Supporting Information for

Solubility of Selected Polymers in Cyclohexane: Comparison between Flory-Huggins Interaction Parameters Calculated Using Three Different Molecular Dynamics Simulation Approaches

Gabriel P. Costa,[1] Stanislav R. Stoyanov,[2,*] Qi Liu,[1] Phillip Choi.[1,3,*]

[1]*Department of Chemical and Materials Engineering, University of Alberta, Edmonton, AB T6G 2G6, Canada;*
[2]*Natural Resources Canada, CanmetENERGY Devon, 1 Oil Patch Drive, Devon, Alberta T9G 1A8 Canada;*
[3]*Faculty of Engineering and Applied Science, University of Regina, Regina, SK S4S 2A0, Canada.*

[*] Corresponding authors: phillip.choi@uregina.ca (PC) and stanislav.stoyanov@nrcan-rncan.gc.ca (SRS)

Table of content

1. Degree of Polymerization

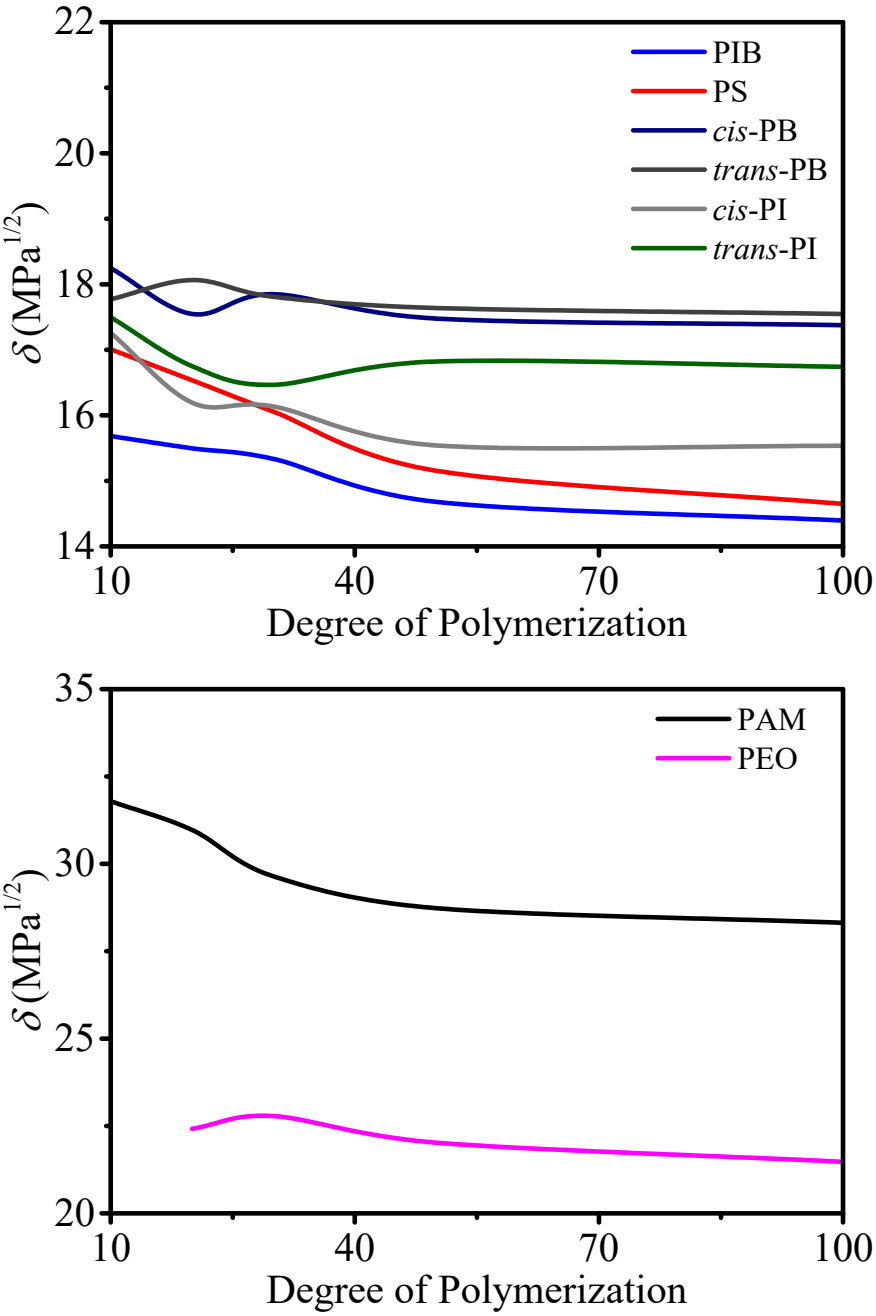

Figure S1. Chain length dependence of the Hildebrand solubility parameters at 298 K.

2. Radial distribution function

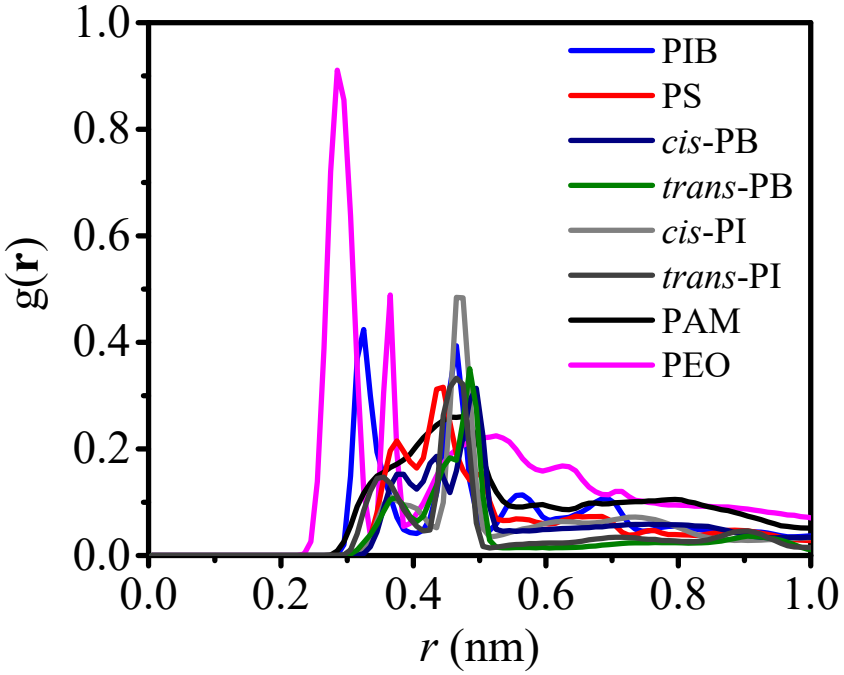

Figure S2. Radial distribution function o the functional groups over a radius of 1 nm.

3. Initial and final spatial disposition of PEO

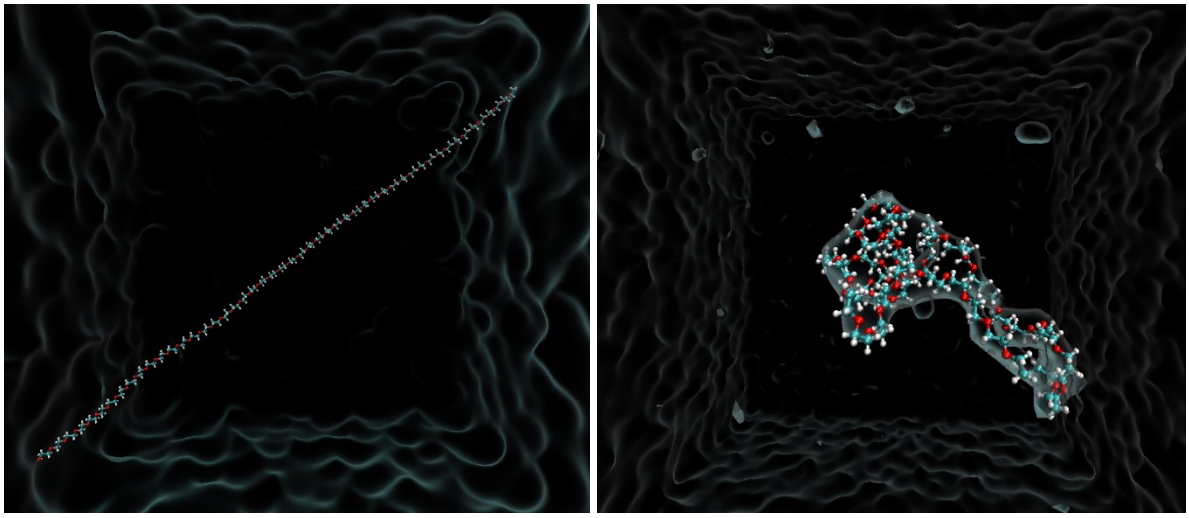

Figure S3. Snapshot of the initial (left) and final (right) conformation of PEO in cyclohexane solution after 50 ns of simulation. The snapshots were obtained using the VMD software.[1]

4. Mean square displacement

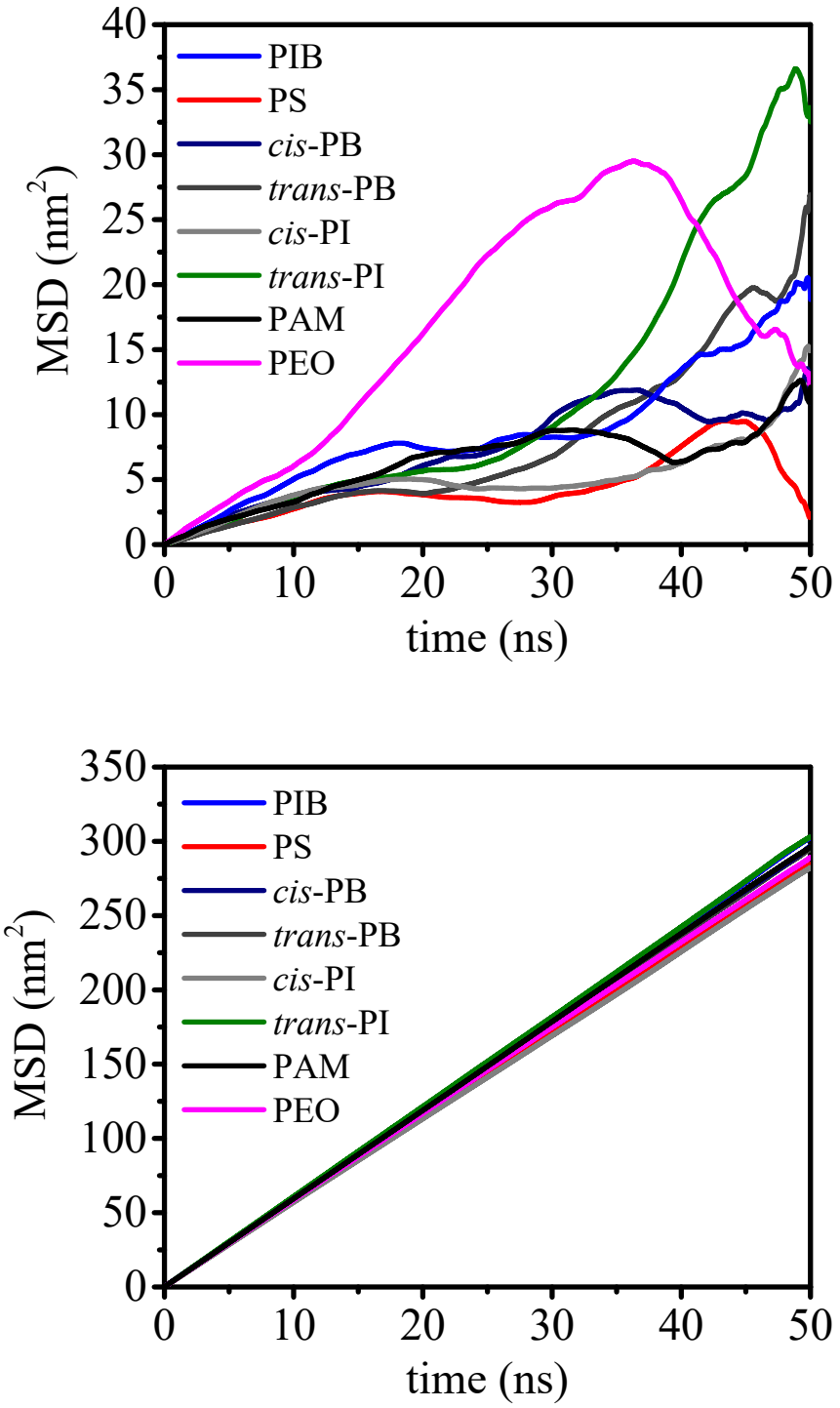

Figure S4. Mean square displacement of the polymer (top) and the solvent (bottom).

References

1 W. Humphrey, A. Dalke and K. Schulten, VMD: Visual molecular dynamics, *J Mol Graph*, 1996, **14**, 33–38.