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How Reliable Are Soft Potentials? Ensuring Thermodynamic Consistency Between Hierarchical Models of Polymer Melts JAMES MC-CARTY, MARINA GUENZA, University of Oregon — The use of soft effective potentials to represent macromolecular systems has become widespread in the areas of biophysics and materials science. A survey of the field reveals a vast array of various phenomenological potentials whose ability to provide quantitative information about several different properties of the same system is not evident. This talk will present a formally sound approach to obtain soft potentials for realistic models of simple linear polymer melts which reproduce the correct center of mass distribution of particles as well as the correct equation of state of the underlying system of interest. Furthermore, an analytical potential allows us to rigorously address the implications of coarse-graining on the entropy and free energies of the system and to account for the reduced degrees of freedom and smoothed energy landscape implicit to coarse-grained models. Finally, the transferability of the method to other systems and potential applications will be discussed.

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