

Modeling Materials at the Nanoscale – a Quantum Dynamical Perspective

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Abstract

Description of complex chemical transformations of nano-scale molecular systems (such as polymers, biological materials, nano-devices) poses a significant challenge for predictive theory and simulations. The multiscale character of physics and chemistry behind processes related to fabrication and functioning of such materials often requires techniques and methods capable to span through several scales of time or space. For example, electron transfer in organic heterojunctions occurs on the femtosecond time scale, transformation of chemical bonding network is typically on the picosecond scale, whereas a relaxation dynamics of soft materials extends to even longer scales. Interplay between all these different scale's phenomena determines efficiency of light harvesting in organic photovoltaic devices. Extending dynamics to longer time scales and to large systems is recognized as a major challenge for science and engineering. We discuss our effort in the development efficient approaches focusing on application to carbon materials.