

Theoretical Study on Nanomaterial Characteristics via Multiscale Simulation

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Recently, molecular modeling and multiscale simulation have received much attention in many research fields due to the elucidation of macroscopic phenomena from atomic scale to continuum scale. Moreover, with the increase of computer technology, the role of multiscale simulation is becoming more important. Accordingly, the multiscale simulation assisted researches can be a promising direction in future research for interdisciplinary effort from both experimental and theoretical parts. In this presentation, the case studies related to nanomaterial characteristics and their applications (*e.g.*, nanophotonics and energy applications) are introduced by using the multiscale simulation from atomic scale to continuum scale. Through the investigation of nanomaterial characteristics, we theoretically analyzed the experimental phenomena and identified the cause. Therefore, this presentation introduces how to investigate the physicochemical properties of nanomaterials for description of experimental phenomena using a variety of simulation methods.