Abstract Submitted
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Many-body effects in systematic coarse graining[1] CHRISTOPH SCHERER, DENIS ANDRIENKO, Max Planck Institute For Polymer Research, Mainz — Particle based coarse-graining (CG) is a systematic way of reduction of the number of degrees of freedom describing a physical system. It involves three steps: choice of the CG degrees of freedom, identification of a merit function which quantifies the difference between the fine- and coarse-grained representations, and determination of the CG potential energy surface (PES). The entire procedure is sensitive to the number and types of basis-functions employed in the CG representations: for example, the incorporation of nonbonded three-body interactions in a coarse-grained water model helps to reproduce both thermodynamic and structural properties [1,2]. In this work, we investigate the effect of extending the basis set to three-body interactions for several organic solvents and formulate clear criteria for when these many-body terms are required. The coarse-graining scheme is implemented in the VOTCA-CSG toolkit [3]. [1] V. Molinero, E. B. Moore, J. Phys. Chem. B, 113, 4008 (2009) [2] L. Larini, L. Lu, G.A. Voth, J. Chem. Phys. 132, 164107 (2010) [3] V. Rhle, C. Junghans, A. Lukyanov, K. Kremer, D. Andrienko, J. Chem. Theory. Comput. 5, 3211 (2009)

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