Theoretical and Physical Chemistry Institute

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LECTURE

"Understanding the properties of aqueous systems and their interactions with nanoporous materials and sustainable ionic liquid solvents to develop environmental, energy storage and geological applications: A computational modelling perspective"

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Water is the key compound for our existence on this planet and it is involved in nearly all chemical, biological and geological processes. Access to clean water is one of the most challenging questions for mankind in the coming century, in particular with the prospect of global warming. Over the last years the rational design of nanoporous materials for processes requiring the capture and release of water, such as the screening of traces of water, the control of the humidity in the air and the delivery of drinking water in remote areas, has become an issue of crucial importance. Several nanoporous materials, such as metal-organic frameworks (MOFs) have been recently envisaged to address ongoing challenges pertaining to water adsorption related applications.

Water is also considered to be among the most important classes of green solvents, due to its efficiency in replacing toxic organic solvents and tuning the properties of novel sustainable solvents such as ionic liquids, which exhibit a wide applicability in electrochemical energy storage and battery applications. A deeper understanding of the modification of ionic liquids' properties upon water addition can therefore provide valuable information with significant practical implications.

Understanding the properties of aqueous systems at extreme temperature and pressure conditions is also a key issue for geological and space-science applications. Despite long-lasting efforts new intriguing properties are still being described, and even the phase diagram of water, although systematically explored in the past, is far from being complete.

In this lecture, our recent research efforts to address fundamental issues related to these topics, by employing computational molecular modelling techniques, will be systematically presented and discussed. Future perspectives and open problems will be also discussed.