NDSU Physics Seminar

"Molecular Simulation of Self-Assembly on the Nanoscale"

Dr. Jerome Delhommelle

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Wednesday, November 18th at 4:00 p.m.

South Engineering 221, NDSU
(refreshments at 3:45 p.m. in room 216)

We review recent work on the molecular simulation of the crystallization process. The aim of this work is to obtain a complete understanding of the molecular mechanisms underlying crystal nucleation and growth, and, in particular, to shed light on the polymorph selection process. For this purpose, we carry out three different types of molecular simulation: (i) to determine the phase diagram of the simulated system, (ii) to simulate the crystal nucleation event and (iii) to gain a direct access to the crystal growth mechanism. We present results obtained on a variety of systems, ranging from model systems to colloidal systems and metal nanoparticles and discuss new leads to improve the accuracy of simulation methods for the determination of phase diagrams.

All are welcome!