

## ***Tuning the optical properties of nanoconfined chromophores: a molecular understanding of environment effects***

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### **ABSTRACT**

Nanoconfinement can lead to significant modifications of the dynamical, optical, and physicochemical properties of confined species, which can be exploited for a wide range of applications [1]. Layered double hydroxides (LDHs) are a class of claylike layered systems, the structure of which comprises positively charged mixed-metal hydroxides with a charge-compensating anions in the expandable interlayer space, this latter allowing the intercalation of different guest species. [2]. Due to their optical transparency, LDHs are considered as promising candidates for modulating and improving the optical properties of luminescent complexes. Indeed, recent experimental studies on ruthenium/LDH hybrids have shown that intercalating Ru complexes in LDH leads to significant improvement of their thermal and photostability [3]. However, a molecular interpretation of the role played by the confined environment, which is key to fine tuning the effect on intercalated compounds, is still missing. Furthermore, the dynamics of the hydrogen bond network of the confined water is still unclear and its role in this effect is yet to be understood.

To reach this goal, we propose to adapt and apply a successful strategy that we recently developed [4], based on an integrated multilevel approach providing an ad hoc intramolecular force field for the Ru complex ground and excited states to be used in classical molecular dynamics simulations. Such simulations are coupled with TD-DFT calculations of the optical properties of the chromophore in its local environment. Our current work addresses the following fundamental questions: is it possible to disentangle the role of nanoconfinement vs. that of the complex-surface interaction? What is the local structure of intercalated water? How is the nature of the electronic excited states of the complex affected by the local environment (especially with respect to charge transfer)?

### **REFERENCES**

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