

The Relationship between Structure and Performance of Different Polyimides Based on Molecular Simulations

Supplementary Materials

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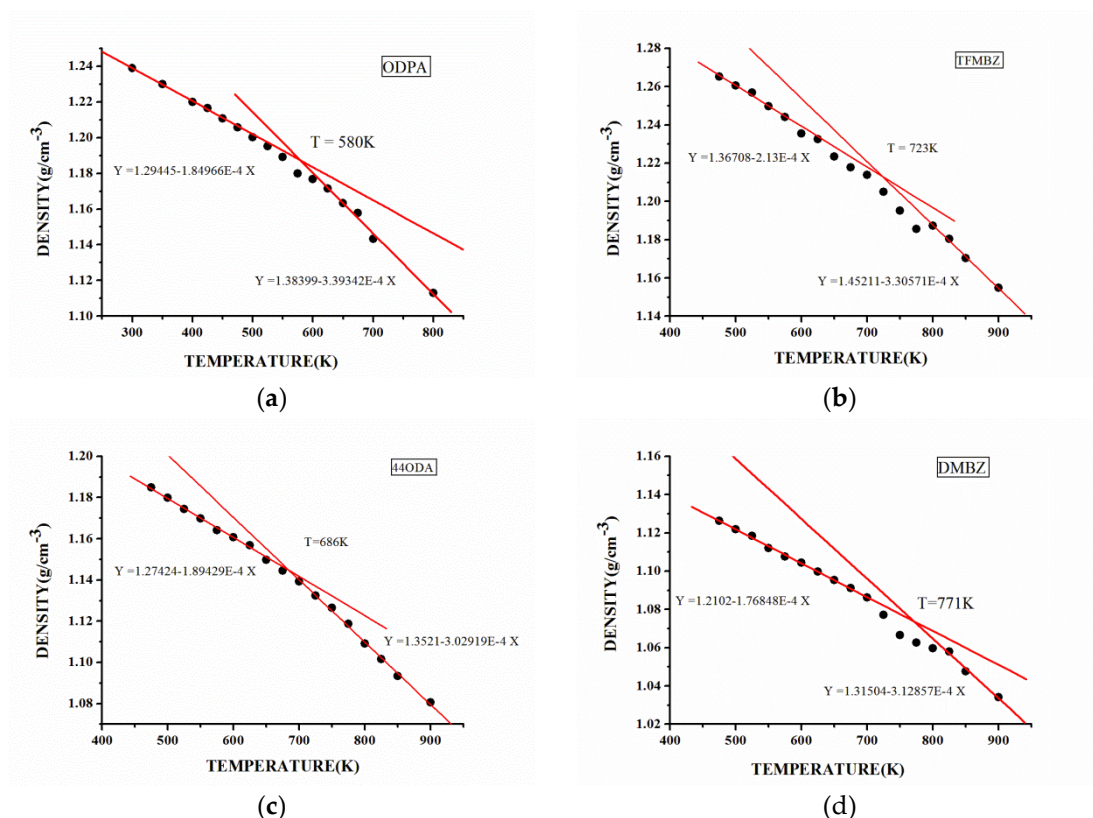
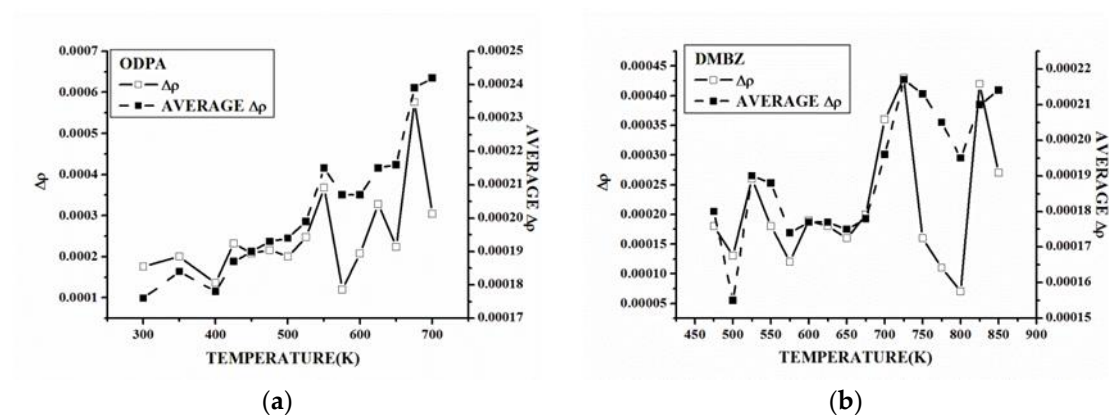
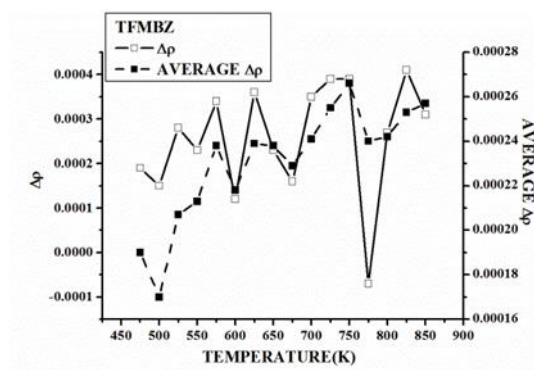
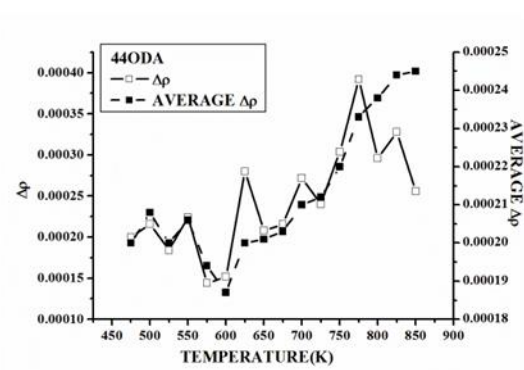


Figure S1. Linear fitting results of density variation with temperature of each simulated model. (a) ODPA-APB; (b) α -BPDA-TFMBZ; (c) α -BPDA-4,4-ODA; (d) α -BPDA-DMBZ.



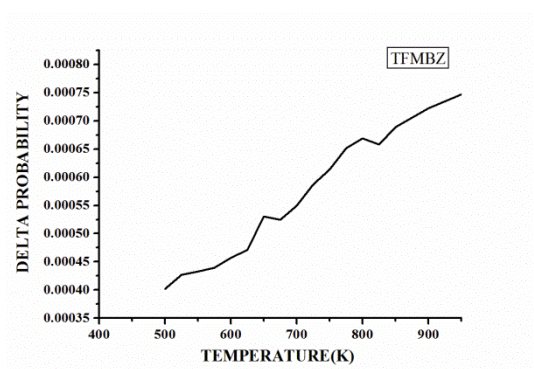


(c)

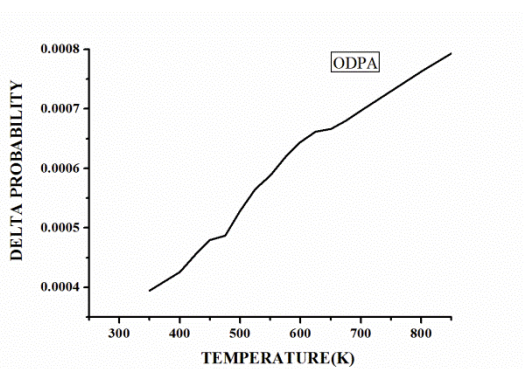


(d)

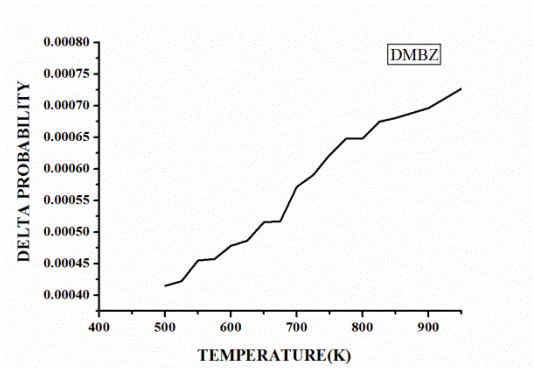
Figure S2. $\Delta\rho$ - T curves and $\Delta\rho$ mean value curves with temperature of each system: (a) ODP-APB; (b) α -BPDA-DMBZ; (c) α -BPDA-TFMBZ; (d) α -BPDA-4,4-ODA.



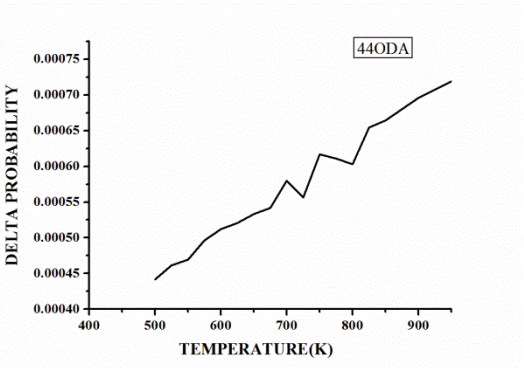
(a)



(b)



(c)



(d)

Figure S3. Temperature variation of dihedral angle distribution in main chain structure: (a) α -BPDA-TFMBZ; (b) ODP-APB; (c) α -BPDA-DMBZ; (d) α -BPDA-4,4-ODA.