

## **Unravelling the effect of nanoconfinement on molecular properties: a theoretical and experimental study of hybrid layered double hydroxides**

Matter that is confined on a nanoscale displays very different physical properties compared to the bulk. Achieving the control of the factors affecting this very special behavior is relevant in many scientific domains. In particular, nanoconfined water exists in natural biological (proteins, ion channels) and geological (porous rocks, clays) systems, as well as in devices that are developed in Chemistry and Engineering (nanofluidic, nanofiltration, nanomedicine). Among natural systems such as clays, some materials, named Layered Double Hydroxides (LDHs), are intensively used due to the versatility of their possible applications.[1] They comprise inorganic layers having a positively charged surface and packing together, including water and negative ions in the interlamellar region to allow a neutral environment. Anions of very different nature can be intercalated to obtain hybrid systems: inorganic, organic as well as biological molecules and macromolecules (amino acids, enzymes, DNA, etc.). Technology based on these materials can be developed in the field of catalysis, in medical applications (drug delivery), as absorbents of specific pollutants, in the development of nanomaterials.

The anion positions within the interlayer domain and their dynamics are key factors to develop novel systems for biocompatible materials and for environmental chemistry. Moreover, understanding the structure and the dynamics of water confined in systems of nanometric size represents a challenge for researchers, since the use of materials such as the LDHs in technological and industrial applications strongly depends on it (exchange and intercalation properties, conduction, reactivity, etc.). In the past few years, the LCPME Laboratory has provided original strategies to synthesize hybrid LDHs and spectroscopic methods (Infrared, Raman) to obtain information about the nature of the ions and on the intermolecular interactions within the layers.[2] Methodologies based on molecular modeling and tailored on the description of the environment effect on spectroscopic properties were developed in the SRSMC Laboratory, in which multiscale methods are also used to describe the dynamics and the reactivity in large scale systems.[3]

In this PhD project, we shall propose an interdisciplinary approach to provide a molecular understanding of the key phenomena taking place in the interlamellar region, depending on the nature of the anion and on the thermodynamic conditions influencing the size and the nature of the nanoconfined system. It is known that, by changing the scale and the nature of confinement, it is possible to observe changes in the physical- chemical properties of water, such as conductivity, transport properties, dynamics. Besides, when the intercalated anion is a molecule that might be relevant for biocompatible materials, it is extremely important to understand whether its relevant properties are maintained under confinement. To assess this important issue, we shall profit of a longstanding collaboration with Prof. Adolfo Bastida (Murcia University, Spain). These studies will provide crucial advances toward an improved use of LDHs based technologies, addressing fundamental problems such as the anion intercalation mechanism and the kinetics of intercalation and release.

### **References**

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