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Sala de la Biblioteca

Molecular Modelling Techniques Applied to Supramolecular Chemistry

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Molecular modelling techniques (e.g., classical molecular dynamics and quantum chemical calculations) can be used to get insight on the properties of a wide range of chemical systems. In this talk I will show how these techniques can be used to describe supramolecular polymerizations involving coordination compounds [1] or organic molecules, and will discuss the cooperativity of the corresponding aggregations. Different inter-molecular interactions, namely, aromatic (pi–pi), CH–pi, M–Cl and metallophilic interactions are shown to stabilize the investigated supramolecules. Hybrid materials formed by organic dyes or coordination compounds and zeolites will also be discussed here.

[1] N. A. M. S. Caturello, Z. Csók, G. Fernández, R. Q. Albuquerque, Chem. Eur. J. 22 (2016) 17681-17689.