

Slow dynamics of water in confinement

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WATER AND WATER SYSTEMS "

3nd course within the School of Neutron Science and Instrumentation

Erice, Italy, 22nd July - 31st July 2016

Outline of the talk

- Water anomalies and water phase diagram
- •Glassy behaviour of supercooled water: MCT slow dynamics and thermodynamics

•Water in Vycor, MD simulations: MCT glassy behaviour

•Water in MCM-41, MD simulations, MCT glassy behaviour and fragile to strong crossover linked to thermodynamics and to the bulk behaviour, structure and entropy.

•Hydration water with protein and disaccaride, MD simulations in the supercooled region. Similarities and differences with hydrophilic confinement.

Conclusions

Water anomalies

Isothermal compressibility and constant pressure specific heat show an apparent divergence at $T_s \sim -48^{\circ}C$.

$$\chi \propto \left(\frac{T}{T_s} - 1\right)^{\gamma}$$

$$K_T$$
 γ=-0.35
 c_p γ=-0.26



Experiments

Water phase diagram and liquid-liquid critical point (LLCP) hypothesis



[P.H. Poole, F. Sciortino, U. Essmann, H.E. Stanley, Nature (1992)]

[O. Mishima, and H. E. Stanley, Nature (1998)]

But also possible singularity free scenarios [S. Sastry, P.G. Debenedetti, F. Sciortino, H.E. Stanley PRE (1996]



Water: A Tale of Two Liquids

Paola Gallo, Katrin Amann-Winkel, Charles Austen Angell, Mikhail Alexeevich Anisimov, Frédéric Caupin, Charusita Chakravarty, Erik Lascaris, Thomas Loerting, Athanassios Zois Panagiotopoulos, John Russo, Jonas Alexander Sellberg, Harry Eugene Stanley, Hajime Tanaka, Carlos Vega, Limei Xu, and Lars Gunnar Moody Pettersson

Chemical Reviews 116, 7463-7500 (2016) DOI: 10.1021/acs.chemrev.5b00750



Glass Transition in supercooled water



[Complex dynamics of glass forming liquids: a mode coupling theory, W. Götze, Oxford (2009)]

Single particle dynamics

 \cdot van Hove self density density correlation function (second moment is the MSD)

$$G_{S}(r,t) = \frac{1}{N} \left\langle \sum_{i=1}^{N} \delta(\mathbf{r} + \mathbf{r}_{i}(0) - \mathbf{r}_{i}(t)) \right\rangle$$

$$G_{S}(t=0) = \delta(\mathbf{r})$$

$$G_S(t \to \infty) \to 0$$

\bullet The FT of $G_{\rm S}$ is the intermediate scattering function

$$F_{S}(Q,t) = \left\langle \sum_{i=1}^{N} e^{iQ \cdot [\mathbf{r}_{i}(t) - \mathbf{r}_{i}(0)]} \right\rangle$$

Normal liquid: Debye relaxation

 $F_s(Q, t \to \infty) \approx f \exp\left(-\frac{t}{\tau}\right) \quad \tau$ Relaxation time

Supercooled simple liquid



The Kohlrausch-Williams-Watts (KWW) formula describes the slow α relaxation of the MCT.

MCT: $F_S(Q, t \to \infty) = f_q \exp\left[-\left(\frac{t}{\tau}\right)^{\beta}\right]$ $\tau \propto \frac{1}{D} \propto (T - T_C)^{-\gamma}$

Crossover temperature $T_c \qquad \gamma > 1.5$



MCT in a nutshell

- If we have a sistem with fast and slow variables well separated the Mori-Zwanzig formalism can derive the exact equations of motions for the slow degrees of freedom
- Vibrations inside the cage are fast and $\alpha\mbox{-relaxation}$ is slow.
- Within this formalism MCT approximations: $\phi(Q,T)$ intermediate scattering function. Equation of motion and MCT approximation for the retarded memory nucleus:

$$\begin{split} \ddot{\phi}(q,t) + \Omega^2(q)\phi(q,t) + \Omega^2(q) \int_0^t M(q,t-s)\dot{\phi}(q,s)ds &= 0 \quad \text{with} \quad \Omega^2(q) = \frac{q^2k_BT}{mS(q)} \\ \\ M^{MC}(q,t) &= \int d^3q' V(q,q')\phi(q',t)\phi(q,t) \end{split}$$

MCT in a nutshell

- The vertices depend only on static quatities, S(q), density.
- If S(q) peaks (increasing ρ or decreasing T), vertices V(q,q') increases and correspondingly the memory function.
- Ultimately, ideal glass transition and structural arrest.



MCT solution for HS (in this case there is a critical packing fraction)

SPC/E Potential

(Berensden et al. 87)

Rigid molecule , charged sites and OO LJ



MSD



P=-80 MPa T_c=198.7K da D γ =2.73 T_c=T_s

Gallo, Sciortino, Tartaglia, Chen, Phys. Rev. Lett. 1996. Sciortino Gallo Tartaglia Chen Phys. Rev. E 1996.



FIG. 2. $F_s(Q_{\max}, t)$ vs time (symbols as in Fig. 1). Solid lines are calculated according to Eq.(1). The inset shows the T dependence of the exponent β associated with the slow relaxation.

Confirmed by experiments by Torre, Bartolini, Righini, Nature (2004)

Relaxation times



FIG. 3. $1/\tau_l$ vs Q. Solid lines are guides for the eye. Inset is $\tau_l DQ^2$ vs Q at different T. (Symbols as in Fig. 1.)

F(Q,t) hydrogens



FIG. 2. Semilogarithmic plot of F(Q,t) of hydrogen atoms for all the temperatures investigated at Q_{max} . The error bars are shown only for one temperature for clarity. Lower T are on the top. In the inset only the early times are shown for all the temperatures and for hexagonal ice (thick line) at T=194 K along a selected Q direction at Q_{max} . Early ice features are only slightly sensitive to the Q direction. After Q=0.2 ps ice displays an oscillating behavior, vibrational contributions, around an asymptotic value due to the absence of diffusion.

Relaxation times



FIG. 14. Diamonds represent the full width at half maximum of the $S_H(Q, \omega)$ as a function of Q for different temperatures. Circles represent the values of τ extracted from the fit of the late α region to a stretched exponential. We see, as expected, that these values become more and more different as Q grows and T decreases, i.e., as the exponential of the long-time relaxation becomes more and more stretched.

Water in confined geometry



Water in confined geometry

In many systems of interest for technological and biophysical problems water is confined or at contact with surfaces

What is the role of confinement and or of the substrate in modifying properties of water? How is the hydrogen bond network modified ?

How do static and dynamical properties change ?

How does thermodynamics change?

Strong need for model systems





Vycor



- quite sharp distribution of pores
 - hydrophilic surface
- its pores do not change size when filled with water

• strong capability to adsorb water, its equilibrium hydration at ambient conditions is 25% of its dry weight

Simulation cell

A cubic cell of vitreous silica is obtained by MD
In the cell a cylindrical pore of diameter 40 Å is carved





>The surface of the pore is corrugated and hydrogenated

Preparation of the surface

Cut out all the Si not bound to 4 O at least

Bridging oxygens

No-bridging ox saturated with hydrogens



Simulation of water in Vycor

> The surface of the pore is corrugated and hydrogenated



> Water (SPC/E) is simulated inside the cylinder in interaction with the atoms of the hydrophilic surface

Simulation of water in Vycor

>Water inside the cylinder interacts with the atoms of the substrate by a site-site empirical potential



Hydrophilic condinement: MD of water confined in a Vycor glass pore

site-site model

A cubic block of glass SiO_2 was realized by means a MD simulation quenching liquid SiO_2 to room temperature.

From the cube a cylindrical cavity is carved.

•The surface is treated and hydrogenated to mimic a Vycor glass pore.

•Water is inserted in the cavity









Hydrophilic confinement: density profiles



Spohr, Hartning, Gallo, Rovere, J. Mol. Liq. 1999

Intermediate scattering function at ambient temperature for different hydrations



The long time behaviour cannot be fitted with the KWW

Hydrophilic confinement: Bound and free water





Free water upon supercooling



Fitting formula for the free water simular to the bulk

$$F_{S}(Q,t) = [1 - A(Q)] \exp(-(t / \tau_{s})^{2}) + A(Q) \exp(-(t / \tau)^{\beta})$$

curve described by two relaxation processes:

- short relaxation time τ_s
- long relaxation time $\boldsymbol{\tau}$

A(Q) is the Debye-Waller factor

β(T) Kohlrausch exponent

Power law behaviour of the relaxation time



Diffusion coefficient of free water



Free water upon supercooling for N_W =1500



Gallo, Rovere, Spohr, J. Chem. Phys. 2000

MCT parameters from the
simulation
$$N_W=2600$$
> Along z: $T_C=185.3 \quad \gamma=2.11$
> in xy plane: $T_C=194.6 \quad \gamma=1.90$ $N_W=1500$ > Along z: $T_C=167.6 \quad \gamma=3.8$
> in xy plane: $T_C=170.4 \quad \gamma=3.4$

Increase of the free volume \rightarrow **decrease** of T_C

Bulk water P_{amb} : $T_C = 186.3 \quad \gamma = 2.29$

Results in agreement with experiments: JM Zanotti, MC Bellissent-Funel, SH Chen PRE (1999)
Fragile to Strong transition in water and the LLCP

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P.G. Debenedetti, F.H. Stillinger, *Nature* **410**, 259 (2001)



[1] K. Ito, C. T. Moynihan and C. A. Angell, Nature 398, 492 (1999).

[2] L. Xu, P. Kumar, S. V. Buldyrev, S.-H. Chen, P. H. Poole, F. Sciortino and H. E. Stanley, Proc. Natl. Acad. Sci. USA **102**, 16558 (2005).

[3] L. Liu, S.-H. Chen, A. Faraone, C.-W. Yen and C.-Y. Mou, Phys. Rev. Lett. **95**, 117802 (2005); A. Faraone, L. Liu, C.-W. Yen C.-Y. Mou and S.-H. Chen, J. Chem. Phys. **121**, 10843 (2004).

$$H=G_{\infty} au$$
 (Maxwell's Relation)

Fragile
$$\tau = \tau_0 \exp \left(\frac{\tau_0}{\tau_0} + \frac{\tau_0}{$$

$$T = \tau_0 \exp\left[\frac{DT_0}{T - T_0}\right]$$
$$T = \tau_0 \exp\left[\frac{E_A/k_B}{T}\right]$$

 $\begin{bmatrix} RT \end{bmatrix}$

The occurrence of a fragile-strong transition in water [1,2] has recently been connected to the existence of the second critical point [2,3].

But can it really be experimentally verified in confined water [3], where crystallization can be avoided, that this crossover temperature exists for the bulk? How different is that confined water with respect to the bulk?



Comparison between our QENS results and MD simulation of bulk ST2 model water



[L. Liu, S.H. Chen, *A. Faraone, C.W. Yan and C.Y. Mou, Phys. Rev. Lett.* 95, 117802 (2005). Mallamace et al JCP 2006] .

According to ST2 model of water, the locus of F-S transition coincides with the locus of Cpmax. Also TIP5P supports the connection between the Widom line and F-S xu et al. PNAS 2005.

Model details for our simulation of water in MCM-41

Cubic cell of silica with a cylindrical cavity carved inside to mimic the properties of a single pore of a MCM-41 system

≻Box length: 42 Å

- > Pore diameter: 15 Å
- > Water model: SPC/E

Number of water molecules: N=380, N=216

> Interaction between water sites and silica atoms modeled with an empirical potential.

> Range of T explored: 190 K < T < 300 K



MCM (Mobile Crystalline Material) is porous silica with an honey-comb like structure. By changing the length of the template molecule, the width of the channels can be controlled to be within 1 to 10 nm.

Water inside the MCM-41 pore



Total self intermediate scattering function in MCM41



Self intermediate scattering function (SISF) vs. t calculated at the peak of the structure factor $Q_{MAX} \approx 2.25 \text{ Å}^{-1}$ for all water molecules in the pore We see a two step relaxation scenario but it cannot be fitted with a strexp!



Overall effective density inside the pore 0.98 gr/cm³, for the free water 1 gr/cm³ 70% is the percentage of free water inside our pore.

Self intermediate scattering function in MCM-41: two separate sets of waters



Self intermediate scattering function of free water in MCM-41



Self intermediate scattering function (SISF) vs. t calculated at the peak of the structure factor $Q_{MAX} {\approx} 2.25$ Å $^{-1}$

Red lines are the fit to the KWW function

Also in QENS we expect only mobile water molecules to contribute to the spectra, experimental resolution is around 10 ns

Evidence of a fragile to strong transition

In the range 280 K > T > 210 K the behaviour of τ can be fitted with the Vogel-Fulcher-Tamman (VFT) law (blue curve in the figure)

$$\tau(T) \propto \exp\left[BT_0 / (T - T_0)\right] \tag{1}$$

this is the signature that in this region the system has a *fragile* behaviour, B is a measure of the fragility and T_0 is the ideal glass transition temperature.

For T< 210 K there is a crossover to a *strong* behaviour described by an Arrhenius formula

$$\tau(T) \propto \exp[E_A / k_B T]$$
 (2)

where E_A is the activation energy.



P. Gallo, M. Rovere, S.-H. Chen, J. Phys. Chem. Lett. 2010

Parameters of the transition

Fragile behaviour from fit to Eq. (1)

T₀=200 K EXP: 190÷200 K [1] BULK SPCE: 210 K [2]

Crossover temperature: T_{cross} = 215 K EXP: 210÷224 K [1]

Strong behaviour from fit to Eq. (2)

Activation energy $E_A = 34 \text{ kJ/mol}$ BULK: 65 kJ/mol [2]

[1] L. Liu, S.-H. Chen, A. Faraone, C.-W. Yen and C.-Y. Mou, Phys. Rev. Lett.
95, 117802 (2005); A. Faraone, L. Liu, C.-W. Yen C.-Y. Mou and S.-H. Chen, J. Chem. Phys. 121, 10843 (2004).
[2] F. Starr, F. Sciortino and H. E. Stanley Phys. Rev. E 60, 6757 (1999).

Response function





Relation between the Widom line and the dynamic crossover

$$T = (218 \pm 5)K$$

MCT test of free water in MCM-41 timetemperature superposition priciple



The shape of the correlators in the late b early a region does not depend on T

$$F^{(s)}(Q,t) = \hat{\phi}_Q(t/\tau_\alpha(T))$$

The master function has the shape of the von Schweidler law

$$\hat{\phi}(t) = f_Q^c - h_Q (t/\tau_\alpha)^b.$$

VS law does not hold for the curves in the strong region

Gallo et al. JPCM 2012

Test on the MCT exponents for free water in MCM-41 is also OK

$$\gamma = \frac{1}{2a} + \frac{1}{2b}$$
$$\lambda = \frac{\Gamma^2(1-a)}{\Gamma(1-2a)} = \frac{\Gamma^2(1+b)}{\Gamma(1+2b)}$$

From one parameter we calculate the others, from b of VS in particular we got a $\gamma = 3.25$

This value coincides with the one obtained from simulations fit

Excess of two body entropy and the FTS transition

- Excess of entropy: $S_{exc} = S S_{IdGas}$
- The excess entropy can be represented as an expansion in terms of **n** -body contributions represented by integrals on the **n** particle distribution functions g_n (r1, ..., r_n)
- Assuming that the main contribution to the particle interaction comes from the two-body terms, the excess entropy per particle $s_{exc}=S_{exc}/N$ is then

$$s_{\text{exc}} \approx s_2 = -2 \pi \rho k_B \int \{g(r) \ln[g(r)] - [g(r) - 1] \} r^2 dr$$

Where g(r) is the Ox-Ox radial distribution function RDF

Radial Distribution functions MD bulk TIP4P



Excess two body entropy bulk water MD bulk TIP4P





Excess of two body entropy and the FTS transition

- The excess entropy is determined by the configurational space available for a system. In this respect it can be connected also to the dynamics of the liquid.
- The relation between the entropy and the transport properties are based on the Rosenfeld scaling.
- The idea behind the Rosenfeld scaling is that liquid diffusion is determined by the combination of collisions and cage effects and the relaxation time can be related to the excess entropy by a relation of the type

$$1/\tau \propto e^{\alpha s_{exc}}$$

- where it is assumed that the cage relaxation can have a frequency proportional to the number of configurations.
- We consider s_{exc} proportional to s_2



Two body excess entroy: fit to the equation in bulk TIP4P

$$s_2/k_B = B + b \ln(\epsilon)$$
 where $\varepsilon = (T-T_c)/T_c$



P. Gallo and M. Rovere, Relation between the two body entropy and the relaxation time in supercooled water, PRE 2015

Free water g(r) for SPC/E free water in MCM-41



First minimum height in MCM41 free water Change of trend at the FTS transition



SPC/E bulk

$$s_2/k_B = B + b\ln\left(\epsilon\right)$$



SPC/E bulk









Gallo, Camisasca, De Marzio, Rovere, in preparation

Anomalous diffusion

Anomalous diffusion of water at contact with disordered surfaces could be interpreted in terms of a disordered distribution of the residence time of water molecules

Transition between a regime with exponential distribution of residence times

to residence time distr. with long tail

$$P(t_{res}) \propto t^{-\mu} \quad \longrightarrow \quad <\Delta r^2 > \propto t^{\mu-1}$$







Dynamics of bound water



P. Gallo, M. Rovere and S.-H. Chen, J. Phys.: Condens. Matter 22, 284102 (2010)

SPECIAL ISSUE "WATER AT INTERFACES"

Guest editors P. Gallo and M. Rovere

Dynamics of bound water



T=300 K Nw=216 Low hydration MCM41



MSD of the outer shells for the low hydration $N_w = 216$ at temperatures T = 300 and 240 K. Straight lines are fits to the subdiffusion behaviour. Both lines have a slope of 0.5. The exponent does not dempend on T (similar to bound water in Vycor) In the inset the MSD are normalized to $t^{0.5}$ to see the convergence to the sublinear behaviour.

Residence Time distribution MCM-41



Log-log plot of the residence time distribution as a function of time for the oxygen atoms of water. The curve for T = 240 K is shifted by a constant factor for clarity. The bold lines are fits with the power law formula $\psi(t) = at^{-\mu}$ with $\mu = 1.5$.
Residence Time distribution MCM-41



Log-log plot of the MSD for the inner shells of the system with $N_w = 380$ at T = 300 K. In the inset at the bottom: linear-log plot of the RTD for the inner shells fitted with an exponential decay. In the inset at the top: log-log plot of the RTD for the outer shells fitted with a power law decay. Aqueous solutions of lysozyme and trehalose



Lysozyme is part of the innate immune sistem can be found in tears, saliva, human milk etc.

- Increase in protein thermal stability with trehalose (see for expample Exp. G. Bellavia, S. Giuffrida, G. Cottone, A. Cupane and L. Cordone J. Phys. Chem. B 115, 6340 (2011).
- Trehalose interacts preferentially with water and stiffens the protein (see for example Exp/Sim. A. Lerbret, F. Affouard, A. Hédoux, S. Krenzlin, J. Siepmann, M. C. Bellissent-Funel and M. Descamps J. Phys. Chem. B 116, 1103 (2012).)
- See review paper L. Cordone, G. Cottone, A. Cupane, A. Emanuele, S.Giuffrida, and M.Levantino, Curr. Org. Chem. 19, 1684 (2015).

Total intermediate scattering functions for water in the bulk phase and in Lyz-Tr(aq) at Q_{max}



$$F^{(s)}(Q,t) = (1 - (f1 - f2)) \exp[-(t / \tau_{short})^{2}] + f1 \cdot \exp[-(t / \tau_{\alpha})^{\beta_{\alpha}}] + f2 \cdot \exp[-(t / \tau_{long})^{\beta_{long}}]$$

- Similar to water and trehalose the aqueous solution with Lysozyme and trehalose has an additional slower relaxation [A. Magno and P. Gallo, J. Phys. Chem. Lett. 2, 977 (2011)]
- This slower relaxation comes from hydration water
- Bulk water shows only one slow relaxation (in black in the figures)

D. Corradini, E. G. Strekalova, H. E. Stanley, and P. Gallo, Sci. Rep. 3, 1218 (2013).

Total relaxation times at the peak of the oxygen structure factor



Retardation factor

$$\tau_{long}/\tau_{\alpha} ->4/6$$

$$\tau_{\rm long}/\tau_{\rm a}\simeq 5.7$$

in agreement with experiments on trehalose aqueous solutions

($\tau_{\text{long}}/\tau_{a} \simeq 6.0$ at T = 308 K)

[M. Paolantoni et al., J. Phys. Chem. B
113, 7874 (2009). L. Lupi, L. Comez, M. Paolantoni, D. Fioretto and B. M. Ladanyi, J. Phys. Chem. B 116, 7499
(2012). L. Comez, L. Lupi, A. Morresi, M. Paolantoni, P. Sassi, D. Fioretto, J. Phys. Chem. Lett. 4, 1188 (2013)

How about hydration water?

Two well distinct slow relaxations have been found in aqueous solutions of water and biomolecules and where possible experiments have shown that in particular hydration water has both. See for example references here below.



- S. Perticaroli, L. Comez, P. Sassi, M. Paolantoni, S. Corezzi, S. Caponi, A. Morresi, and D. Fioretto, 5, J. Non. Cryst. Solids 407, 472 (2015).
- D. Corradini, E. G. Strekalova, H. E. Stanley, and P. Gallo, Sci. Rep. 3, 1218 (2013).
- L. Comez, L. Lupi, A. Morresi, M. Paolantoni, P. Sassi, and D. Fioretto, J. Phys. Chem. Lett. 4, 1188 (2013).
- A. Magno and P. Gallo, J. Phys. Chem. Lett. 2, 977 (2011).
- L. Zhang, L. Wang, Y.-T. Kao, W. Qiu, Y. Yang, O. Okobiah, and D. Zhong, Proc. Natl. Acad. Sci. U. S. A. 104, 18461 (2007).
- S. K. Pal, J. Peon, B. Bagchi, and A. H. Zewail, J. Phys. Chem. B 106, 12376 (2002).
- S. K. Pal, J. Peon, and A. H. Zewail, Proc. Natl. Acad. Sci. 99, 1763 (2002).

How about dynamics of our hydration water? Does it show these two relaxations and how does it change with the presence of trehaloses?



Comparison of behaviour of hydration water (water molecules within 6Å from the surface: it is the red hearth-shaped corona in the picture) for Lysozyme in water and the thernary system Lyso+Water+Treha

Slow dynamics gets slower with trehalose and long time tails present already in lyso(aq) get longer



Fit for hydration water both relaxations are found! And both relaxation times have a crossover

$$F^{(S)}(Q,t) = (1 - (f1 - f2)) \exp[-(t / \tau_{short})^{2}] + f1 \cdot \exp[-(t / \tau_{\alpha})^{\beta_{\alpha}}] + f2 \cdot \exp[-(t / \tau_{long})^{\beta_{long}}]$$

α - relaxation times of hydration water



See also Schirò, Cupane, Mallamace and others.

Long relaxation times



Conclusions

•MCT holds for bulk supercooled water [Gallo et al. prl (1996), Sciortino et al pre(1996), Torre et al. Nature (2004)

•Molecular dynamics simulations of <u>supercooled water</u> confined in a silica nanopore modeled with MCM-41 features have been performed down to T=190 [P. Gallo, M. Rovere and SH Chen JPCL (2010)].

•A layer analysis analogous to what done in Vycor [Gallo, Rovere, Spohr PRL 2000, JCP (2000)] was done separating bound water from free water. From the behavior of the relaxation time we find evidence of a fragile-to-strong dynamic transition with a crossover from a non-Arrhenius (Vogel-Fulcher-Tammann) to an Arrhenius behavior at a temperatureT=215 K, results close to the experimental finding and simulations in the bulk.

•Similar to Vycor the MCT test works [Gallo, Rovere, Chen, JPCM 2012].

•Excess entropy of free water and structure of free water inside MCM-41 show behviour that fits the same framework [Gallo, Camisasca, DeMarzio, Rovere, in preparation]

•Similar to Vycor [Rapinesi, Rovere, Gallo JPC 2002] also in MCM-41 the anomalous diffusion is present for the bound water [Gallo, Rovere, Chen, JPCM 2010]

•Water close to the surface of a protein with and without a cryoprotecting agent, two dynamics crossovers [Corradini, Streklova, Stanley, Gallo, Sci. Rep. (2013); Camisasca, De Marzio, Corradini, Gallo in press J.C.P. (2016); Camisasca, De Marzio, Gallo in preparation]





COLLABORATORS

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ROMA TRE GROUP OF: Simulations of Liquids and Soft Matter



	MAIN RESEARCH TOPICS:			
	 Confined water 			
	•	Supercool superheat	and	
	•	Aqueous electrolite	solutions es	of
	•	Ices terrestric extraterr	with 11 estrial	ions, and
	•	Aqueous cryoprese	solutions rvation	for

Prof. PAOLA GALLO (top center), Prof.MAURO ROVERE (top right), Dr. MARIA MARTIN CONDE Post Doc (top left), Dr. GAIA CAMISTASCA PhD (bottom right), Dr. MARGHERITA DE MARZIO PhD (Bottom center right), Dr. ANTONIO IORIO PhD (bottom center left), Dr. PIETRO PUGLIESE PhD here in Erice works on water in carbon nanotubes (bottom left)