

“Assembly and Patterns in the Nanoworld and Beyond”

Wednesday
November 8, 2017
3:00 pm
Wu and Chen Auditorium
Levine Hall



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Abstract

In recent years, nanoscience and nanotechnology have played an ever increasing role in industry, medicine, and materials science and engineering. Because of their size, intermediate between the dimensions of atoms and of bulk matter, nanoscale materials often exhibit unique properties. If one compares a crystal composed of only a few thousands of atoms to a bulk crystal, the fraction of the total number of atoms on the surface of the nanosized crystal is much larger than the corresponding fraction for the bulk solid. This results in a much higher chemical reactivity for the nanosized crystal and, in most cases, in a lower temperature of melting than for the bulk crystal. The unique properties of nanoscale materials have been the subject of intense research over the last decade, as well as their enhanced efficiency. For instance, when their use as catalysts, has been demonstrated. One needs, however, to be able to control the properties of nanomaterials (size, shape and crystalline structure) to fully harness the powerful properties of these materials. In this talk, I will discuss how molecular simulation can help unravel the interplay between kinetics and thermodynamics during the formation of nanomaterials. In particular, I will examine how the control of the properties of the nanoparticles can be achieved during nucleation and growth. Examples of the formation of semiconductor, metal and molecular nanoparticles will be presented.

Bio

Jerome Delhommelle did his undergraduate studies at the Ecole Normale Supérieure (Cachan), and received a B.S. and a M.S. in Physical and Theoretical Chemistry from the University of Paris Sud-Orsay (France). He graduated in 2000 with a Ph.D. in Physical and Theoretical Chemistry (advisor: Prof. A. H. Fuchs) and took up postdoctoral appointments at the Research School of Chemistry at the Australian National University in Prof. D. J. Evans' group, and at Vanderbilt University in Prof. P. T. Cummings' group. He is now an Associate Professor in Chemistry at the University of North Dakota. His research consists of developing molecular simulation methods to analyze the microscopic mechanisms underlying various nonequilibrium processes. His recent research focuses on understanding and controlling polymorphism during crystallization, for which he received a NSF CAREER award in 2011 from the Division of Materials Research, as well as the 2012 OpenEye Outstanding Young Faculty Award from the American Chemical Society.

Fall 2017 CBE Seminar Series

