Computationally-driven materials design

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Bridging atomistic simulations with nanoscale systems

Molecular Dynamics

Enhanced Sampling

Kinetic Monte Carlo

Fuel and emission

Nanoparticle formation

Health applications
In-house multiscale code SNAPS (Stochastic NANoParticle Simulator)

Nanoparticle formation in reactive systems - Chemical growth based on generic reactions

Stochastic nanoparticles characterization
Research Focus

Phase stability

Melting mechanism
Solid phase change
Ion migration
Inorganic nanomaterials
Organic assemblies

Supramolecular structures
Chirality
Computational driven molecular design
Non-equilibrium phases
Heterostructures