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Volume 35, Issue 15, July 1994, Pages 3251-3259

Polymer paper

Estimation of polymer compatibility from molecular mechanics calculations

Andrew R Tiller  ... Boris Gorella 

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[https://doi.org/10.1016/0032-3861\(94\)90130-9](https://doi.org/10.1016/0032-3861(94)90130-9)

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Abstract

A new computational method is presented for the rapid estimation of polymer miscibility. This algorithm (coined FLEXIBLEND) makes use of molecular mechanics calculations on a pair of polymer segments in order to estimate heats of mixing. Specific interactions between polymer segments of different types are accounted for, as are effects due to local chain flexibility. The many assumptions and approximations of such two-segment approaches are discussed, and the new algorithm is used to investigate how miscibility predictions are influenced by segment size and other parameters of the model. Predictions of polymer miscibility in agreement with experiment are presented for miscible and immiscible blends, and detailed error analysis indicates the statistical significance of the FLEXIBLEND results. Balancing the recognized limitations with the computational speed of the method, it is concluded that the new algorithm should be

useful in initial screening of potential blend candidates, and in giving a rough guide as to how changes in chemical structure might alter phase behaviour. The method also provides useful insight as to why two polymers mix or phase-separate. Finally, the FLEXIBLEND results are compared with those of a more rigorous, but computationally more expensive, amorphous cell method for calculating heats of mixing.



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Keywords

polymer miscibility; computer modelling; molecular mechanics

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Current address: Department of Chemistry, University of California-Irvine, Irvine, CA 92717, USA.

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