Molecular Modeling and Simulation in Nanotechnology: Novel Opportunity for Research, Education, and Outreach

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ABSTRACT

Molecular and larger length-scale modeling and simulation are playing an increasingly important role in fundamental understanding of nanoscale phenomena and as well as in technological applications. Detailed information available from molecular simulations provides excellent opportunities for education and outreach when combined with with visualization tools. I will briefly present examples from my group's research that focus on understanding biological structure and function in non-biological contexts (e.g., protein under high pressures, enzymes in non-aqueous media). We have recently developed "Molecularium" -- an education and outreach effort in which molecular level concepts are taught to general public through development of animation movies that are projected in a planetarium dome. The first Molecularium show "Riding Snowflakes" was released to the general public in the NY-capital region on Feb 4th, 2005. I will present the progress and the future directions of this project. Both research and education efforts are funded by the US National Science Foundation.