

Abstract Submitted
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New Molecular Theory for Dense, Thin Polymer Films KARL FREED, James Franck Institute, University of Chicago — The development of a molecular theory for dense polymer systems ranks among the most challenging problems in the statistical mechanics of complex matter. These difficulties become compounded when considering the influence of molecular details on thermodynamic properties of thin polymer films, properties deviating from those of the bulk phases. A new theory of dense polymer films is developed as a significant generalization of methods used to devise the lattice cluster theory, an extension of Flory-Huggins theory that include details of monomer structure and short range correlations (neglected in FH theory) and that has successfully been applied to a wide range of polymer systems. The new theory incorporates the essential “transport” constraints of Helfand and focuses on the strict imposition of excluded volume constraints, appropriate to dense polymer systems, rather than the maintenance of chain connectivity as appropriate for lower densities and implemented in self-consistent theories of polymer adsorption at interfaces. The theory is illustrated by presenting examples of the computed density and chain end profiles for free standing films as a function of bulk density, chain length, temperature, and chain semi-flexibility.

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