

Multiscale Atomistic Modeling of Amorphous Organic Functional Materials for Optical Chemical Sensing and OLED Applications

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Abstract

Atomistic multiscale simulation is applied to modeling amorphous organic functional materials with specific optical or electronic properties. Materials for optical chemical gas sensors and for organic light-emitting devices (OLED's) are considered as examples. The functionality of such materials is provided by constituting molecules that determine their specific functional properties. In the case of sensing devices, these are so-called indicator molecules (IMs) changing their optical response (mostly, luminescence) upon interaction with a target molecule (detected or analyte molecule, AM). The goal of simulation in this case is to predict the optical properties of the entire structure (sensing material) and its response to various AMs. In the case of OLED's, these are light-emitting and electron- or hole-transporting molecules. The goal of simulation here is to predict the main electronic parameters of these molecules that determine the efficiency of a particular OLED. In both cases, the properties of functional molecules strongly depend on their local supramolecular environment, that is, on the microstructure of the amorphous material. Therefore, a multiscale atomistic approach is used, in which molecular dynamics simulations are used to describe the microstructure of the material, and quantum chemical methods are used to calculate the required electronic properties of the functional molecules in the material. Commonly, a statistical treatment is required to obtain the distribution of wanted molecular properties or their averaged values in the real amorphous material. Problems arising at each step of modeling are analyzed, and current approaches to their solution are discussed. The possibilities of modern atomistic simulation methods are considered using specific examples. [1–8]

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Figures

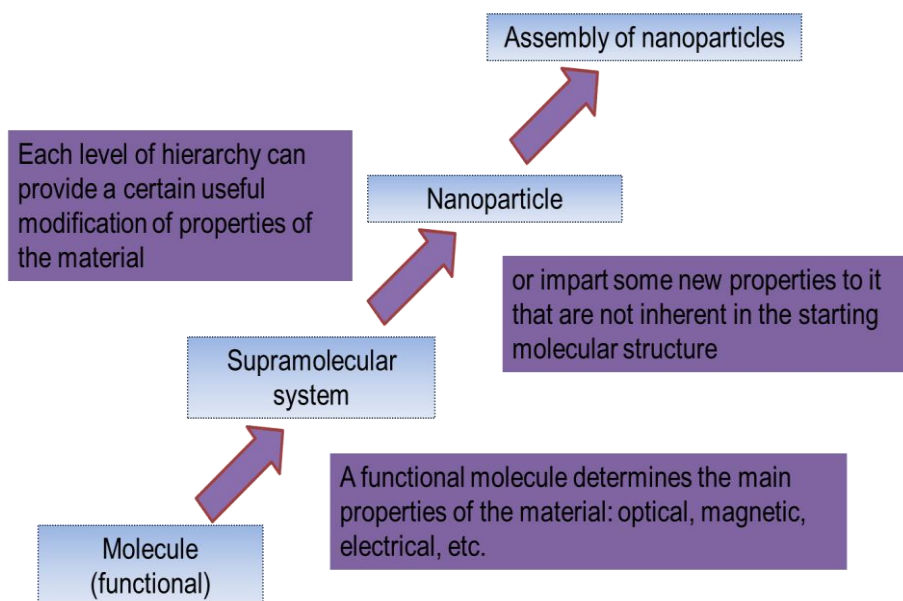


Fig. 1. Hierarchical levels of a functional material for optical chemical sensors

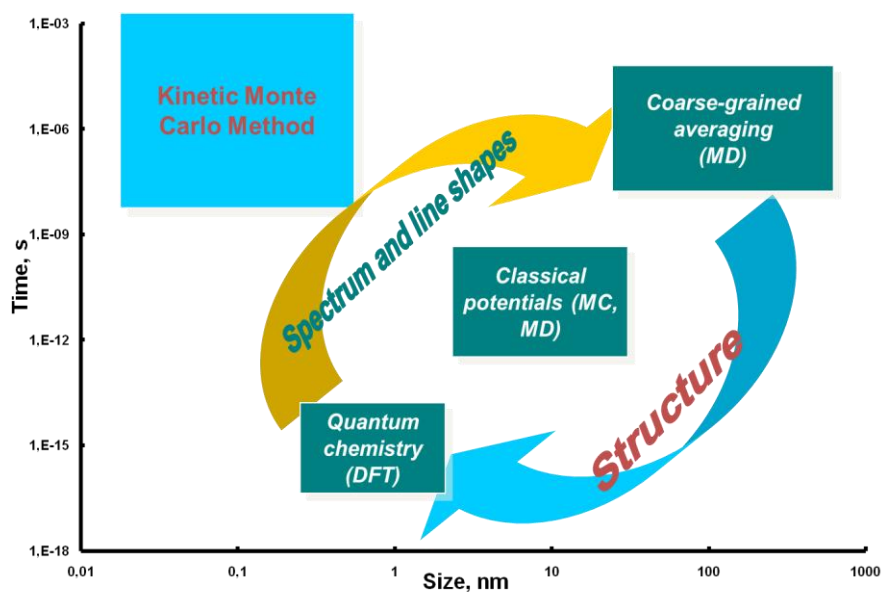


Fig. 2. Scheme of multiscale atomistic simulation of a functional material for optical chemical sensors