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Multiscale atomistic modeling of amorphous organic functional materials for optical chemical sensing and OLED applications

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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.

Biography

Alexander Bagaturyants has completed his PhD at the age of 28 years from Institute of Organoelement Compounds, USSR Academy of Sciences, Moscow and his Dr.Sci. at the age of 48 years from N.N. Semenov Institute of Chemical Physics, USSR Academy of Sciences, Moscow. He is a chief researcher at Photochemistry Center RAS, Moscow and Professor at the Department of Condensed Matter Physics, National Research Nuclear University MEPhI. He has published more than 190 papers in reputed journals.

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Hybrid nano/micro structures of metal oxides: Nano at birth, micron by choice

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Processing of nanopowders for energy storage faces difficulties both in scaling up from the lab scale to the industry as well as eliminating toxicity. As a solution to these problems, the present study investigates into hybrid micro/nano metal oxide powders with a hierarchical morphology. This morphology when employed as supercapacitor electrodes gives an advantage of surface relaxation during the charge/discharge process making it super stable. The study highlights the advantages of nanostructuring of microparticles which can answer the toxicity issues and their potential as a commercial product. This claim in the present study has been validated by cell toxicity study, which establishes that bulk nanostructures are relatively less toxic. These electrodes exhibited high specific mass capacitance value similar to nanostructured particles. Using the material a coin cell device was fabricated and was subjected to electrochemical studies.

Biography

Avinash Balakrishnan had completed his PhD at the age of 28 years from Paichai University, S. Korea and postdoctoral studies from Grenoble Institute of Technology France. He is an Assistant Professor at Amrita Center for Nanosciences. He has published more than 70 papers in reputed journals and edited one book on supercapacitors. He serves as an Associate Editor to Journal of Nanosciences and Nanotechnology. He is also an editor in chief to Advanced Carbon Journal.

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