Real Sociedad Española de Física

ID de la contribución : **110** Tipo : **Oral parallel contribution**

The quest towards supramolecular networks from first principles

miércoles, 19 de julio de 2017 16:05 (20)

How far into molecular complexity can we get from first principles? Can we predict specific recognitions between molecules from the computation of the relevant conformations and interactions? Is it then possible to forsee how assemblies of molecules spontaneously conform functional nanostructures and materials? Will we ever understand the behaviour of living organisms from the investigation of their molecular building blocks? Should we even dare? These are challenging but central questions in the scientific activity of chemical physicist. A modest illustration of this topic can be obtained from an overview of the incursions of our group into molecular recognition and supramolecular aggregation over the last decade.

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Clasificación de la sesión : Molecular Physics at the Edge II

Clasificación de temáticas : Molecular Physics at the Edge