Low-Dimensional Materials: Interplay Between Theory and Experiment

Marek Sierka
Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Löbdergraben 32, D-07743 Jena, Germany

Low-dimensional and nanostructured materials such as clusters, nanoparticles, thin films and nanocrystalline solids are technologically very important systems that often exhibit unique properties. This opens new possibilities for fabrication of highly functional materials with tailored properties. Due to the limitations of both theory and experiments this task can frequently only be achieved combining computer simulations and experimental investigations. In addition, many chemical and physical properties of nanostructured materials arise from processes and features at multiple scales, both spatial and temporal. This makes necessary simulations of material properties using information or models from different levels of theory: quantum mechanics, molecular mechanics and dynamics as well as statistical thermodynamics. The examples presented in my talk include joined theoretical and experimental studies of structure evolution of nanoparticulate iron oxide, development of polymer-based, nanoparticulate carrier materials for targeted therapy of diseases as well as the development of nanostructured glass ceramics for zero thermal expansion materials. In all cases the full characterization and understanding of these systems could only be accomplished combining experiments and simulations employing a multitude of computational tools.