
Seminar

Solids and fluids at interfaces: Novel simulation techniques

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Interfacial free energies are often not accessible experimentally, although they are central quantities for the understanding of nucleation phenomena or wetting behavior. Even in particle-based computer simulations, it is difficult to obtain reliable estimates of interfacial free energies, in particular if solid phases are involved. In my talk, I present thermodynamic integration schemes for the determination of interfacial free energies for solid-liquid interfaces as well as for interfaces between a liquid or crystal with a frozen structured wall, formed by particles frozen into the same equilibrium structure as the liquid or crystal, respectively.

Thursday, Jan 28th 2016

4:00 PM (Tea/Coffee at 3:45 PM)

Seminar Hall, TCIS