Integrated Exploration of Experimentation and Molecular Simulation in Ester-containing Polyimide Dielectrics

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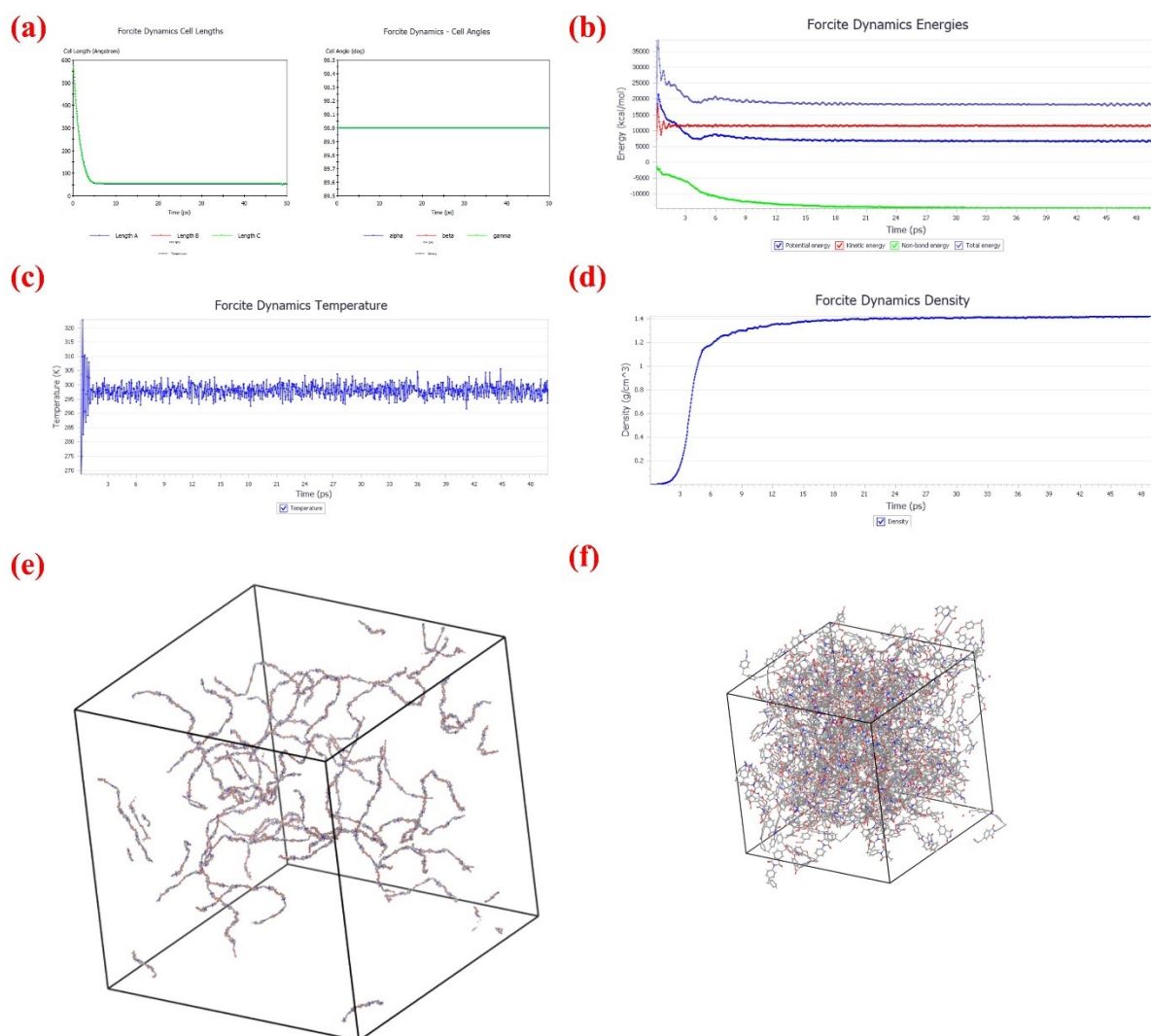
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Snapshots of molecular simulation process of EPI-1 (Figure S1 ~ Figure S4)
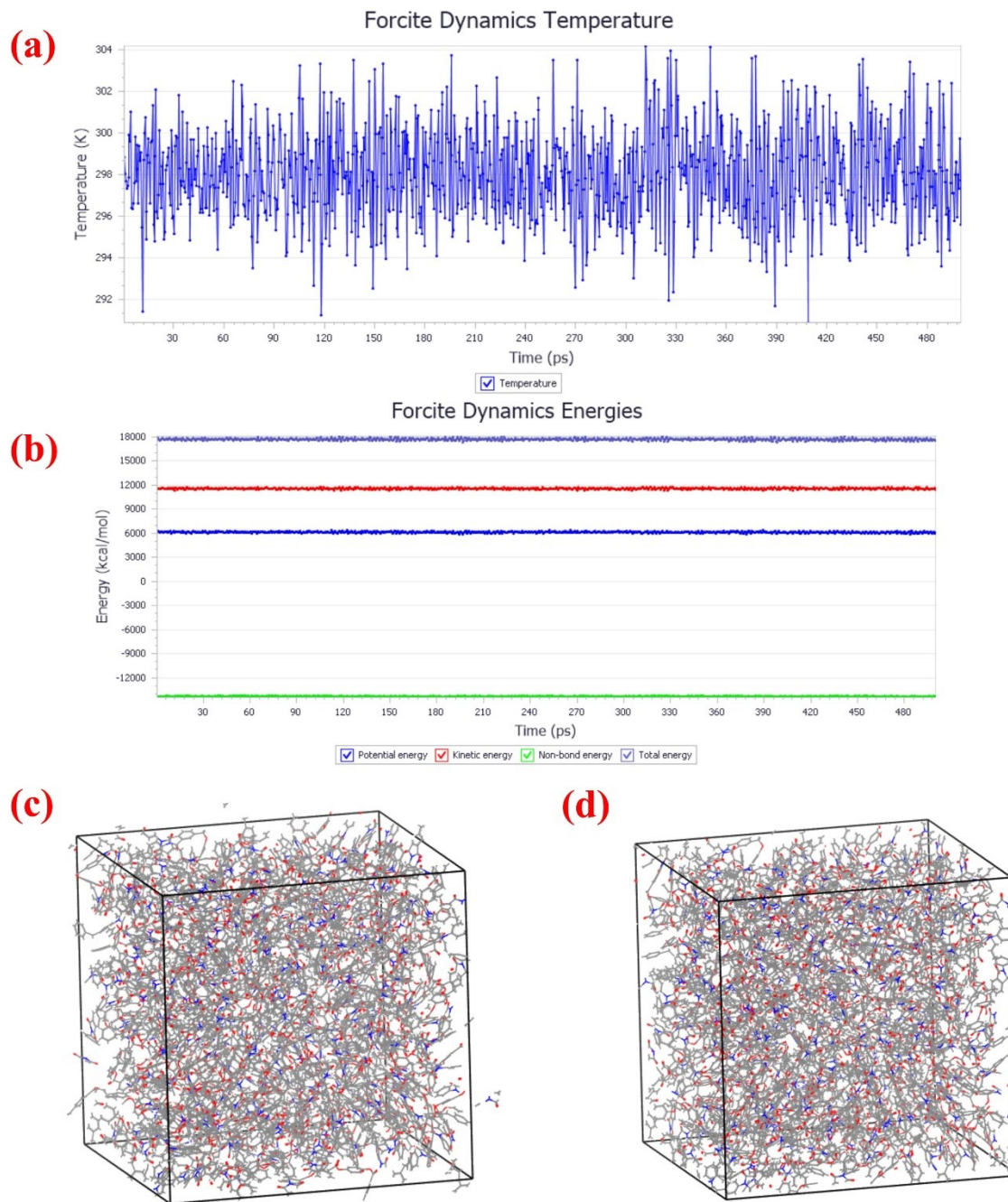

Figure S1 The compress process (NPT: 0.5 GPa, 50 ps) of EPI-1: (a) The cell lengths and angles (b) the dynamics energies (c) the dynamics temperature and (d) the dynamics density as functions of time, respectively; (e) The initial frame (the size of cube: a=b=c=274.158 Å); (f) The end frame (the size of cube: a=b=c=52.8615 Å with a properly amplification).
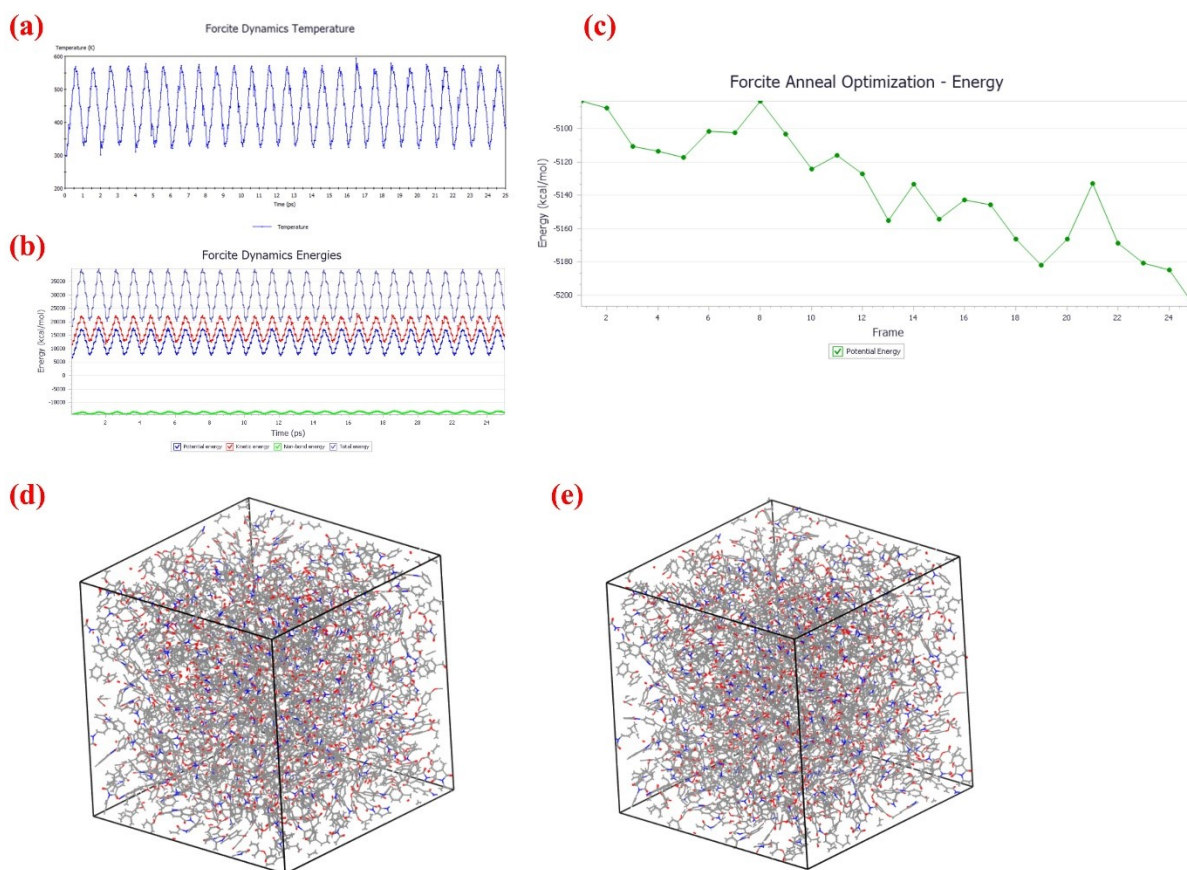
Figure S2 The annealing process (NVT: 298 - 598 K, repeat 25 times) of EPI-1: (a) The dynamics temperature and (b) the dynamics density as functions of time, respectively; (c) The energies of 25 optimizations after the annealing process; (d) The initial frame (the size of cube: a=b=c=52.8615 Å); (e) The frame with the lowest energy (the size of cube: a=b=c=52.8615 Å).
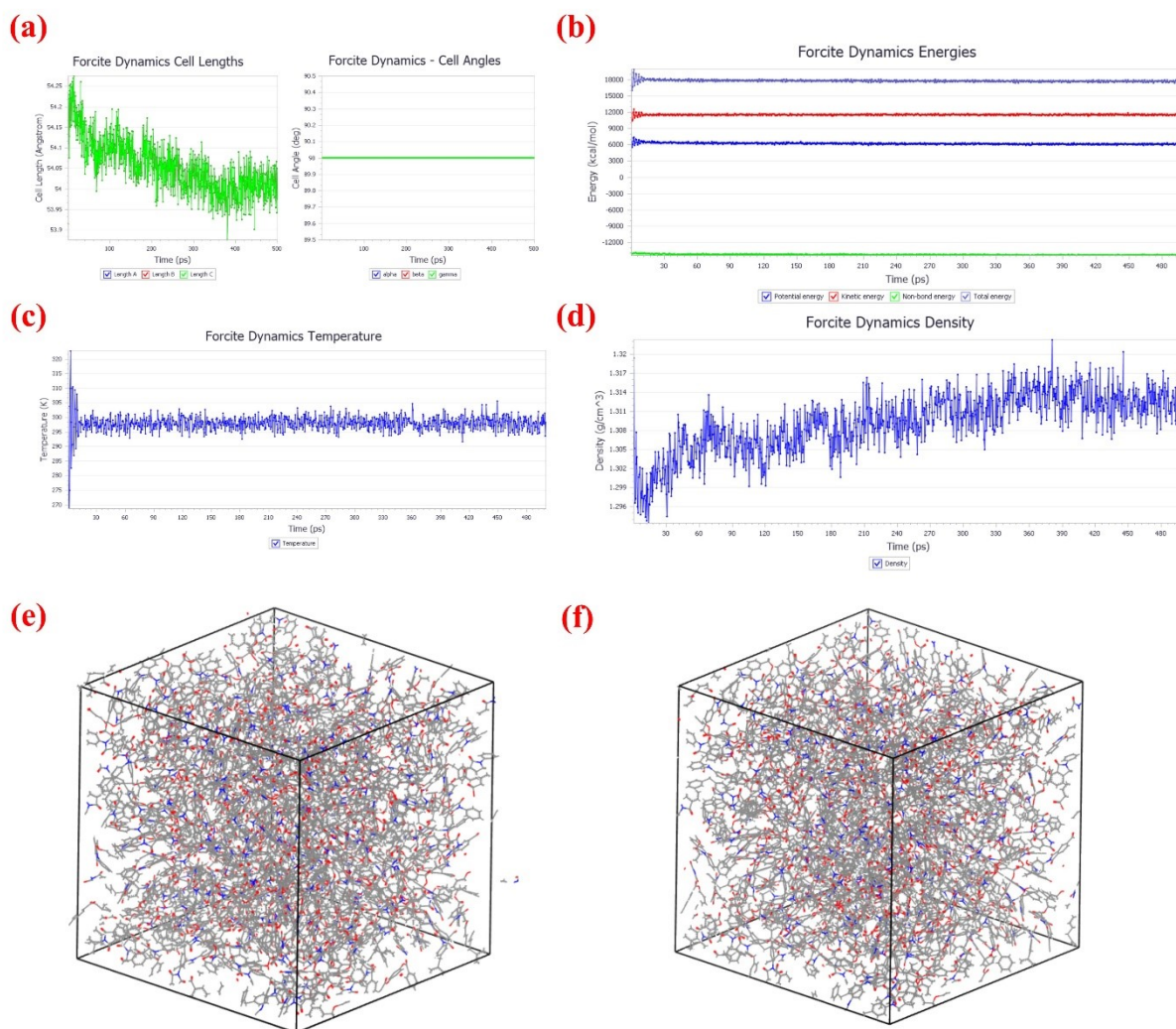
Figure S3 The release process (NPT: 10^{-4} GPa, 500 ps) of EPI-1: (a) The cell lengths and angles (b) the dynamics energies (c) the dynamics temperature changing with time and (d) the dynamics density as functions of time, respectively; (e) The initial frame (the size of cube: a=b=c=52.8615 Å); (f) The end frame (the size of cube: a=b=c=54.3257 Å).
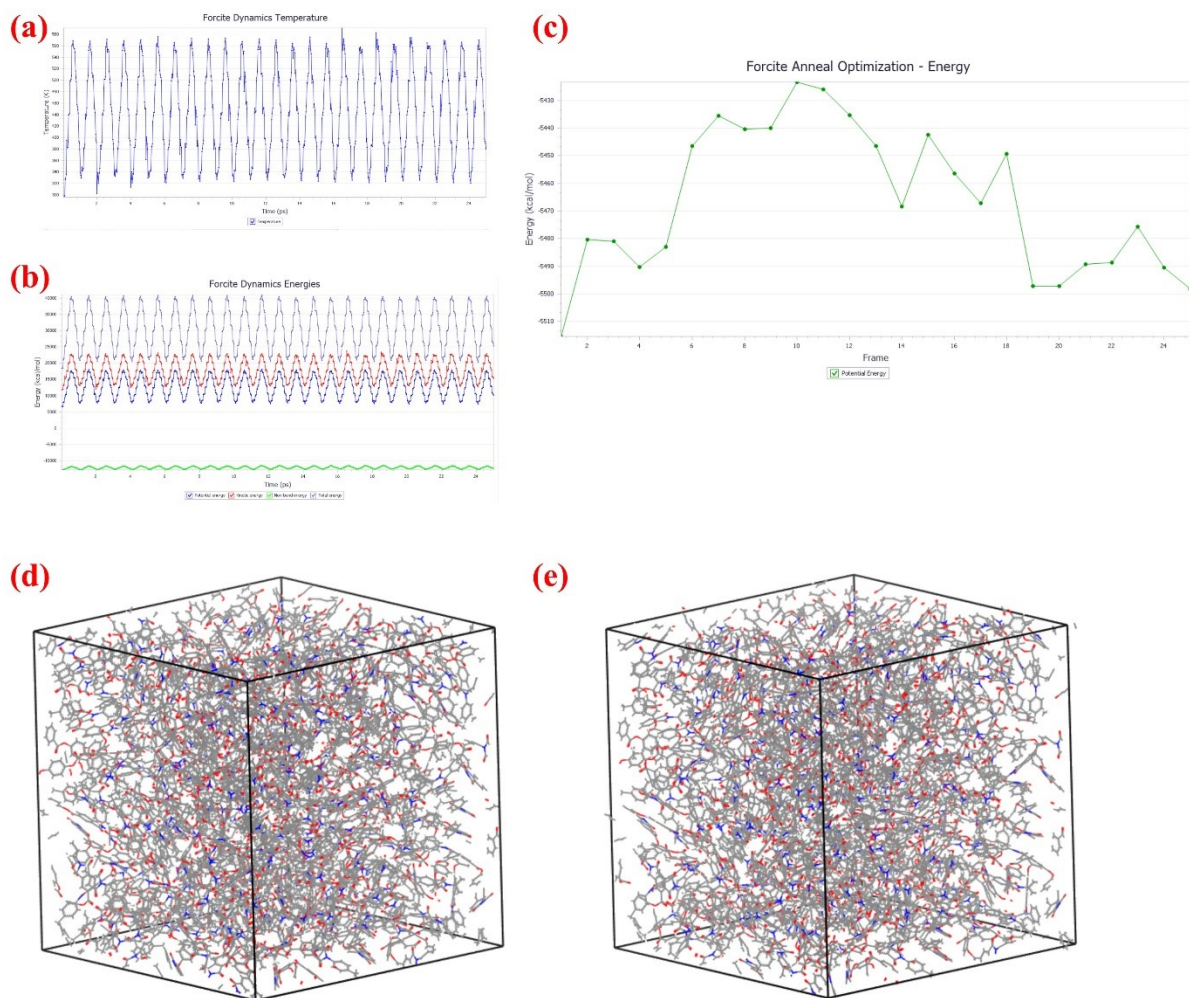
Figure S4 The equilibrium process (NVT, 500 ps) of EPI-1: (a) The dynamics temperature and (b) the dynamics energies as functions of time, respectively; (c) The initial frame (the size of cube: a=b=c=52.8615 Å); (d) The end frame (the size of cube: a=b=c=52.8615 Å).
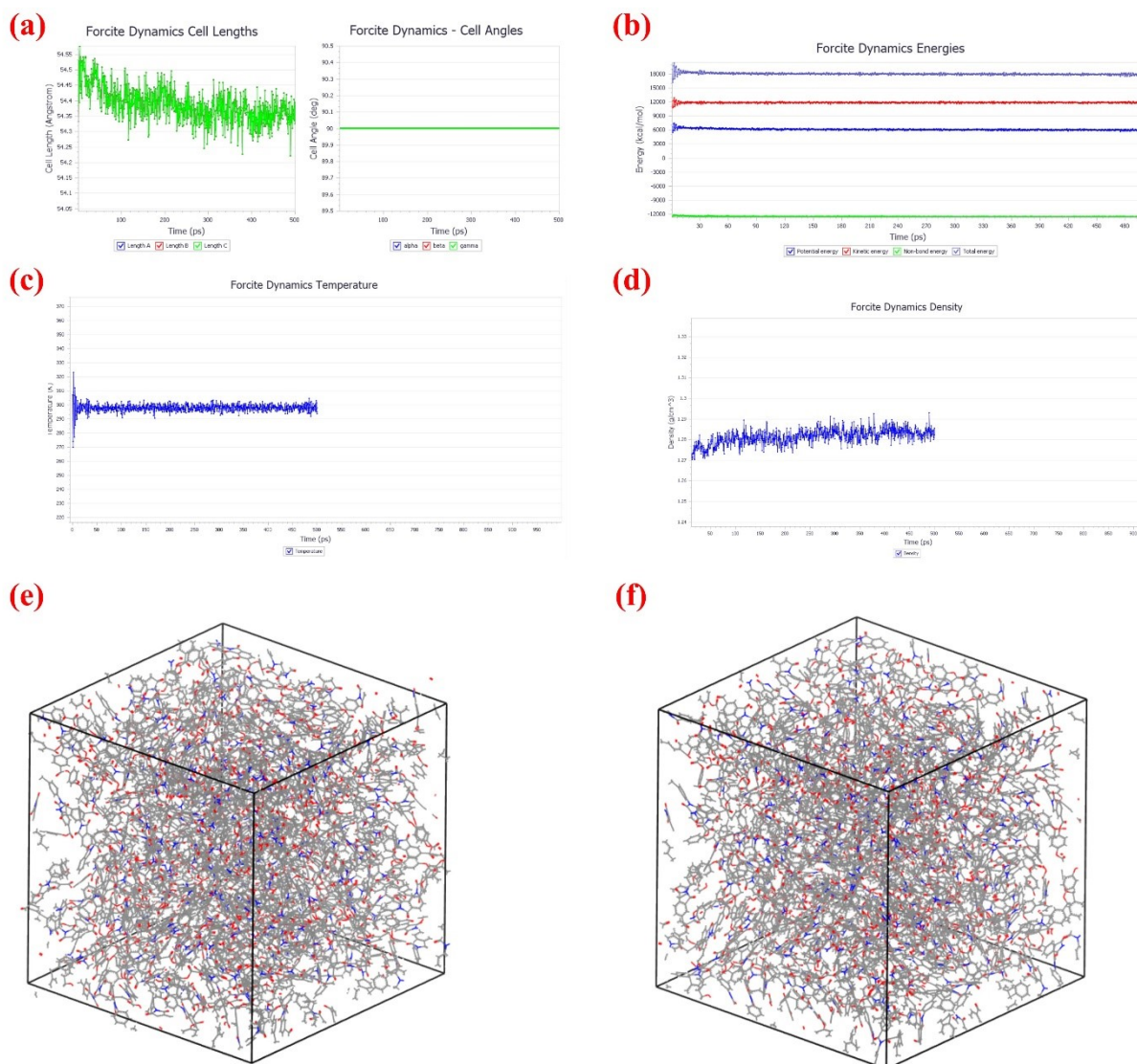
Snapshots of molecular simulation process of EPI-2 (Figure S5 ~ Figure S8)
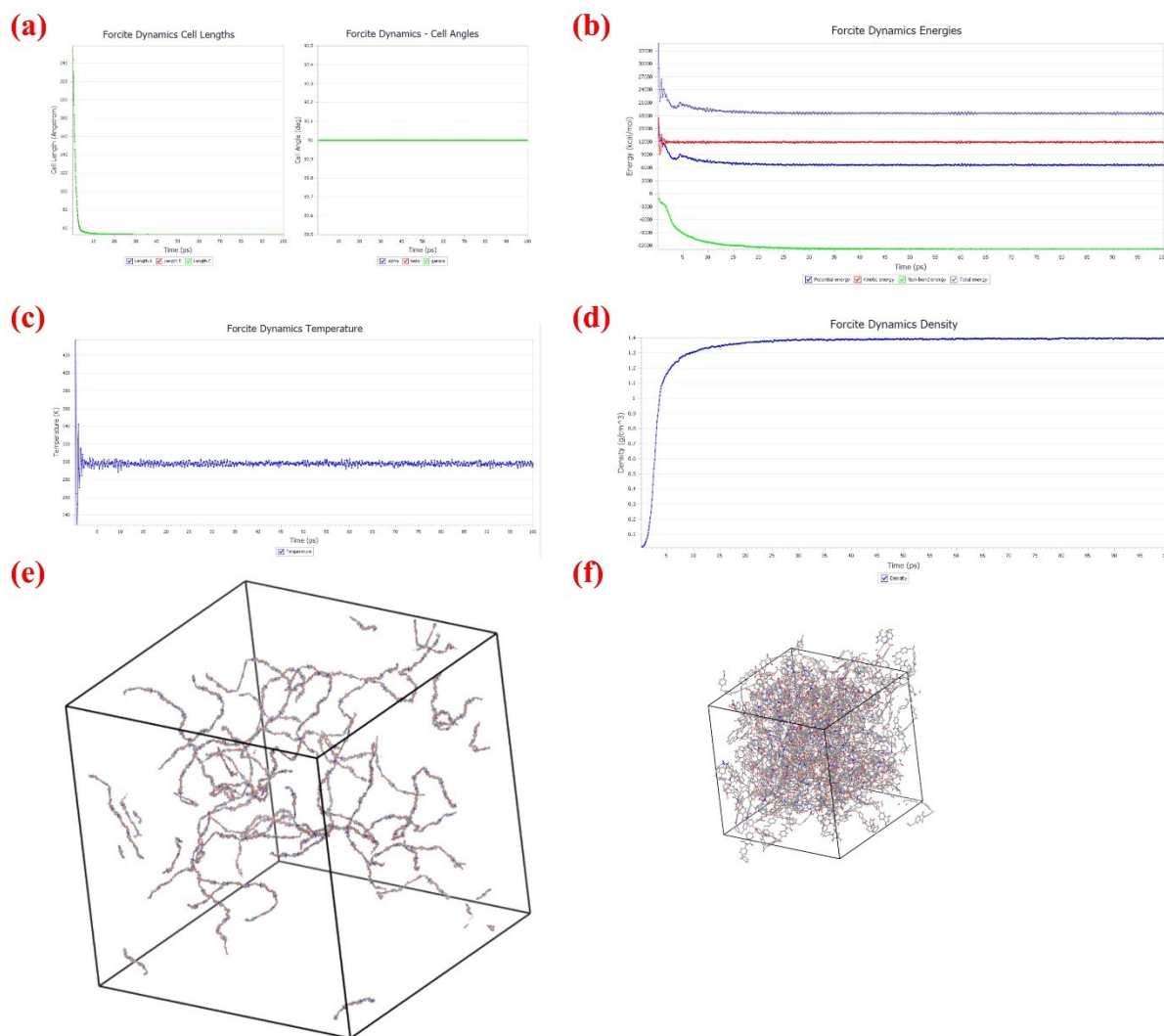
Figure S5 The compress process (NPT: 0.5 GPa, 50 ps) of EPI-2: (a) The cell lengths (b) the dynamics energies (c) the dynamics temperature and (d) the dynamics density as functions of time, respectively; (e) The initial frame (the size of cube: a=b=c=274.158 Å); (f) The end frame (the size of cube: a=b=c=52.6450 Å, with a properly amplification).
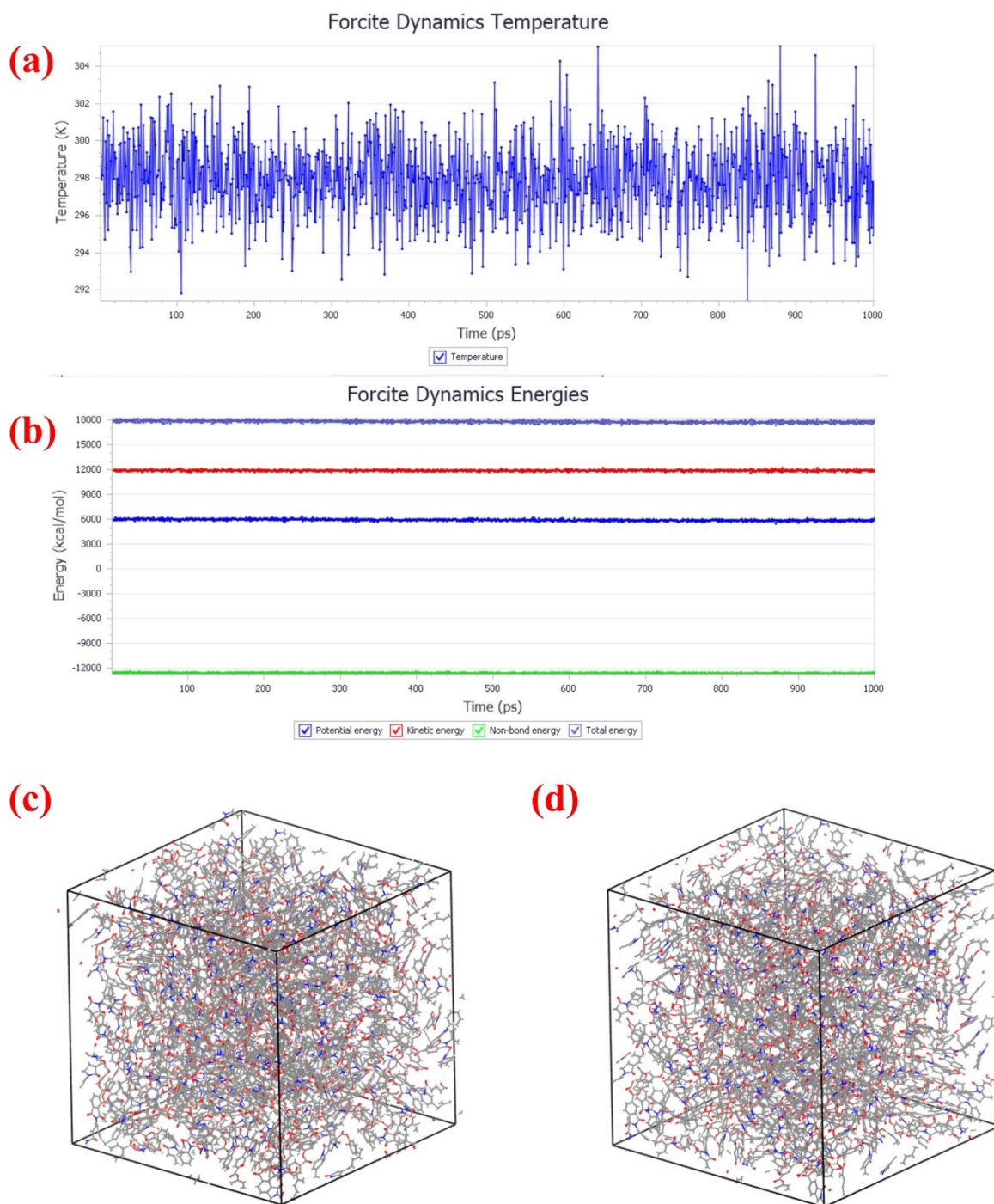
Figure S6 The annealing process (NVT: 298 - 598 K, repeat 25 times) of EPI-2: (a) The dynamics temperature and (b) the dynamics density as functions of time, respectively; (c) The energies of 25 optimizations after annealing process; (d) The initial frame (the size of cube: a=b=c=52.6450 Å); (e) The frame with the lowest energy (the size of cube: a=b=c=52.6450 Å).
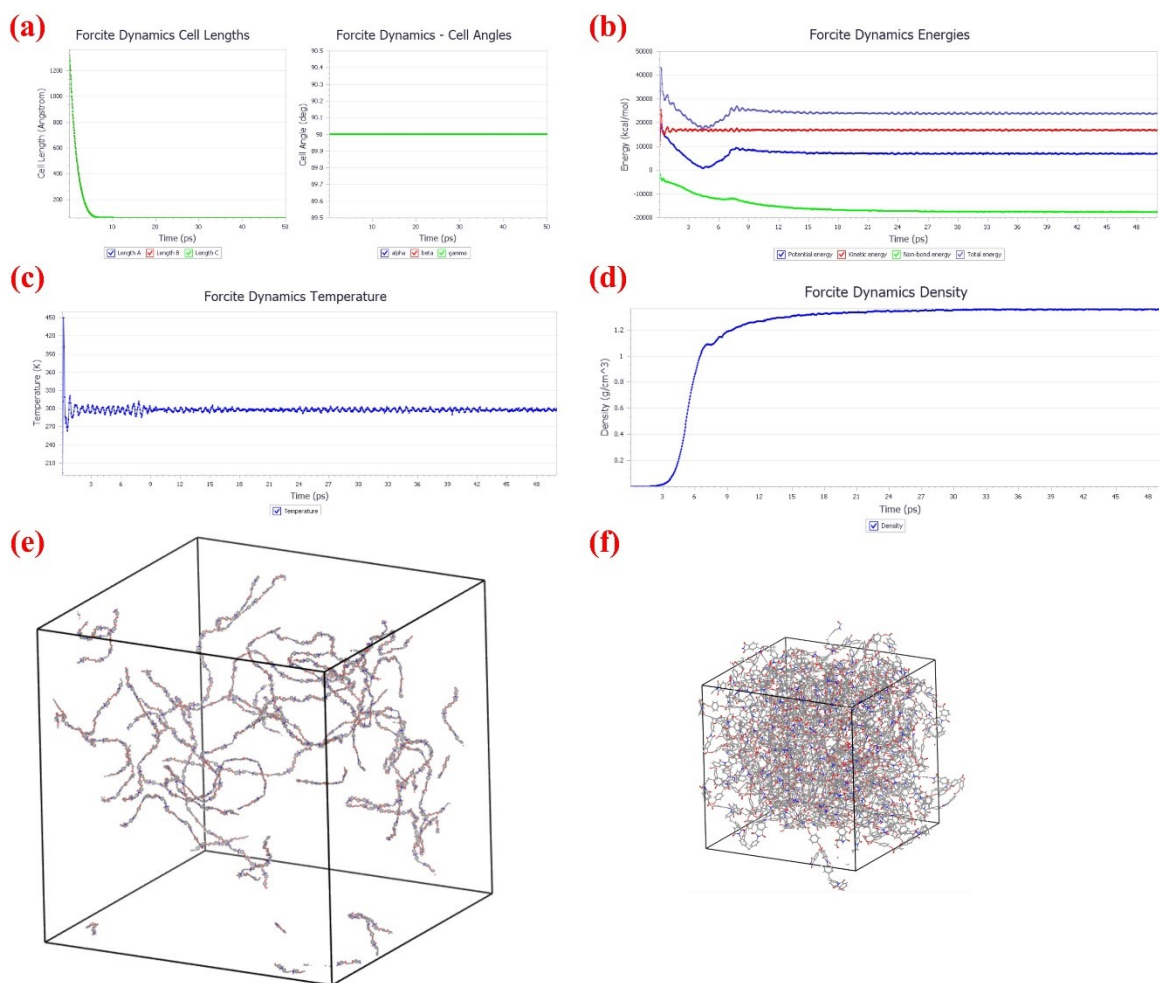
Figure S7 The release process (NPT: 10^{-4} GPa, 500 ps) of EPI-2: (a) The cell lengths and angles (b) the dynamics energies (c) the dynamics temperature and (d) the dynamics density as functions of time, respectively; (e) The initial frame (the size of cube: a=b=c=52.6450 Å); (f) The end frame (the size of cube: a=b=c=53.0987 Å).
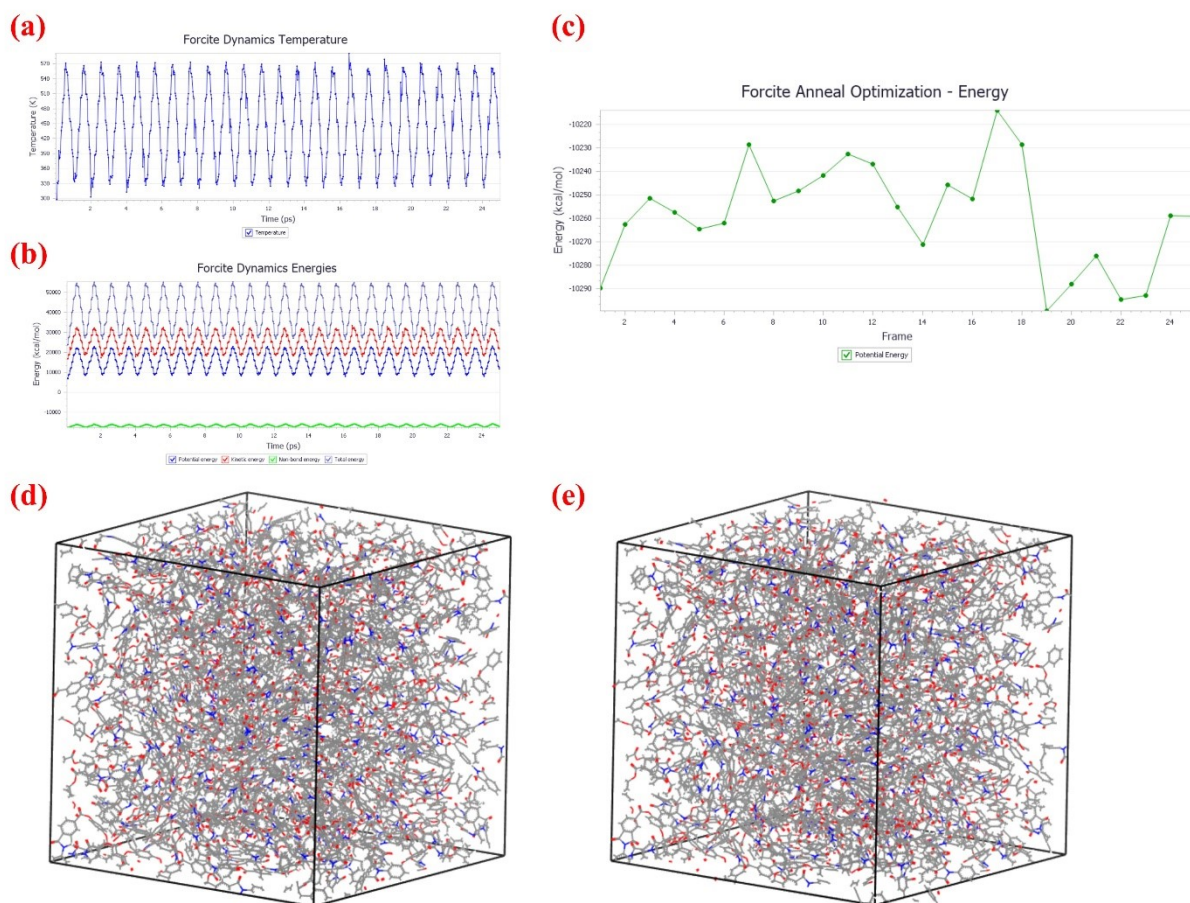
Figure S8 The equilibrium process (NVT, 1000 ps) of EPI-2: (a) The dynamics temperature and (b) the dynamics energies as functions of time, respectively; (c) The initial frame (the size of cube: a=b=c=53.0987 Å); (d) The end frame (the size of cube: a=b=c=53.0987 Å).
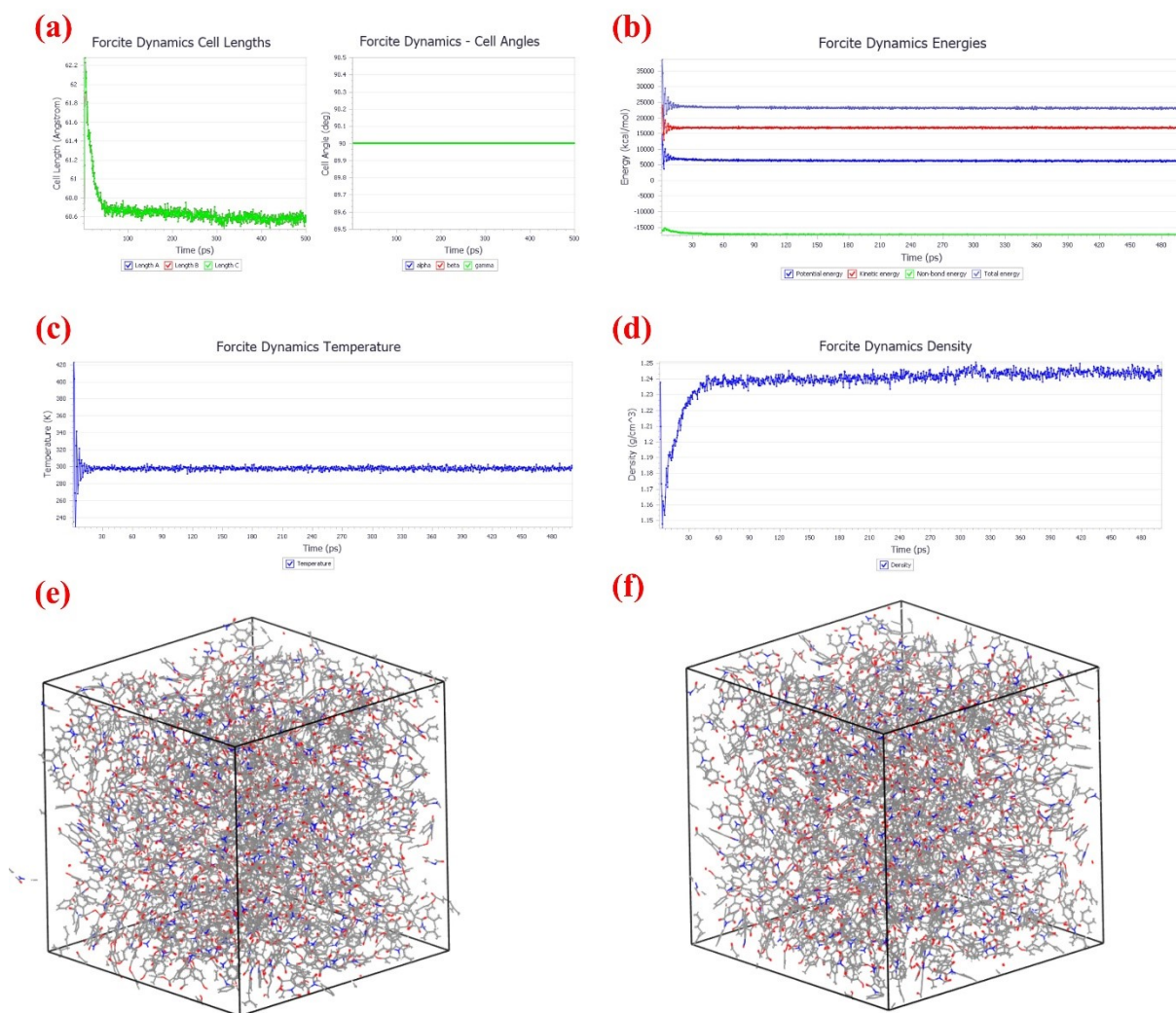
Snapshots of molecular simulation process of EPI-3 (Figure S9 ~ Figure S12)
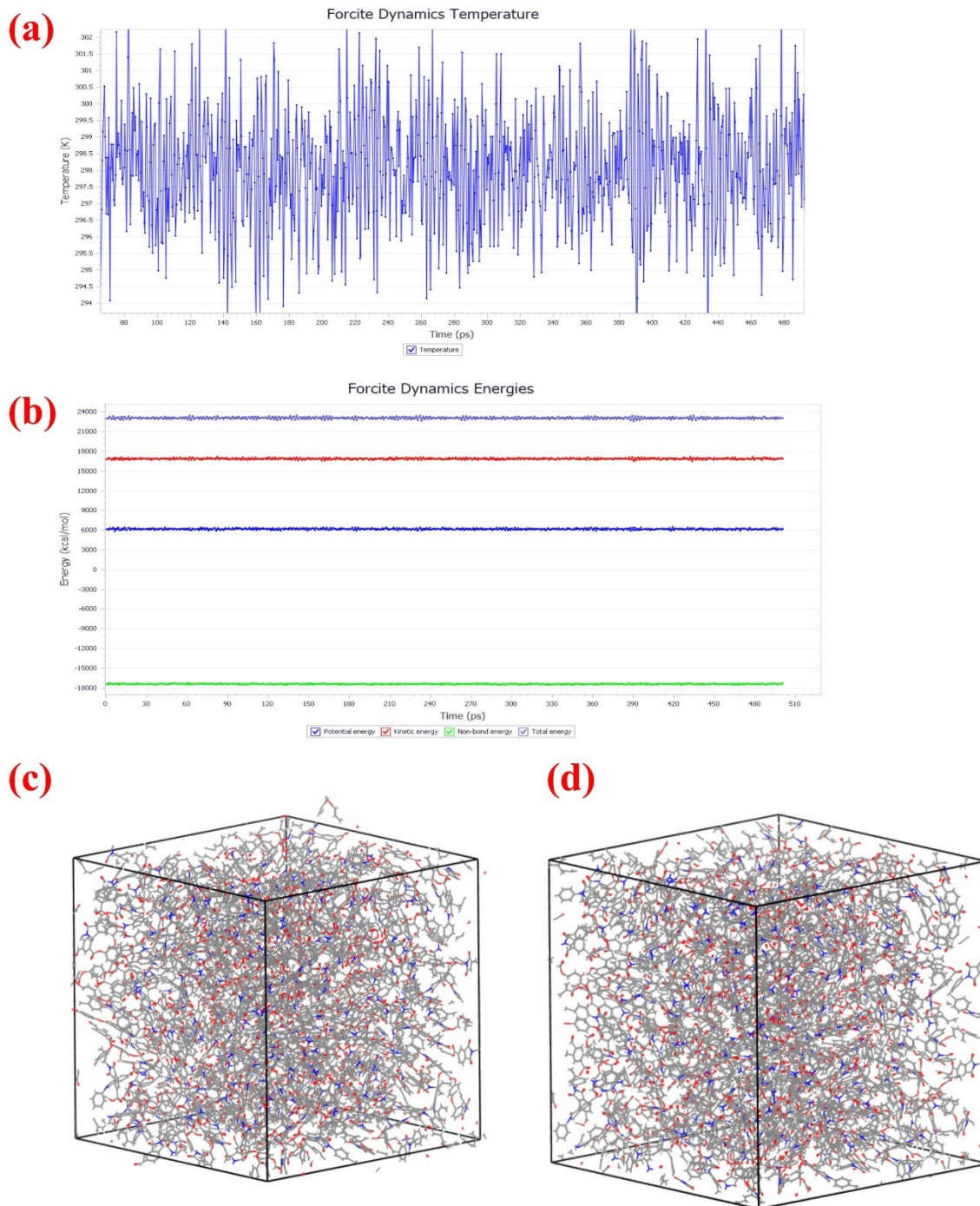

Figure S9 The compress process (NPT: 0.5 GPa, 50 ps) of EPI-3: (a) The cell lengths and angles (b) the dynamics energies (c) the dynamics temperature and (d) the dynamics density as functions of time, respectively; (e) The initial frame (the size of cube: a=b=c=274.158 Å); (f) The end frame (the size of cube: a=b=c=58.8030 Å, with a properly amplification).

Figure S10 The annealing process (NVT: 298 - 598 K, repeat 25 times) of EPI-3: (a) The dynamics temperature and (b) the dynamics density as functions of time, respectively; (c) The energies of 25 optimizations after annealing process; (d) The initial frame (the size of cube: a=b=c=58.8030 Å); (e) The frame with the lowest energy (the size of cube: a=b=c=58.8030 Å).
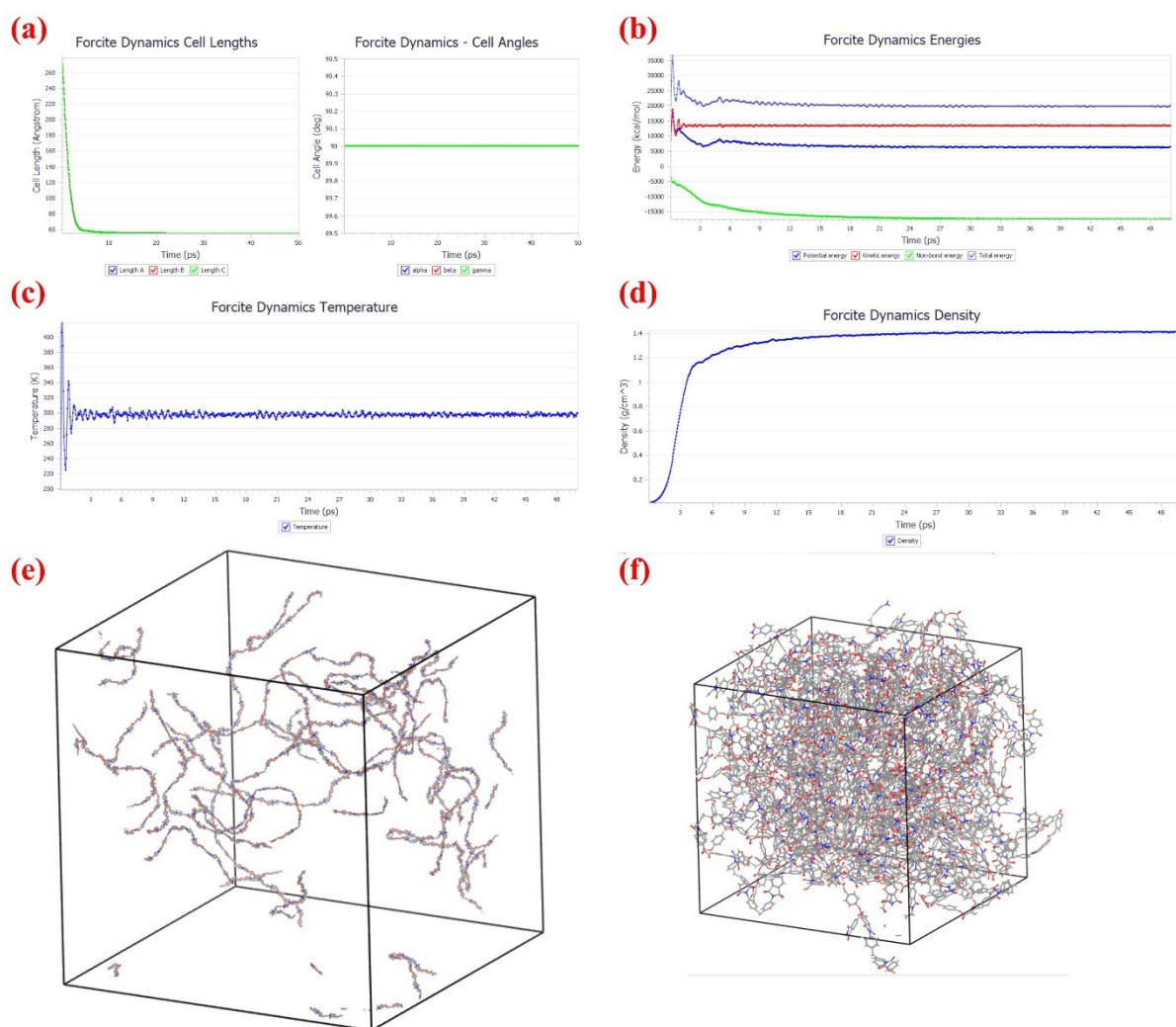
Figure S11 The release process (NPT: 10^{-4} GPa, 500 ps) of EPI-3: (a) The cell lengths and angles (b) the dynamics energies (c) the dynamics temperature and (d) the dynamics density as functions of time, respectively; (e) The initial frame (the size of cube: a=b=c=58.8030 Å); (f) The end frame (the size of cube: a=b=c=60.5495 Å).
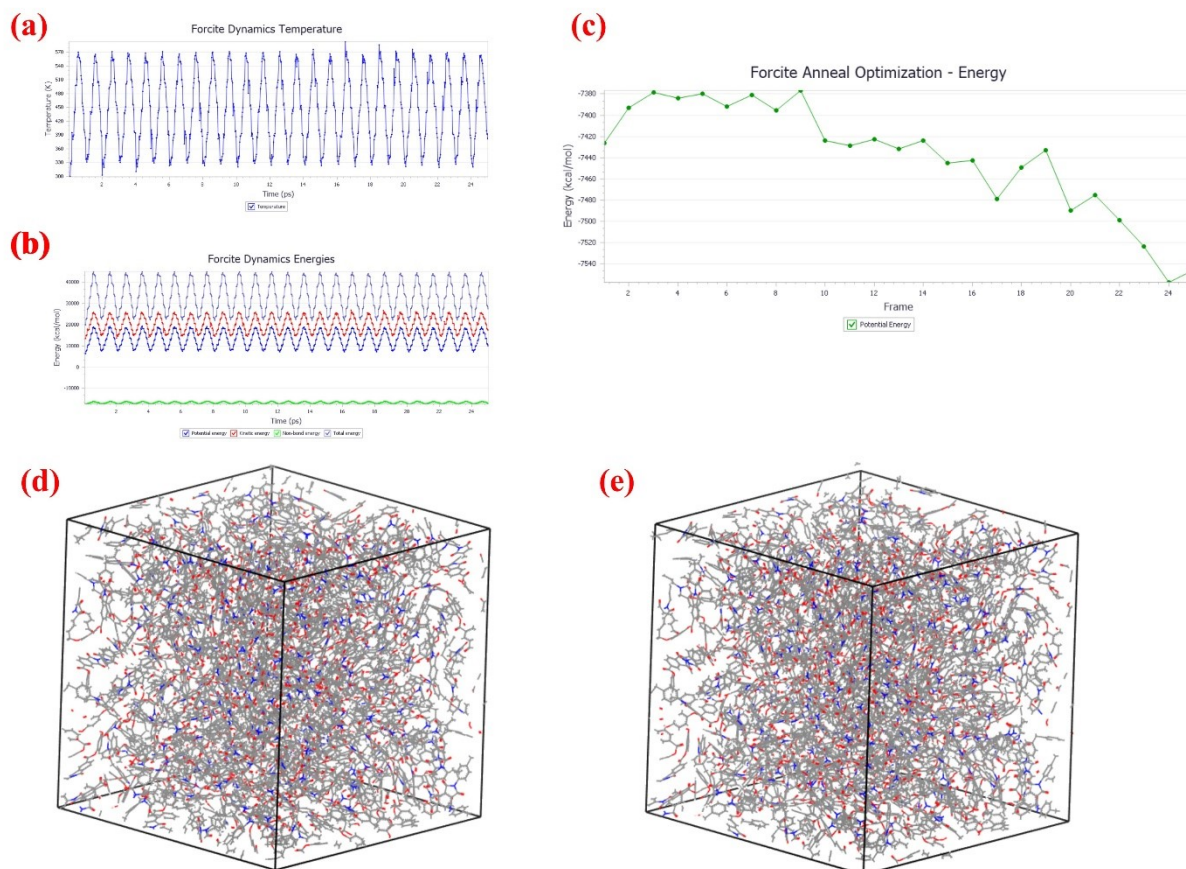
Figure S12 The equilibrium process (NVT, 500 ps) of EPI-3: (a) The dynamics temperature and (b) the dynamics energies as functions of time, respectively; (c) The initial frame (the size of cube: a=b=c=60.5495 Å); (d) The end frame (the size of cube: a=b=c=60.5495 Å).
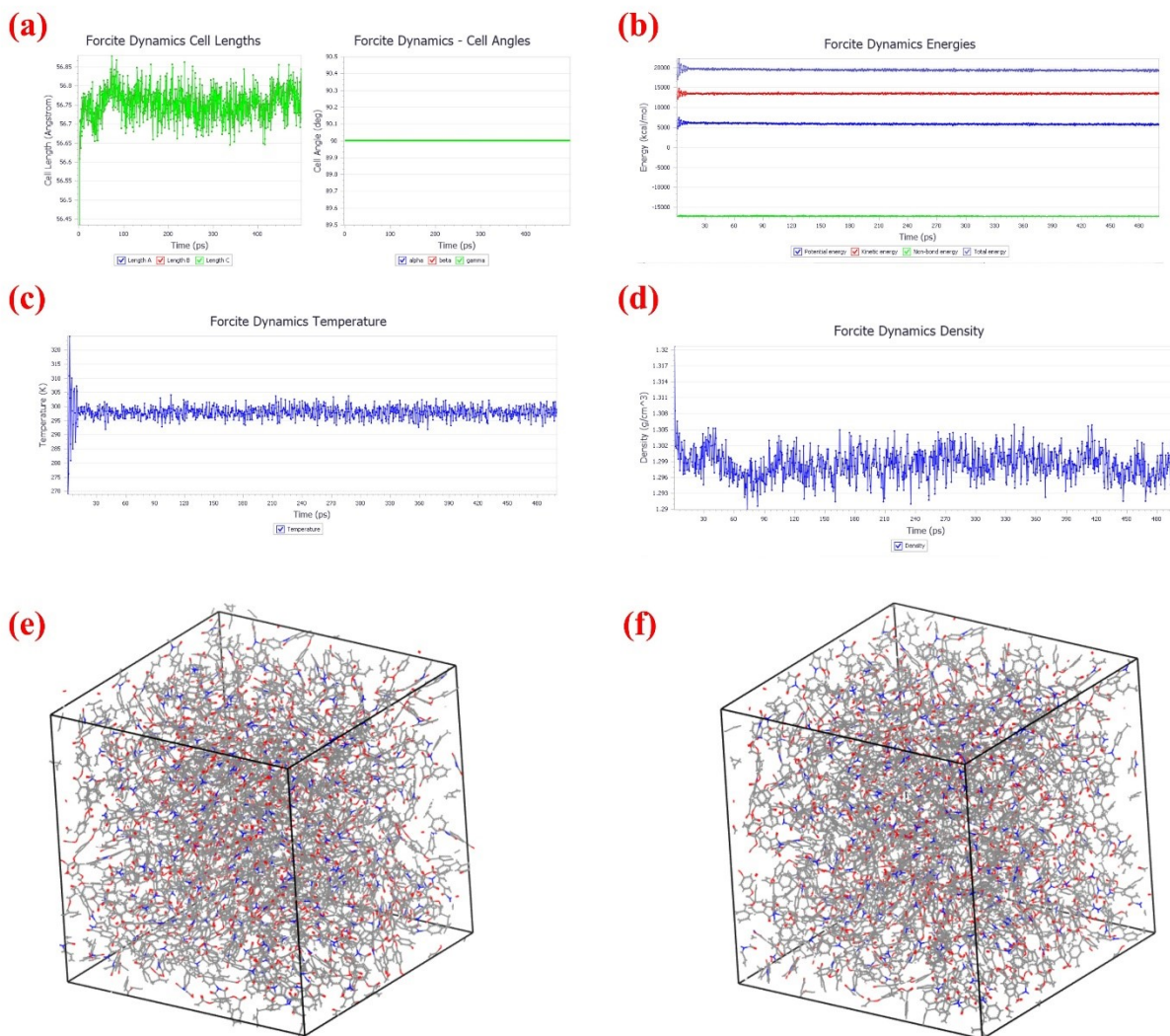
Snapshots of molecular simulation process of EPI-4 (Figure S13 ~ Figure S16)

Figure S13 The compress process (NPT: 0.5 GPa, 50 ps) of EPI-4: (a) The cell lengths and angles (b) the dynamics energies (c) the dynamics temperature and (d) the dynamics density as functions of time, respectively; (e) The initial frame (the size of cube: a=b=c=274.158 Å); (f) The end frame (the size of cube: a=b=c=55.2112 Å, with a properly amplification).
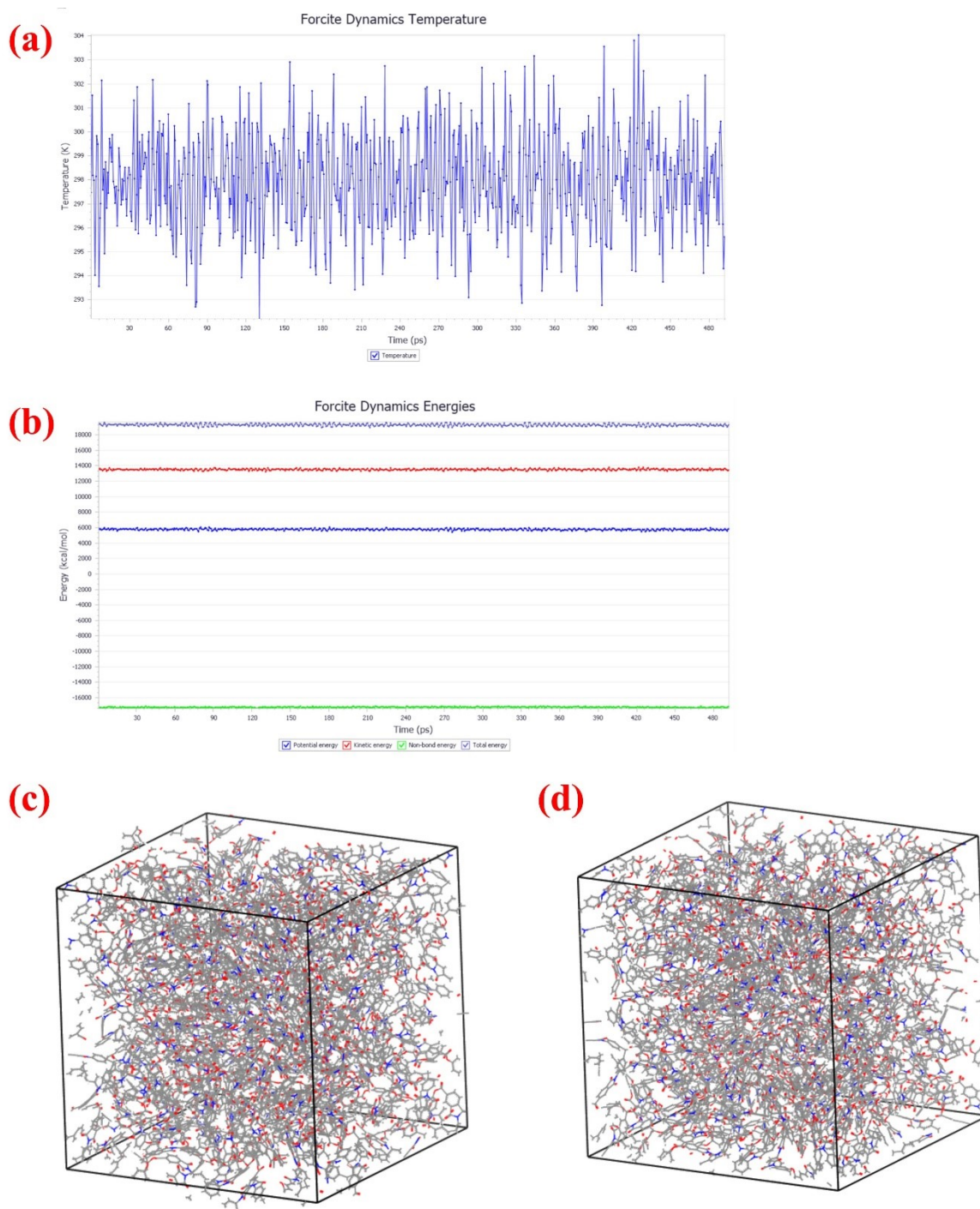
Figure S14 The annealing process (NVT: 298 - 598 K, repeat 25 times) of EPI-4: (a) The dynamics temperature and (b) the dynamics density as functions of time, respectively; (c) The energies of 25 optimizations after annealing process; (d) The initial frame (the size of cube: a=b=c=55.2112 Å); (e) The frame with the lowest energy (the size of cube: a=b=c=55.2112 Å).
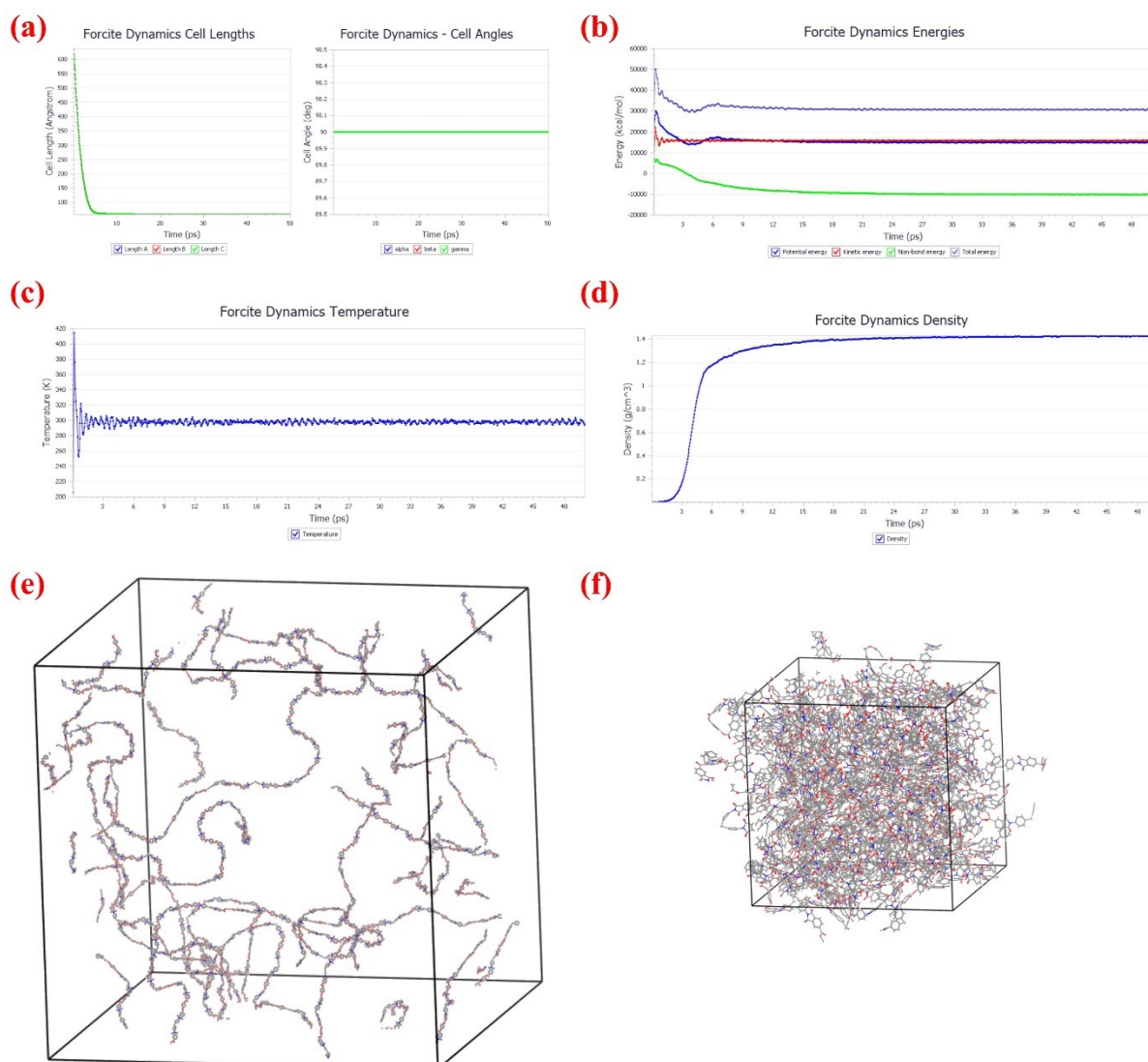
Figure S15 The release process (NPT: 10^{-4} GPa, 500 ps) of EPI-4: (a) The cell lengths and angles (b) the dynamics energies (c) the dynamics temperature and (d) the dynamics density as functions of time, respectively; (e) The initial frame (the size of cube: a=b=c=55.2112 Å); (f) The end frame (the size of cube: a=b=c=56.7748 Å).
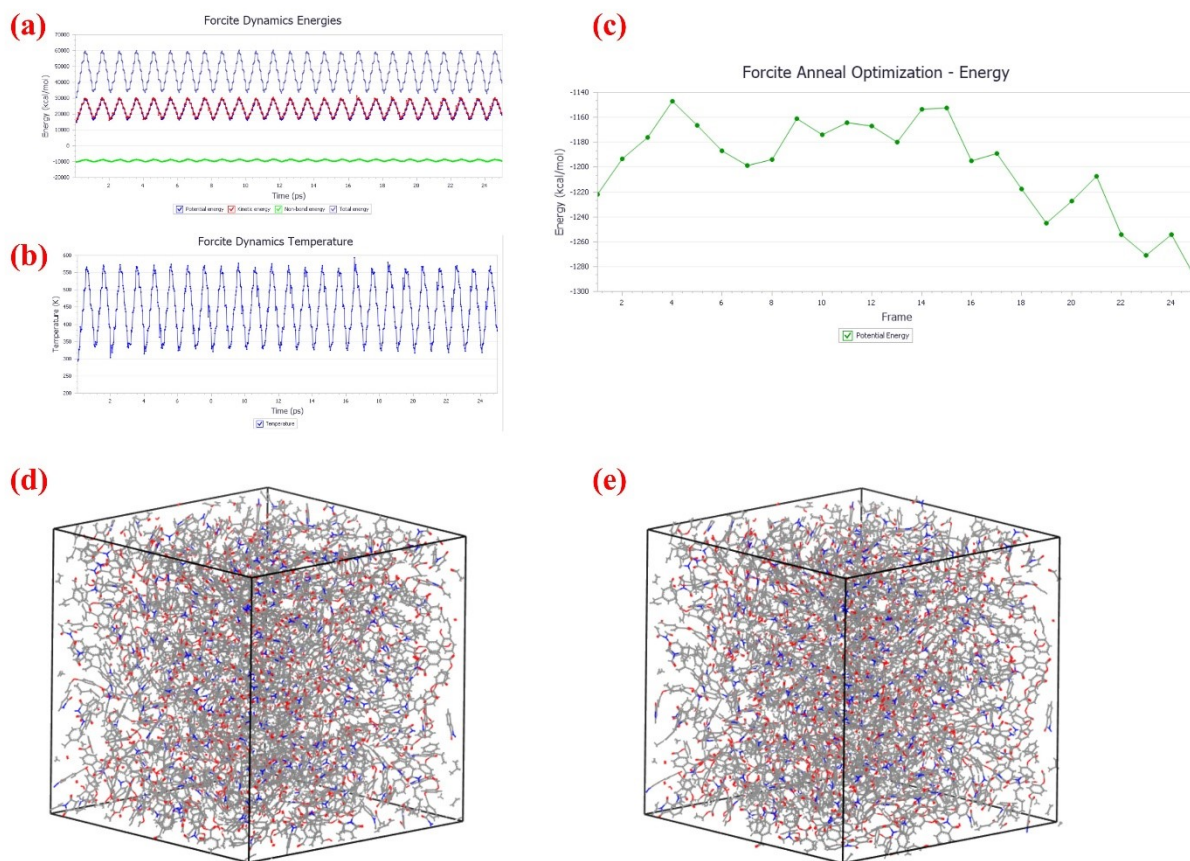
Figure S16 The equilibrium process of EPI-4: (a) The dynamics temperature and (b) the dynamics energies as functions of time, respectively; (c) The initial frame (the size of cube: a=b=c=56.7748 Å); (d) The end frame (the size of cube: a=b=c=56.7748 Å).

Snapshots of molecular simulation process of EPI-5 (Figure S17 ~ Figure S20)


Figure S17 The compress process (NPT: 0.5 GPa, 50 ps) of EPI-5: (a) The cell lengths and angles (b) the dynamics energies (c) the dynamics temperature and (d) the dynamics density as functions of time, respectively; (e) The initial frame (the size of cube: a=b=c=274.158 Å); (f) The end frame (the size of cube: a=b=c=58.3726 Å, with a properly amplification).

Figure S18 The annealing process (NVT: 298 - 598 K, repeat 25 times) of EPI-5: (a) The dynamics temperature and (b) the dynamics density as functions of time, respectively; (c) The energies of 25 optimizations after annealing process; (d) The initial frame (the size of cube: a=b=c=58.3726 Å); (e) The frame with the lowest energy (the size of cube: a=b=c=58.3726 Å).
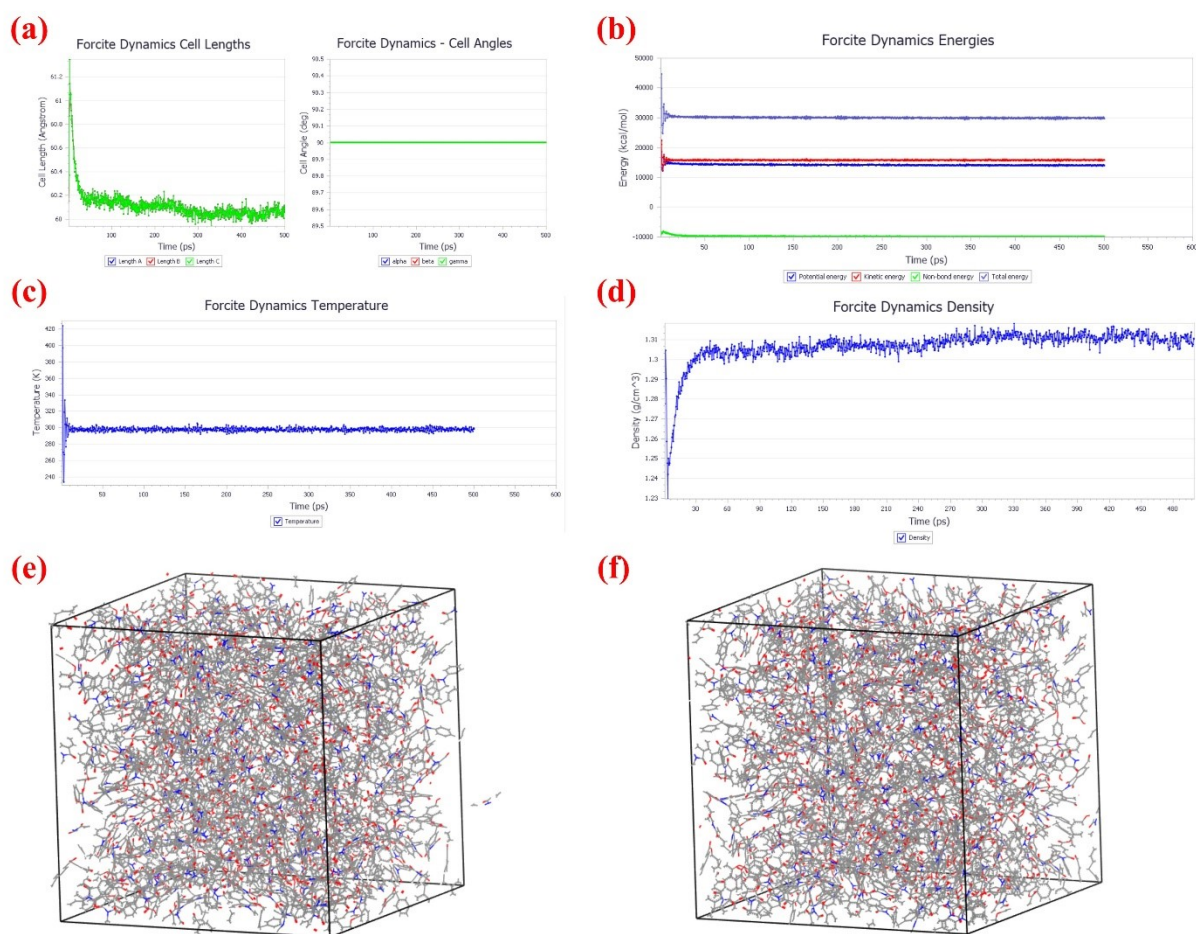
Figure S19 The release process (NPT: 10^{-4} GPa, 500 ps) of EPI-5: (a) The cell lengths and angles (b) the dynamics energies (c) the dynamics temperature and (d) the dynamics density as functions of time, respectively; (e) The initial frame (the size of cube: a=b=c=58.3726 Å); (f) The end frame (the size of cube: a=b=c=60.0594 Å).
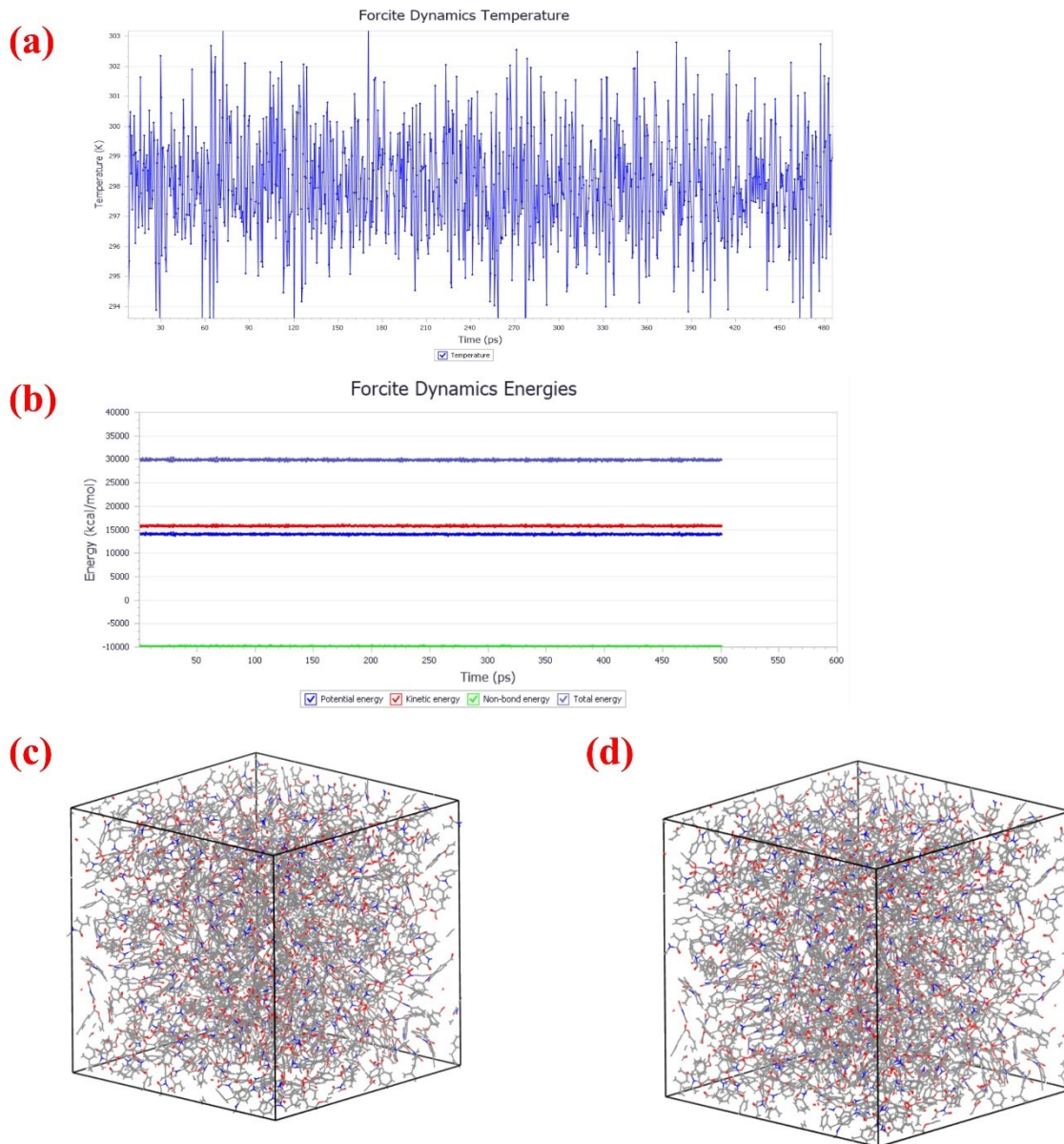
Figure S20 The equilibrium process (NVT, 500 ps) of EPI-5: (a) The dynamics temperature and (b) the dynamics energies as functions of time, respectively; (c) The initial frame (the size of cube: a=b=c=60.0594 Å); (d) The end frame (the size of cube: a=b=c=60.0594 Å).
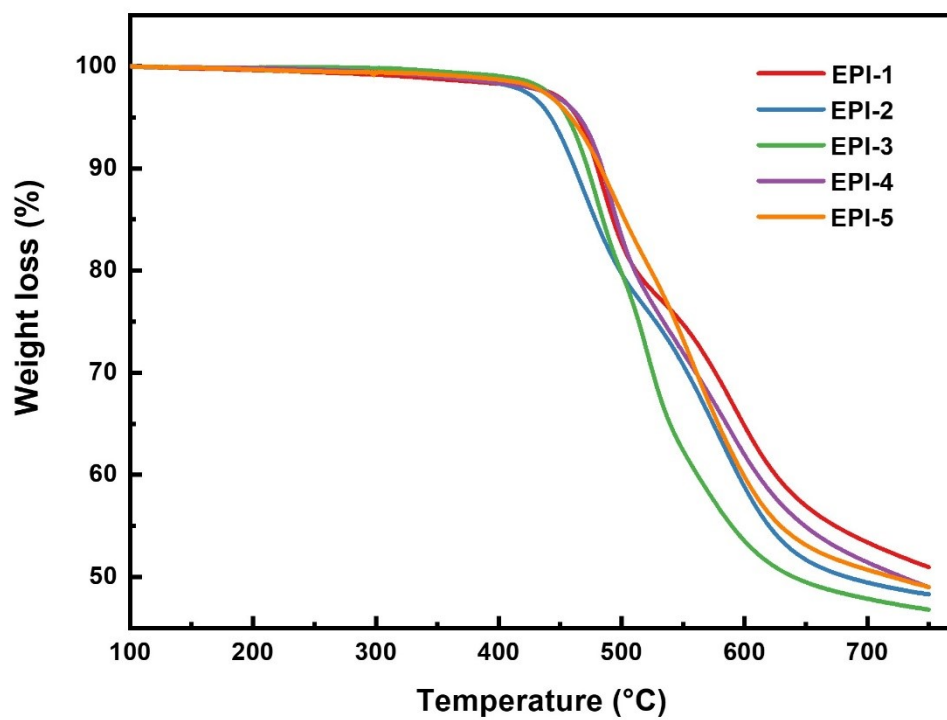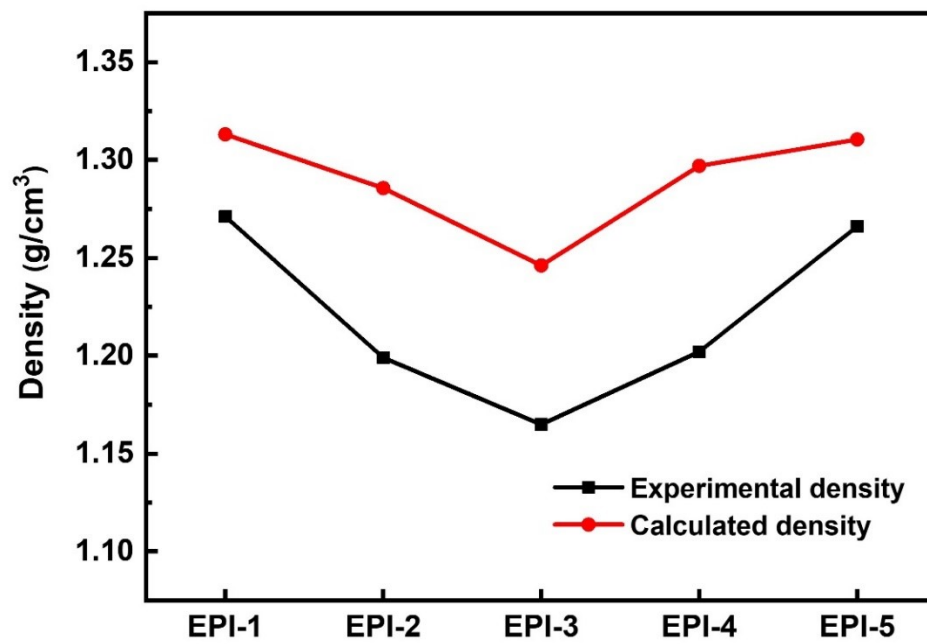
Figure S21 TGA curves (N_2 atmosphere) of ester-containing polyimides
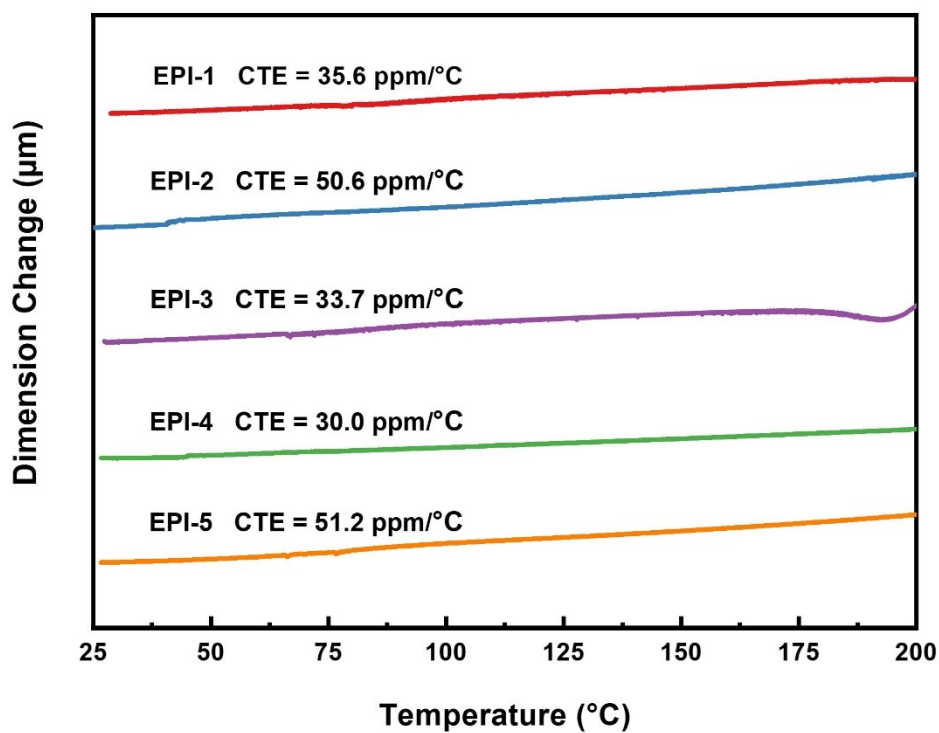
Figure S22 TMA curves of ester-containing polyimides

Table S1 thermal properties of ester-containing polyimides

polyimides	$T_{5\%}$ (°C)	CTE (ppm/°C)	T_g (°C)
EPI-1	464	35.58	316
EPI-2	442	50.63	338
EPI-3	456	33.72	200
EPI-4	465	29.98	246
EPI-5	458	51.18	247

Figure S23 The density of EPIs from both experimentation and calculation.