University of Texas at San Antonio

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3:15p.m.-4:15p.m.

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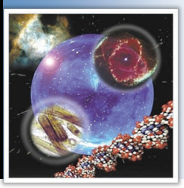
Growth, Transformation, and Assembly of Nanoscale Materials: Insights from Simulation

Achieving the controlled synthesis of colloidal nanomaterials with selected shapes and sizes is an important goal for a variety of applications that can exploit their unique properties (e.g., optical, catalytic, magnetic, etc.). In the past decade, a number of promising solution-phase synthesis techniques have been developed to fabricate various nanostructures. A deep, fundamental understanding of the phenomena that promote selective growth and assembly in these syntheses would enable tight control of nanostructure morphologies in next-generation techniques. I will discuss our efforts to understand how colloidal nanostructures assume selected shapes during their synthesis. Two ideas will be presented and explored using computer simulations and first-principles calculations based on density-functional theory. To highlight one of our research directions, I will discuss our efforts to understand the workings of structure-directing molecules, which facilitate the formation of selective nanoparticle shapes. I will also discuss a second set of efforts aimed at understanding the origins of oriented attachment, a mechanism whereby selective nanostructures are formed via nanoparticle aggregation.



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