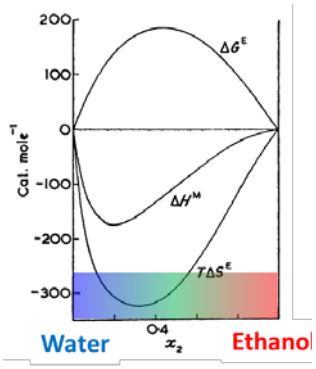
Multi-scale investigation of a scientific cold case: the Water-Ethanol solubility mystery

UMR 6251 - CNRS - Rennes University- France
Physical-Chemistry of Self-assemblies and liquid mixtures

Nowadays, water-ethanol solutions are used in many industrial processes as well as in fundamental research. All these observation make the appearance of *déjà vu*. But careful discussions with perfume industrials or spirit experts point out robust and popular beliefs, such as the over-week maturation required after the perfume mixing, or the taste-opening of distilled whiskey by a water droplet.

From a fundamental perspective, the water-ethanol system is the famous textbook example of non-ideal mixture (cf figure). **Most of the macroscopic experimental observations are in favour of large-scale segregation**. For example, Franks[1,2] explains that the positive excess Gibbs Enthalpy (ΔG^E) of $+0.3k_BT$ "*is always encountered in systems which separate*" and give the example of the butanol/water mixture that exhibits two macroscopic coexisting phases with the same ΔG^E. A few papers pointed out the existence of heterogeneities,[3] without exploring large space scale and slow dynamics. ***Half a century later, this scientific case is still unresolved.***



Excess Thermodynamic Properties of Mixing[1]

The PhD project will be focused on experimental techniques able to characterize both multi-scale **structures and dynamics of these heterogeneities** at the *atomic scale* (Vibrationnal and Nuclear techniques), at the *molecular supramolecular scale* (X-ray Scattering in house and on Synchrotron Sources), and *macroscopic scales* (varied light scattering techniques).

The PhD student will work in collaboration with groups in Prague (P. Stepanek), NYC (O. Gang), synchrotron SOLEIL (T. Bizien). In Rennes, the PhD Student will benefit from complementary experimental techniques (Raman, FTIR, NMR, X-ray Scattering, original optical set-up) as well as state of international leader in liquid mixture molecular dynamic (A. Ghoufi).

1] Franks, F. & Ives, D. Structural Properties of Alcohol-Water Mixtures. *Quarterly Reviews* **20,** 1 (1966).
2] Franks, F. & Desnoyers, J. Alcohol-Water Mixtures Revisited. *Water Science Reviews* **1,** 171–232 (1985).
3] Dixit, S., *et al*, Molecular segregation observed in a concentrated alcohol-water solution. *Nature* **416**, 829–832 (2002).

Profile: ***Open mind*** and enthusiastic candidate, having obtained a master's degree in the ***Physical Chemistry, Soft-Matter Physics*** *or equivalent*.	**Conditions:** 36 month fellowship starting **fall 2023**, The net take home salary is about ~1600 euros/month
Application sent by e-mail, must include a CV, a cover letter highlighting the elements in line with the project, a short description of the Master's internship, transcripts and the contact information of two or three references.	**Contact :** franck.artzner@univ-rennes.fr Physics department, Rennes University Brittany, FRANCE https://ipr.univ-rennes.fr/interlocuteurs/franck-artzner

Selected recent papers :

Physical Properties and Hydrogen-Bonding Network of Water-Ethanol Mixtures from Molecular Dynamics Simulations. *J. Phys. Chem. B* **120,** 793–802 (2016). Atomic view of the histidine environment stabilizing higher-pH conformations of pH-dependent proteins. *Nat. Commun.* **6,** 7771 (2015). Origin of transparency in scattering biomimetic collagen materials. *Proc. Natl. Acad. Sci. U. S. A.* **117,** 11947–11953 (2020). Atomic structure of Lanreotide nanotubes revealed by cryo-EM. *Proc. Natl. Acad. Sci. U. S. A.* **119,** e2120346119 (2022). *Design, synthesis, and characterization of protein origami based on self-assembly of a brick and staple artificial protein pair, Proc. Natl. Acad. Sci. USA, **120** (11) e2218428120 (2023).*