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Effect of chain stiffness on structural and thermodynamic properties of polymer melts JUTTA LUETTMER-STRATHMANN, University of Akron — Static and dynamic properties of polymers are affected by the stiffness of the chains. In this work, we investigate structural and thermodynamic properties of a lattice model for semiflexible polymer chains. The model is an extension of Shaffer's bond- fluctuation model [1] and includes attractive interactions between monomers and an adjustable bending penalty that determines the Kuhn segment length. For isolated chains, a competition between monomer-monomer interactions and bending penalties determines the chain conformations at low temperatures. For dense melts, packing effects play an important role in the structure and thermodynamics of the polymeric liquid. In order to investigate static properties as a function of temperature and chain stiffness, we perform Wang-Landau type simulations and construct densities of states over the two- dimensional state space of monomer-monomer and bending contributions to the internal energy. In addition, we present first results from an algorithm for equation-of-state effects in lattice models.
[1] J. S. Shaffer, J. Chem. Phys. 101, 4205 (1994).

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