

Abstract Submitted  
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**The conditional reversible work method for molecular coarse graining of soft matter** NICO VAN DER VEGT, EMILIANO BRINI, GREGOR DEICHMANN, Technische Universität Darmstadt, COMPUTATIONAL PHYSICAL CHEMISTRY GROUP TEAM — I will discuss a recently introduced systematic coarse-graining method that provides transferable coarse-grained potentials for scale-bridging simulations of soft matter systems. The method [1-3] is based on direct calculation of pair potentials in the gas or liquid phase with thermodynamic integration or free energy perturbation methods and has been coined the Conditional Reversible Work (CRW) method. I will discuss the CRW method in the general context of systematic coarse graining, a recent extension to dynamically-consistent coarse-grained simulations [4], and show some practical examples, including coarse-grained simulations of molecular liquids and polymers.

[1] E. Brini, N.F.A. van der Vegt, J. Chem. Phys. 137, 154113 (2012).

[2] E. Brini, V. Marcon, N.F.A. van der Vegt, Phys.Chem.Chem.Phys. 13, 10468-10474 (2011).

[3] E. Brini et al. Soft Matter 9, 2108-2119 (2013).

[4] G. Deichmann, V. Marcon, N.F.A. van der Vegt, submitted

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