Properties of water at nanoscale will help to design innovative technologies

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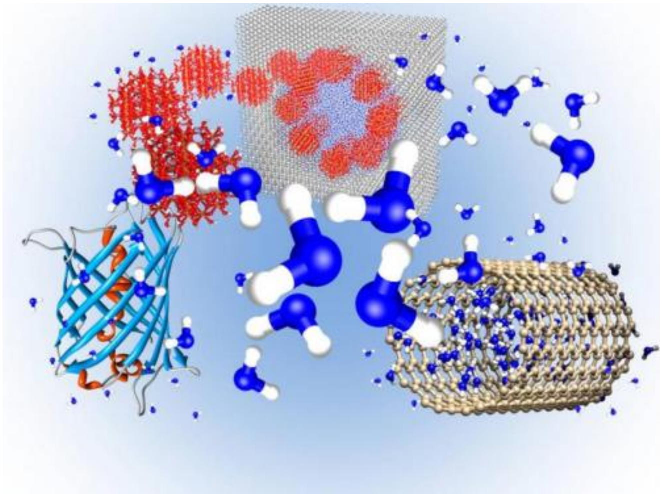

This shows nanopores, nanotubes, proteins and nanoparticles. Credit: Politecnico di Torino

Mechanical engineers from both Department of Energy at Politecnico di Torino and Translational Imaging Department at Houston Methodist Research Institute have modeled and provided a novel insight of the surprising water properties at the nanoscale, even if many other intriguing water characteristics are still far to be fully unveiled. A broad range of technological applications may benefit from these findings, from engineering to biomedical field, as recently shown in a scientific paper published on *Nature Communications*.

Swimming in a honey pool. That's the sensation a water molecule should "feel" while approaching a solid surface within a nanometer (i.e. less than a ten-thousandth of hair diameter). The reduction in water mobility in the very close proximity of surfaces at the nanoscale is the well-known phenomenon of "nanoconfinement", and it is due to both electrostatic and van der Waals attractive forces ruling matter interactions at that scale.

In this context, scientists from Politecnico di Torino and Houston Methodist Research Institute have taken a further step forward, by formulating a quantitative model and a physical interpretation able of predicting the nanoconfinement effect in a rather general framework. In particular, geometric and chemical characteristics as well as physical conditions of diverse nanoconfining surfaces (e.g. proteins, carbon nanotubes, silica nanopores or iron oxide nanoparticles) have been quantitatively related to mobility reduction and "supercooling" conditions of water, namely the persistence of water in a liquid state at temperatures far below 0°C, when close to a solid surface.

This result has been achieved after two years of in silico (i.e. computer-based) and in vitro (i.e. experiment-driven) activities by Eliodoro Chiavazzo, Matteo Fasano, Pietro Asinari (Multi-Scale Modelling Lab, Department of Energy at Politecnico di Torino) and Paolo Decuzzi (Center for the Rational Design of Multifunctional Nanoconstructs at Houston Methodist Research Institute).

This study may soon find applications in the optimization and rational design of a broad variety of novel technologies ranging from applied physics (e.g. "nanofluids", suspensions made out of water and nanoparticles for enhancing heat transfer) to sustainable energy (e.g. thermal storage based on nanoconfined water within sorbent materials); from detection and removal of pollutant from water (e.g. molecular sieves) to nanomedicine.

The latter is the field where the research has indeed found a first important application. Every year, almost sixty millions of Magnetic Resonance Imaging (MRI) scans are performed, with diagnostic purposes. In the past decade, MRI technology benefitted from various significant scientific advances, which allowed more precise and sharper images of pathological tissues. Among other, contrast agents (i.e. substances used for improving contrast of structures or fluids within the body) importantly contributed in enhancing MRI performances.

This research activity has been able to explain and predict the increase in MRI performances due to nanoconfined contrast agents, which are currently under development at the Houston Methodist Research Institute. Hence, the discovery paves the way to further increase in the quality of MRI images, in order to possibly improve chances of earlier and more accurate detection of diseases in millions of patients, every year.

Additional results and applications of nanoconfinement effect on nanomedicine will be published soon, thanks to a multidisciplinary collaboration between biomedical (Houston Methodist), engineering (Politecnico di Torino) and chemical (Rice University, Houston–TX) research groups. In particular, iron oxide contrast agents loaded in silicon or polymeric nanovectors are currently investigated, because they can be first magnetically concentrated in human diseased tissues and then employed for enhancing MRI performances. Moreover, such a nanoconstructs own theranostic properties, which means that they can be used for diagnostic (i.e. MRI) and therapeutic (i.e. temperature triggered drug release or hyperthermia treatments) purposes at the same time, which is a significant step forward in the war on cancer.

Provided by Politecnico di Torino