455c Thermodynamics of Symmetric Dimers: Lattice Dft Predictions and Simulations

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Lattice density functional theory (DFT) is developed for symmetric dimers with nearest neighbor interactions. Equations of equilibrium are analyzed in the region of multiple solutions. Comparison with Monte Carlo simulations is discussed in terms of phase diagram, including first order and order-disorder transitions. It is shown that mean field approximation gives useful analytical solutions which are accurate over a wide range of densities and temperatures.