Supporting Material

Prediction of the Glass Transition Temperature in Polyethylene Terephthalate/Polyethylene Vanillate (PET/PEV) Blends: A Molecular Dynamics Study

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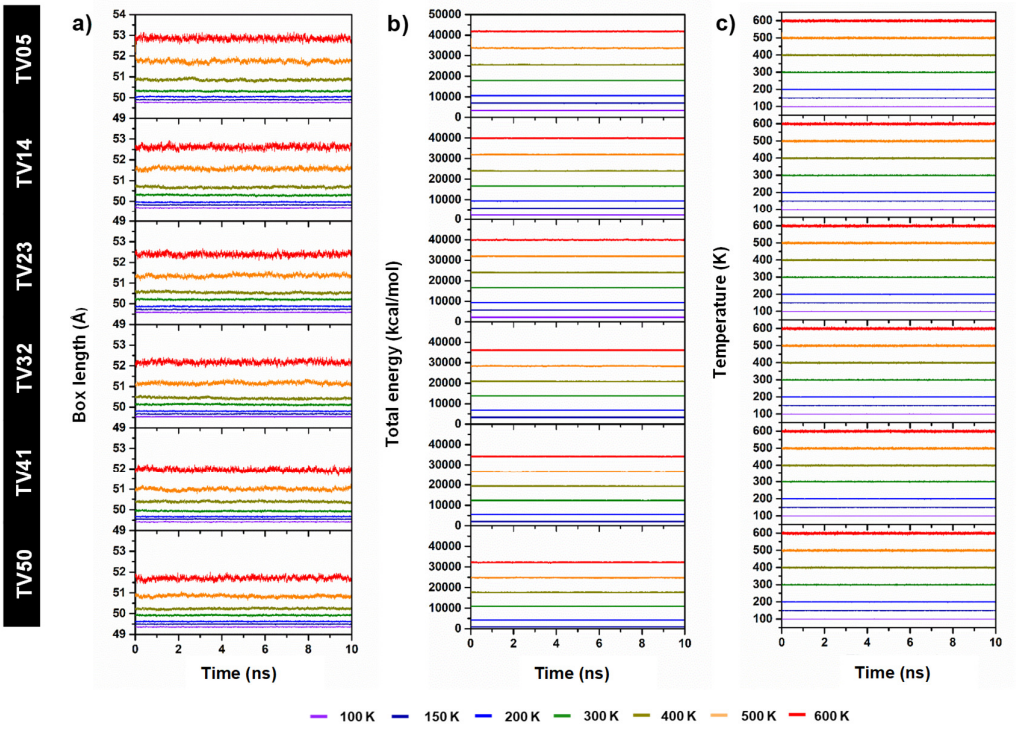


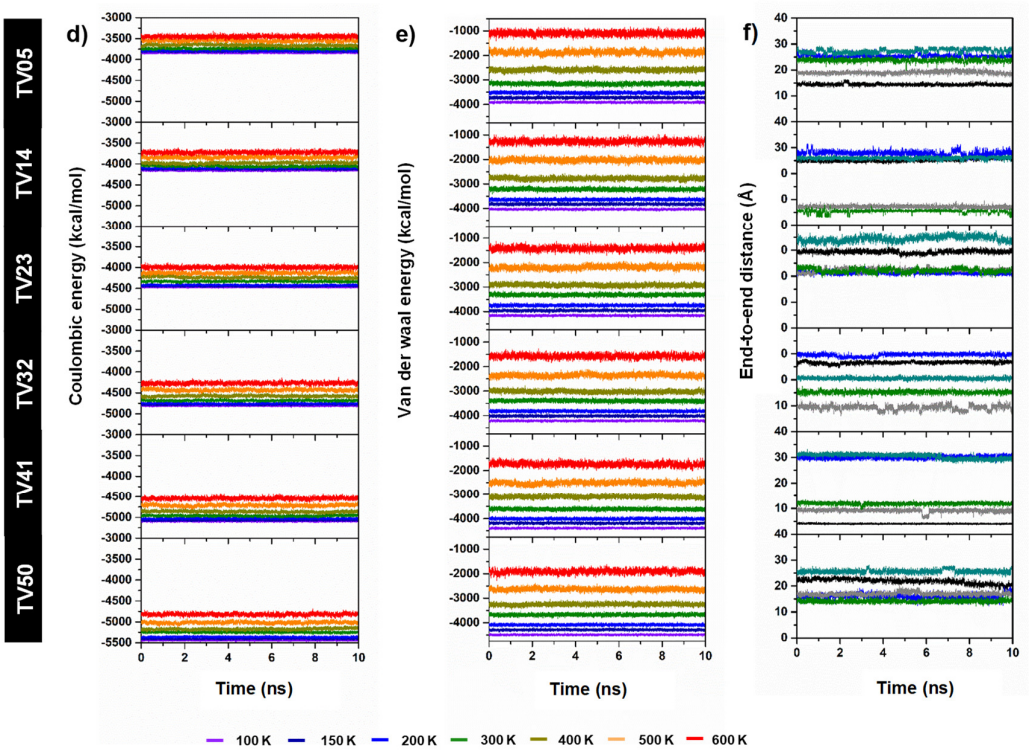
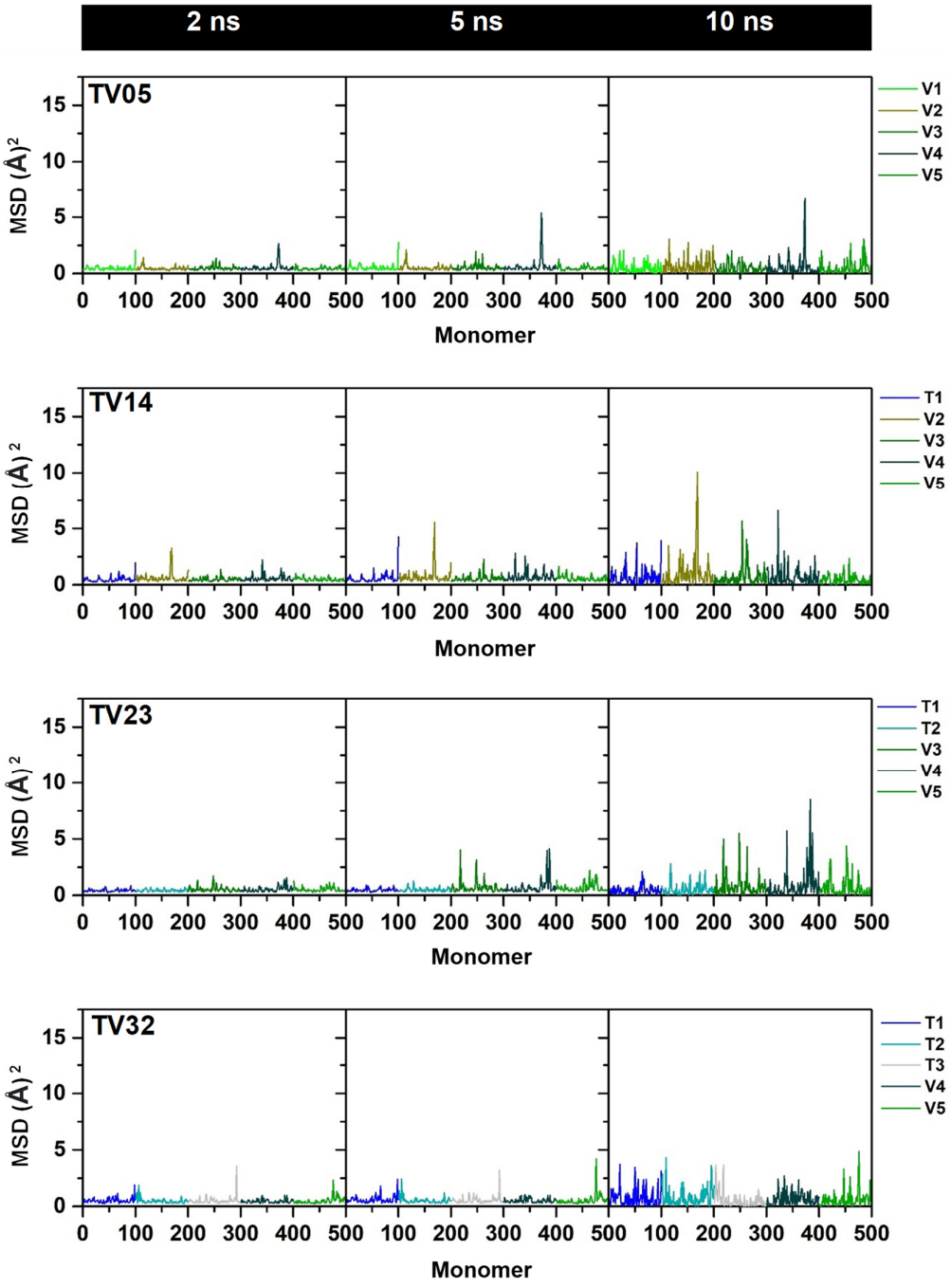


Figure S1. The investigation of system equilibrium (**a**) box length (Å) of production run from 1 to 10 ns, (**b**) temperature, (**c**) total energy profile (kcal/mol), (**d**) coulombic energy(kcal/mol), (**e**) van der Waal energy (kcal/mol) and (**f**) end-to-end distances (Å) for each chain.


2 ns
5 ns
10 ns
TV05
V1
V2
V3
V4
V5
MSD (Å)²
Monomer
TV14
T1
V2
V3
V4
V5
TV23
T1
T2
V3
V4
V5
TV32
T1
T2
T3
V4
V5
0
5
10
15
0 100 200 300 400 500 100 200 300 400 500 100 200 300 400 500

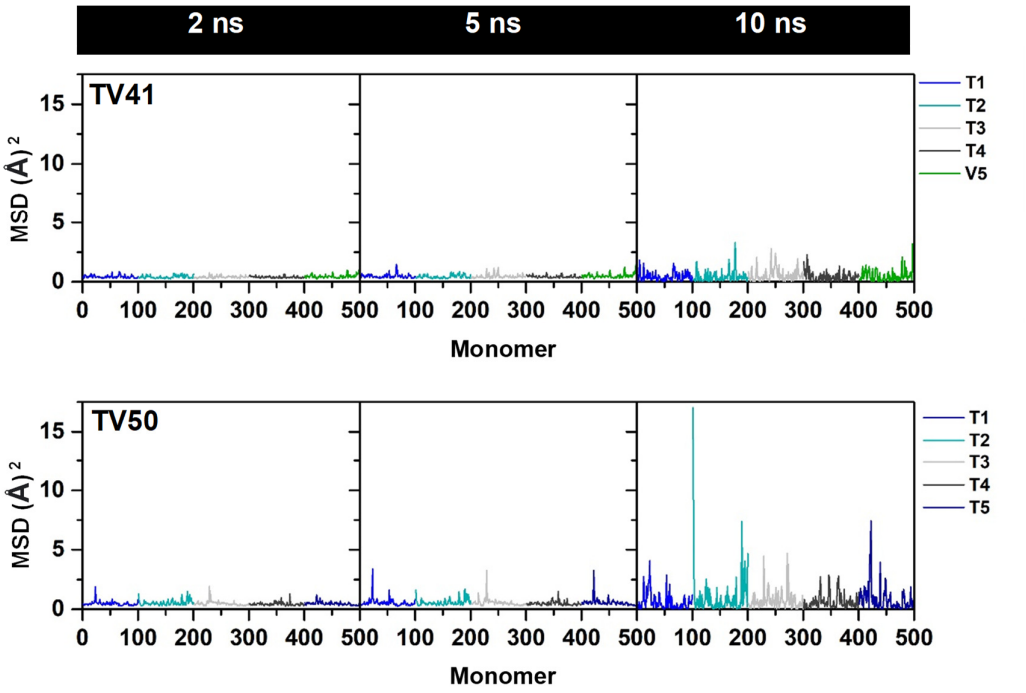


Figure S2. Mean square displacement (MSD) of PET/PEV blend at 2 ns, 5 ns, and 10 ns of last 10-ns production run. T represented PET chain and V represented PEV chain.

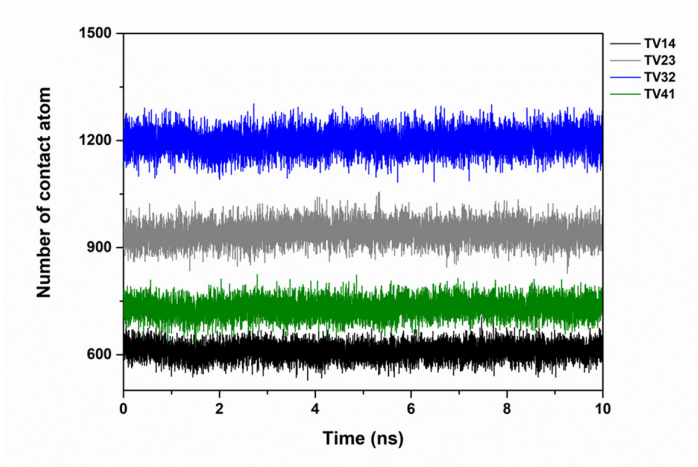


Figure S3. The number of contact atom at 6 Å, which represent hydrophobic interaction.

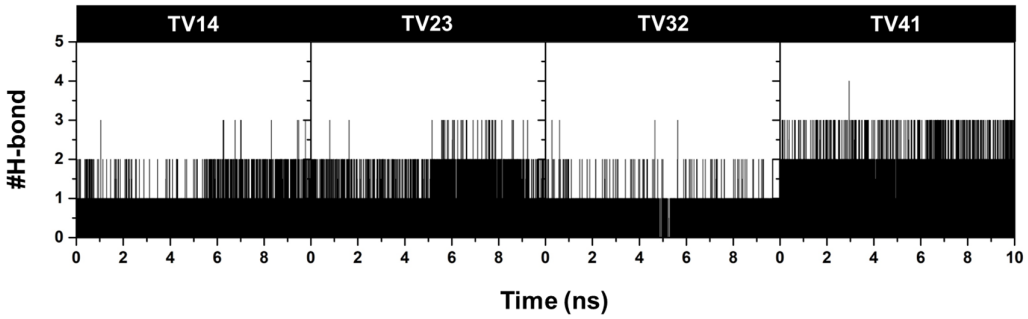


Figure S4. The number of hydrogen bonds formed between PET and PEV chains per time using a cut-off of 3.0 Å for CH…O and an angle of 180±20 degrees for CH-H…O.