Multiscale Molecular Modeling:
A Tool for the Design of Hybrid Organic/Inorganic Nano Structured Materials

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A current challenge of physical, chemical and engineering sciences is to develop theoretical tools for predicting structure and physical properties of complex nano structured materials. However, despite all efforts, progress in the prediction of macroscopic physical properties from structure has been slow. Major difficulties relate to the fact that the final properties of the material strongly depend on the nanostructure of the matrix and the interactions of the nano fillers with the matrix. The investigation of the nanostructure via computer simulation is not straightforward and cannot be done using one single tool: in principle the structure could be described by atomistic simulation, but we do not have enough computer power to do that for complex system such as nanocomposites. Given these concepts, it is than necessary to carry out calculations for realistic time scales fast enough to be useful in design by following a coarse graining approach. This requires coupling established techniques, each computationally efficient at a given scale in a multiscale approach, resulting in a useful and efficient design for engineers. This is achieved by incorporating the methods and results of the lower scales (e.g., molecular dynamics) to mesoscale simulations and finally transfer the mesoscale structure calculated into a micro Finite Element (FEM) code for the estimation of the macroscopic properties.

In this seminar, focus will be given to the development of a multiscale molecular simulation framework, with the ultimate goal of developing a computationally-based nanocomposite designing tool specific for hybrid organic/inorganic systems (H-O/I). Many examples of the application of this recipe to PCNs and other H-O/I materials will be presented and discussed. The global perspective of the seminar is the complete integration of all available simulation scales, in a hierarchical procedure to provide an efficient and robust simulation protocol for the successful design of H-O/I systems of industrial interest and the prediction of their final performance.