

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Transferability of structure, thermodynamics, and dynamics in coarse-grained macromolecular liquids¹ MOHAMMADHASAN DINPAJOOH, MARINA GUENZA, University of Oregon — The Integral Equation Coarse-Graining (IECG) approach is an analytically solved theory of coarse-graining for the structure, thermodynamics, and dynamics of macromolecular liquid, either in equilibrium or out of equilibrium. We present here a brief overview of the method and recent developments that optimizes computational efficiency, as well as applications of the IECG to liquids of macromolecules and their mixtures.

¹This work was supported by the National Science Foundation Grant CHE-1362500.

Marina Guenza
University of Oregon

Date submitted: 17 Jan 2017

Electronic form version 1.4