

Abstract Submitted
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**Coil-globule transition of macromolecules in mixed solvent:
A semi-grand canonical molecular dynamics approach** DEBASHISH
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formational transition of macromolecules in mixed solvents are intimately linked to
large local concentration fluctuations of solvent components. The numerical stud-
ies in the field are limited to the closed boundary schemes, which, however, suf-
fer from severe system size effects. To overcome this discrepancy, we have devel-
oped a semi-grand canonical molecular dynamics scheme for complex fluids [1]. Our
method makes use of the adaptive resolution scheme (AdResS) [2] with a metropo-
lis particle exchange criterion. In AdResS, an all-atom region, containing macro-
molecule, is coupled to a coarse-grained (CG) reservoir. The semi-grand canoni-
cal particle exchange is performed in the CG region. As the applications of the
method, we study the concentration driven reentrant collapse and swelling tran-
sition of poly(N-isopropylacrylamide) (PNIPAm) and poly(N,N-diethylacrylamide)
(PDEAm) in aqueous methanol and demonstrate the role of the delicate interplay
of the different intermolecular interactions. [1] D. Mukherji and K. Kremer, Macro-
molecules, DOI:10.1021/ma401877c (2013). [2] M. Praprotnik, L. Delle Site, and K.
Kremer, J. Chem. Phys. 123, 224106, (2005).

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