Nano tools for macro problems: multiscale molecular modeling of nanostrucured systems

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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 organic inorganic nano composite from the knowledge of a few input parameters. This task is particularly crucial in the design and fabrication of nano and bio-nano devices and systems which is the new horizon of nanotechnology for the forthcoming 5 years. Indeed, nanotechnology roadmap is moving from passive nanostructures to active nanostructures and eventually to Nano systems. The complexity of such systems and devices does not allow to follow the try-and-error procedure for the design, due to incredible amount of resources needed to obtain the desired results.

Recent development in computer HW and SW as well as in theories and algorithms allow us to investigate complex systems in the field of material and life science, using the computer as a virtual microscope, allowing us to 'see' the nanostructure and to predict macroscopic properties and behavior, without the need of constructing the nanosystem.

This paper deals with the application of multiscale molecular modeling to different Nano systems selected form the material science and the life science sectors. Despite the very different systems studied and the different application, the multiscale modeling protocol is rather general and applicable with small adjustments from nanostructured plastics to DNA/siRNA therapeutics in cells.

The concept of multiscale molecular modelling is briefly summarized in figure 1 (1), in which it is explained how different methods and algorithms may be integrated to calculate properties at different time and length scale. The challenge is to 'integrate' the methods, so that the ultimate property may be estimated taking into account all the phenomena pertaining at a smaller scale.

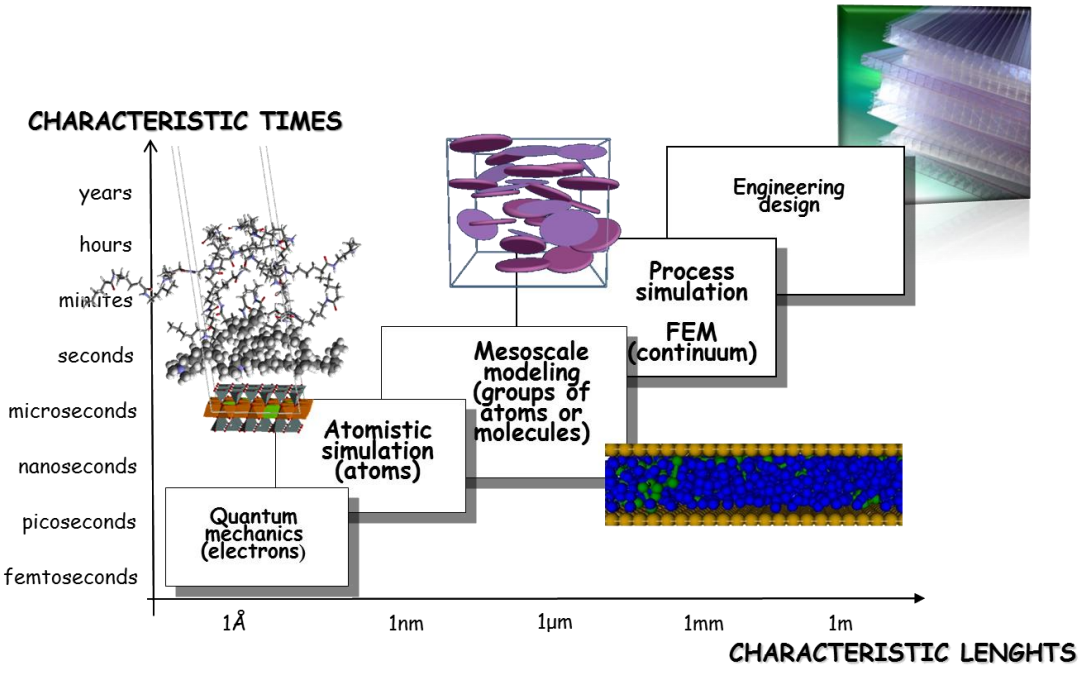

Figure 1: the concept of multiscale modelling.

The proposed computational procedure of the multiscale simulation and modeling is based on the following ansatz: 1) fully atomistic molecular dynamics simulations are perform to retrieve fundamental structural and energetical information at the molecular level; 2) the data gathered at point 1) are mapped into the corresponding structural and energetical information necessary to run

coarse-grained simulations at a mesoscopic level; 3) the main output of point 2), i.e., the system mesoscopic morphologies and density distributions finally constitute the input for finite element calculations and macroscopic properties predictions. The core step in the entire computational recipe is undoubtedly constituted by point 2), or the mesoscale level simulations. In mesoscale modeling, the familiar atomistic description of the molecules is coarse-grained, leading to beads of material (representing the collective degree of freedom of many atoms). These beads interact through pair-potentials which capture the underlying interactions of the constituent atoms (2). The primary output of mesoscale modeling are phase morphologies with size up to the micron level. These morphologies are of interest per se, although little prediction of the material properties is available with the mesoscale tools. Finite element modeling then comes into play, and the material properties of interest can be calculated accordingly by mapping the material structures formed at the nanometer scale onto the finite element grid and coupling this information with the properties of the pure components that comprise the complex system. Using standard solvers the finite element code can then calculate the properties of the realistic structured material (3).

In this paper we apply the above mentioned methodology to examples of interest to material science and life science. The first example is related to the enhancement of mechanical and barrier properties if a nanofiller is dispersed into a polymer matrix: the role of multiscale modeling for the development of the material in the stage of screening the best design is evidenced (4). The second example, important for the opto electronic industry, is related to the prediction of the dispersion of gold nanoparticles into a di block copolymer system forming different nano structures. In this case it is relevant to understand how it is possible to influence the self-assembly of the nanoparticles in the diblock copolymer structure (5). The third example is about drug delivery using bio compatible di/tri block copolymers. In this case it is relevant to predict the phase behavior of the polymer system and the ability of the polymer to form micelles and the load a drug. The last example is related to nanovectors in which we combined multiscale molecular simulations and experimental approaches to define mode and molecular requirements of the interaction of nucleic acid-based therapeutics and dendrimer/dendron-based delivery agents. This type of investigation can provide valuable information to devise optimal delivery systems that would increase the efficacy of DNA/siRNA therapeutics in cells and laboratory animals and move them toward clinical applications.

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