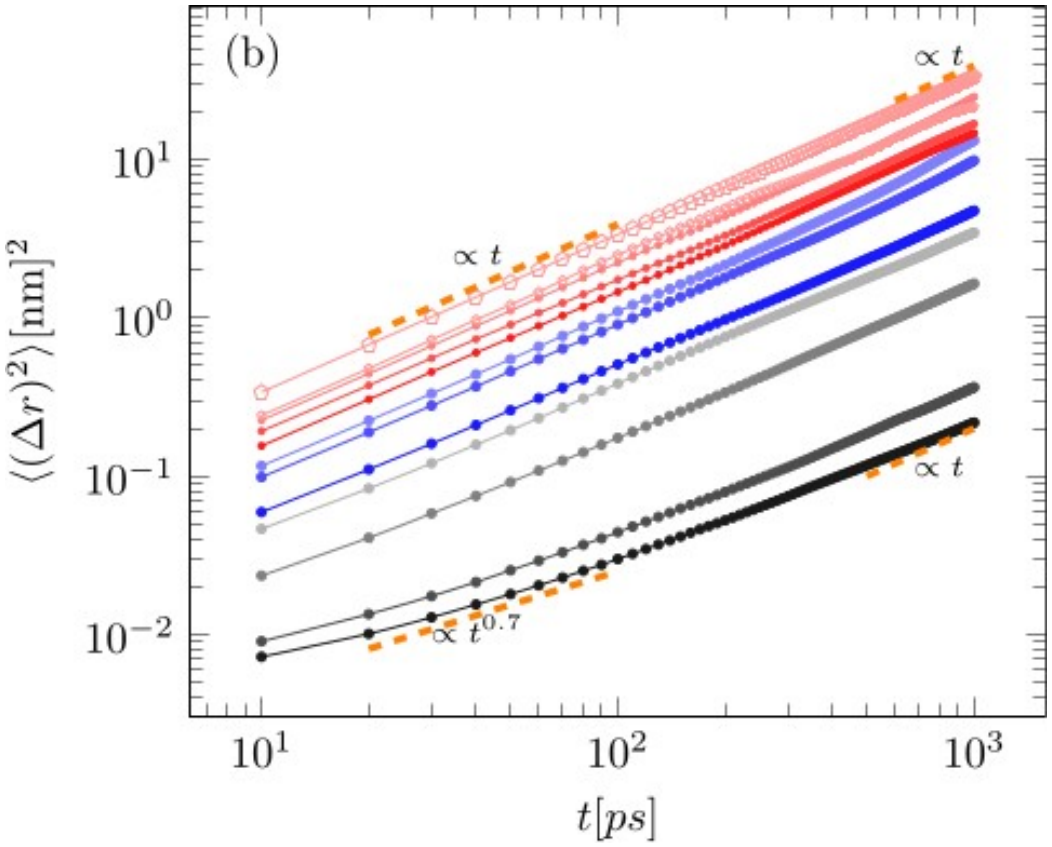
**M. A. F. dos Santos, M. A. Habitzreuter, M. H. Schwade, R. Borrasca, M. Antonacci, G. K. Gonzatti, P. A. Netz, and MCB**
**Journal of Chemical Physics 150 235101 (2019).**



# RDF minor groove

M. A. F. dos Santos, M. A. Habitzreuter, M. H. Schwade, R. Borrasca, M. Antonacci, G. K. Gonzatti, P. A. Netz, and MCB

Journal of Chemical Physics 150 235101 (2019).



# RDF major groove

**M. A. F. dos Santos, M. A. Habitzreuter, M. H. Schwade, R. Borrasca, M. Antonacci, G. K. Gonzatti, P. A. Netz, and MCB**

**Journal of Chemical Physics 150 235101 (2019).**

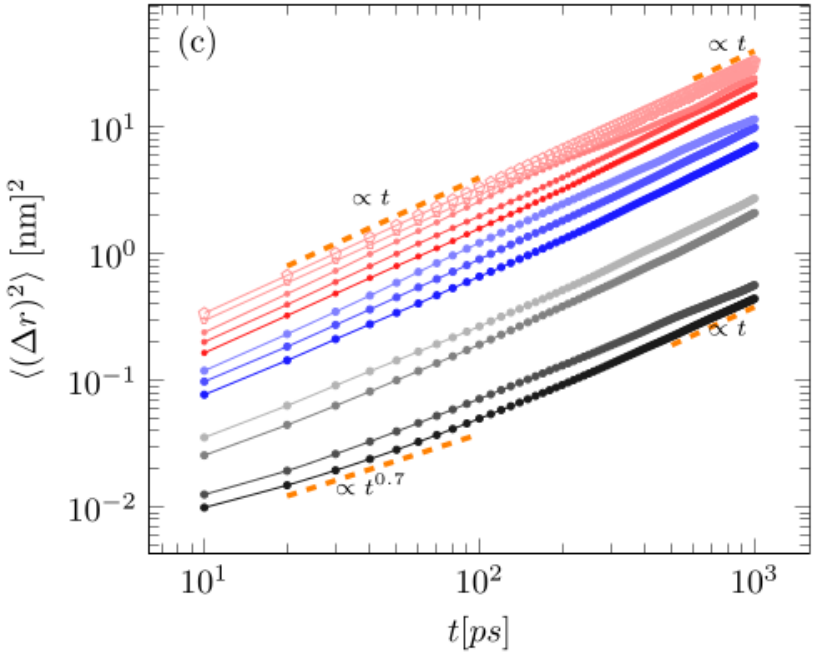



**FIG. 2**. Mean squared displacement (MSD) of water molecules in the (a) bulk, (b) minor, and (c) major grooves, at different temperatures. Dark black filled circles—190 K, black filled circles—200 K, gray filled circles—210 K, light gray filled circles—220 K, dark blue filled circles—230 K, blue filled circles—240 K, light blue filled circles—250 K, dark red filled circles—260 K, red filled circles—270 K, light red filled circles—280 K, small open pentagon—290 K, and large open pentagon—300 K.

# RDF major groove

**M. A. F. dos Santos, M. A. Habitzreuter, M. H. Schwade, R. Borrasca, M. Antonacci, G. K. Gonzatti, P. A. Netz, and MCB**

**Journal of Chemical Physics 150 235101 (2019).**

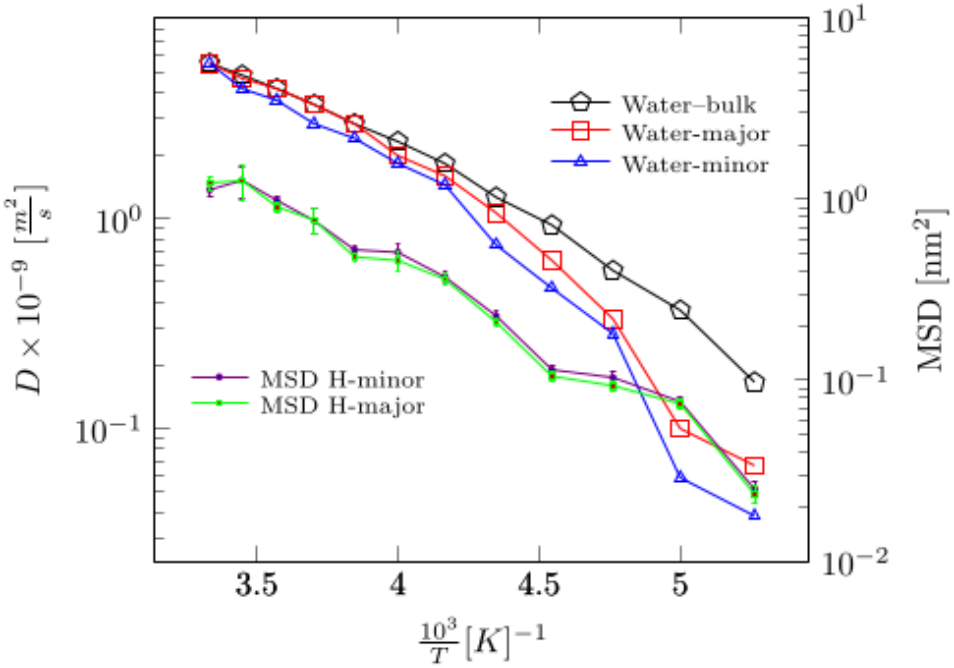



**FIG. 3**. (left axis) Diffusion coefficient vs the inverse of temperature for water in the bulk (black pentagons), in the major (red squares), and in the minor (blue triangles) grooves. (right axis) MSD of the hydrogen atoms of DNA-grooves at $t = 8 \times 10^2$ ps. The error bars for the MSDs (green lines and purple lines), estimated by computing 5 separate MSDs in various $10^3$ ps blocks of the trajectories.