מכון ויצמן למדע
WEIZMANN INSTITUTE OF SCIENCE

Ben May Center for
Chemical Theory and Computation

Ben May Lecture Series

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Statistical Mechanics of Interfaces: Still a Challenge?

Basic concepts related to interfaces between coexisting phases in thermal equilibrium can be traced back to the classic work of Gibbs, van der Waals, Landau, Cahn and Hilliard. Yet, these concepts still pose problems that are not well understood. The concept of an (intrinsic) interfacial profile is a key one for computing the interfacial free energy, but turns out to be ill-defined due to the inherent difficulties in separating the intrinsic profile from capillary wave broadening. A related problem is the failure of the idea of a free energy of homogeneous states inside the two-phase coexistence region in systems with short range forces.

These difficulties can be avoided by computer simulation methods. Yet, the latter suffer from subtle finite size effects, which will be demonstrated in this lecture by extensive Monte Carlo simulations for 2D and 3D Ising models. It will be shown that one can understand them in terms of fluctuation phenomena associated with interfaces, such as translational degrees of freedoms of domains and "domain breathing". Correcting for these finite size effects, one can obtain accurate estimates for interfacial free energies, also for off-lattice models of fluids. Finally, it will be demonstrated that these concepts can be carried over to the study of curved interfaces (of droplets or bubbles, respectively), allowing the estimation of Tolman's length.

Thursday **April 2, 2020**

14:00 AM Gerhard M.J. Schmidt Lecture Hall

For more information and accessibility issues,
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