Hierarchical Multiscale Modeling and Control of Nanomaterials

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In this talk, recent developments from our work on coarse-grained kinetic Monte Carlo simulations and hierarchical multiscale simulation will be discussed. These tools enable simulation of realistic systems in terms of length and time scales, while retaining the correct level of fluctuations as indicated via simulations and theory (large deviation principles). The conceptual developments of coarse-graining will be reviewed and their computational efficiency will be illustrated. In conjunction with nonlinear dynamics and optimal control theory, multiscale modeling becomes in invaluable toolbox for scale-up of materials' self-organization. An example of pattern formation leading to quantum dots (e.g., Pb on Cu) will be presented along with control strategies for nanomaterials processing.