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Application of multiscale theory and modeling to nanoscience and nanotechnology

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Within past two decades, computational modeling and simulations has become an important part of applied research. It has become possible because of big step forward in development of modern computational methodology and improvements in computer hardware and software. Computational modeling allows one to represent the system with high level of details, to understand the physics of the processes and make predictions which can be used for further rational design.

However, the application of computational methods to nanoscience and nanotechnology has some specialties. Typically nano-sized system has several characteristic lengths and timings and so the different approximations have to be applied to different levels of description. That led to the necessity of use of multiscale approaches to represent the nanosystem in the better way. However, the development of methods which efficiently couple multiple scales is still state of the art, because there is no uniform approach on how to combine the different theories. Typically system is subdivided by several overlapping levels each of which includes the averaged description of the rest of the system.

In that work, I am going to present the collective efforts of National Institute for Nanotechnology (Edmonton, Canada) in application of different multiscale approaches to real nano systems in the different areas: nano-electronics, nano-catalysis, polymer- and surface chemistry.

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