

# **Influence Of Monomer Sequence On Microstructure Of Nonadditive Hard Chain Copolymers: Simulation And Equation Of State**

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## **Summary**

Influence of copolymer structure on self-assembly of the copolymer was investigated by introducing nonadditive size interactions among different type segments in copolymers composed of touching hard spheres. The copolymer structures investigated are diblock, alternating, multiblock, and random. The copolymers were simulated using discontinuous molecular dynamics simulation. Equations of state of the different model copolymers were developed using the TPT1 theory. Diblock copolymers were found to self assemble readily at high values of the nonadditivity parameter  $\Delta$  and at high densities. Multiblock and random copolymers self assembled to a smaller extent and the alternating copolymer self-assembled only at very high  $\Delta$  and densities. The TPT1 equation of state provided good prediction of the compressibilities of the different copolymer systems at negative and small positive values of  $\Delta$ . Deviations between the model and simulation results were observed at high  $\Delta$  and high densities. Deviations were associated with self-assembly of the copolymers. (C) 2003 American Institute of Physics.

## **References:**

1. ABUSHARKH BF, 2000, MACROMOLECULES, V33, P1345
2. ABUSHARKH BF, 2000, MACROMOLECULES, V33, P9437
3. ADAMS DJ, 1975, J CHEM PHYS, V63, P1900
4. ALBLAS BP, 1984, J NONCRYST SOLIDS, V61, P201
5. ALDER BJ, 1959, J CHEM PHYS, V31, P459
6. AMAR JG, 1989, MOL PHYS, V67, P739
7. BANASZAK M, 1992, MACROMOLECULES, V25, P3406

8. BARRAT JL, 1991, J CHEM PHYS, V95, P1281
9. BELLEMANS A, 1980, MOL PHYS, V39, P781
10. BESOLD G, 1999, COMPUT PHYS COMMUN, V122, P542
11. CHIEW YC, 1990, MOL PHYS, V70, P129
12. COSTANTINO M, 1991, J PHYS CHEM-US, V95, P9034
13. DAVID EF, 1994, J CHEM PHYS, V100, P7784
14. EHRENBERG V, 1990, PHYSICA A, V169, P365
15. FREDRICKSON GH, 1987, J CHEM PHYS, V87, P697
16. FRIED H, 1991, J CHEM PHYS 2, V94, P8349
17. GAZZILLO D, 1989, J PHYS-CONDENS MAT, V1, P3469
18. GAZZILLO D, 1991, J CHEM PHYS, V95, P4565
19. GROOT RD, 1998, J CHEM PHYS, V108, P8731
20. HAMAD EZ, 1996, J CHEM PHYS, V105, P3222
21. HAMAD EZ, 1996, J CHEM PHYS, V105, P3229
22. HAMAD EZ, 1997, J CHEM PHYS, V106, P6116
23. HAMAD EZ, 1997, MOL PHYS, V91, P371
24. HAMAD EZ, 1999, J CHEM PHYS, V111, P5599
25. HAYNES CA, 1993, AICHE J, V39, P1539
26. HOFFMANN A, 1997, J CHEM PHYS, V106, P6709
27. HOFFMANN A, 1997, J CHEM PHYS, V107, P7559
28. HONNELL KG, 1987, J CHEM PHYS, V87, P664
29. JUNG JK, 1994, J CHEM PHYS, V100, P9064
30. JUNG JY, 1995, J CHEM PHYS, V102, P1349
31. LARSON RG, 1994, MACROMOLECULES, V27, P4198
32. LEIBLER L, 1980, MACROMOLECULES, V13, P1602
33. MALAKHOV AO, 1992, MACROMOLECULES, V25, P6262
34. MANSOORI GA, 1971, J CHEM PHYS, V54, P1523
35. MATSEN MW, 1994, PHYS REV LETT, V72, P2660
36. MATSEN MW, 1997, J CHEM PHYS, V106, P2436
37. MATSEN MW, 2002, J PHYS-CONDENS MAT, V14, R21
38. MELNYK TW, 1975, MOL PHYS, V29, P891
39. MURAT M, 1999, MACROMOLECULES, V32, P595
40. OHTA T, 1986, MACROMOLECULES, V19, P2621
41. RAPPAPORT DC, 1979, J CHEM PHYS, V71, P3299
42. RAPPAPORT DC, 1987, J PHYS A, V11, L213
43. SCHAIK HM, 1992, J CHEM PHYS, V97, P8561
44. SCHOUTEN JA, 1985, CHEM PHYS LETT, V114, P40
45. SCHULL KR, 1992, MACROMOLECULES, V25, P2122
46. SCHULTZ AJ, 2002, J CHEM PHYS, V117, P10329, DOI 10.1063/1.1519839
47. SEMENOV AN, 1985, ZH EKSP TEOR FIZ, V61, P733
48. SMITH SW, 1996, J CHEM PHYS, V104, P5616
49. TENNE R, 1978, PHYS REV A, V17, P2036
50. VANHINSBERG MGE, 1993, FLUID PHASE EQUILIBR, V88, P115
51. WERTHEIM MS, 1984, J STAT PHYS, V35, P19
52. WERTHEIM MS, 1987, J CHEM PHYS, V87, P7323

53. WHITMORE MD, 1990, J CHEM PHYS, V93, P2946

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