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Estimation of χ parameter from molecular simulations ASHWIN RAVICHANDRAN, CHAU-CHYUN CHEN, RAJESH KHARE, Texas Tech University — The χ parameter introduced in Flory-Huggins theory is widely used to determine polymer miscibility and its value is generally obtained by fitting to experimental data. In spite of its wide usage, techniques for predicting χ parameter from the knowledge of molecular structure are not yet well established. In this work, we apply molecular simulations to estimate the value of the χ parameter for a polymer blend system. In particular, we propose to use the approach suggested by Schweizer & Curro [*Journal of Chemical Physics*, **91**, 5059 (1989)] which estimates χ parameter in terms of the direct correlation functions. The χ parameter thus obtained is related to the molecular structure factor, thereby making comparisons with experiment possible. Molecular dynamics simulations with atomistically detailed models are performed to estimate the value of the χ parameter. Results will be presented for the application of this formalism to the binary blend of polyisobutylene (PIB) and polybutadiene (PBD) for which experimental data are available [*Industrial & Engineering Chemistry Research*, **47**, 3551 (2008)]. Finally, important structural features of the condensed phase which influence the value of the χ parameter will be discussed.

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