

Cyberinfrastructure for Phase-Space Mapping

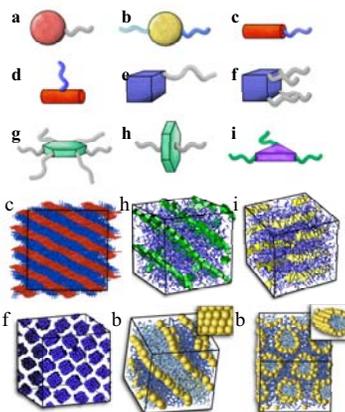
Free Energies, Phase Equilibria and Transition Paths

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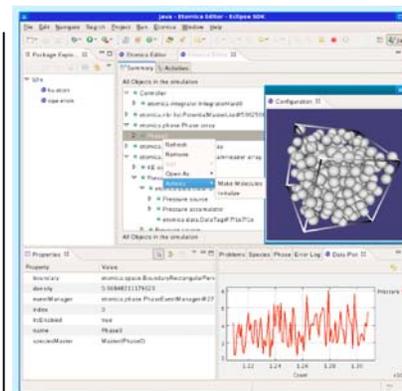
Aim: routine calculation of free energies, phase equilibria, and transition paths by molecular simulation

Approach:

- Develop consensus Application Programming Interface (API) for molecular simulation
- Implement API (or facades of it) in new and established codebases
- Develop targeted library components that interact with API-compliant code
- Construct general-purpose GUI that interacts with API components

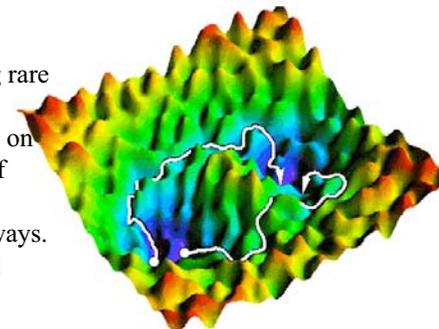


Examples of model tethered nanoparticles and the phases into which they self-assemble. (S. Glotzer)



Etomica graphical framework being developed for molecular simulations. (D. Kofke)

Schematic energy surface of a complex system. Understanding rare transitions requires finding and analyzing trajectories that move on such a surface from one basin of attraction to another. There are many (possibly torturous) pathways. A representative sampling of all possible routes is required. (D. Chandler)



Co-PIs: Chandler (Berkeley); Cummings (Vanderbilt); Gelb (Wash.-St. Louis); Glotzer (Michigan)