Supporting Information

Comparative studies on structure, sensitivity and mechanical properties of CL-20/DNDAP cocrystal and composite by molecular dynamics simulation

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Table of contents

Table S1 Cell parameters of CL-20/DNDAP cocrystal at different temperatures

T/K	*a*/nm	*b*/nm	*c*/nm	*α*/(°)	*β*/(°)	*γ*/(°)	*ρ*/(g /cm^{-3})	*V*/nm^3
198	1.282	2.212	1.312	89.19	105.36	91.14	1.928	3.585
248	1.290	2.217	1.314	88.83	105.83	90.96	1.912	3.614
298	1.311	2.153	1.346	90.63	106.04	89.30	1.893	3.651
348	1.322	2.151	1.344	89.82	106.70	89.87	1.887	3.662
398	1.329	2.180	1.338	90.18	106.15	89.37	1.856	3.724
Exp.(298 K)[a]	1.302	2.262	1.296	90.00	104.65	90.00	1.871	3.694

[a] Cited from ref. 1..

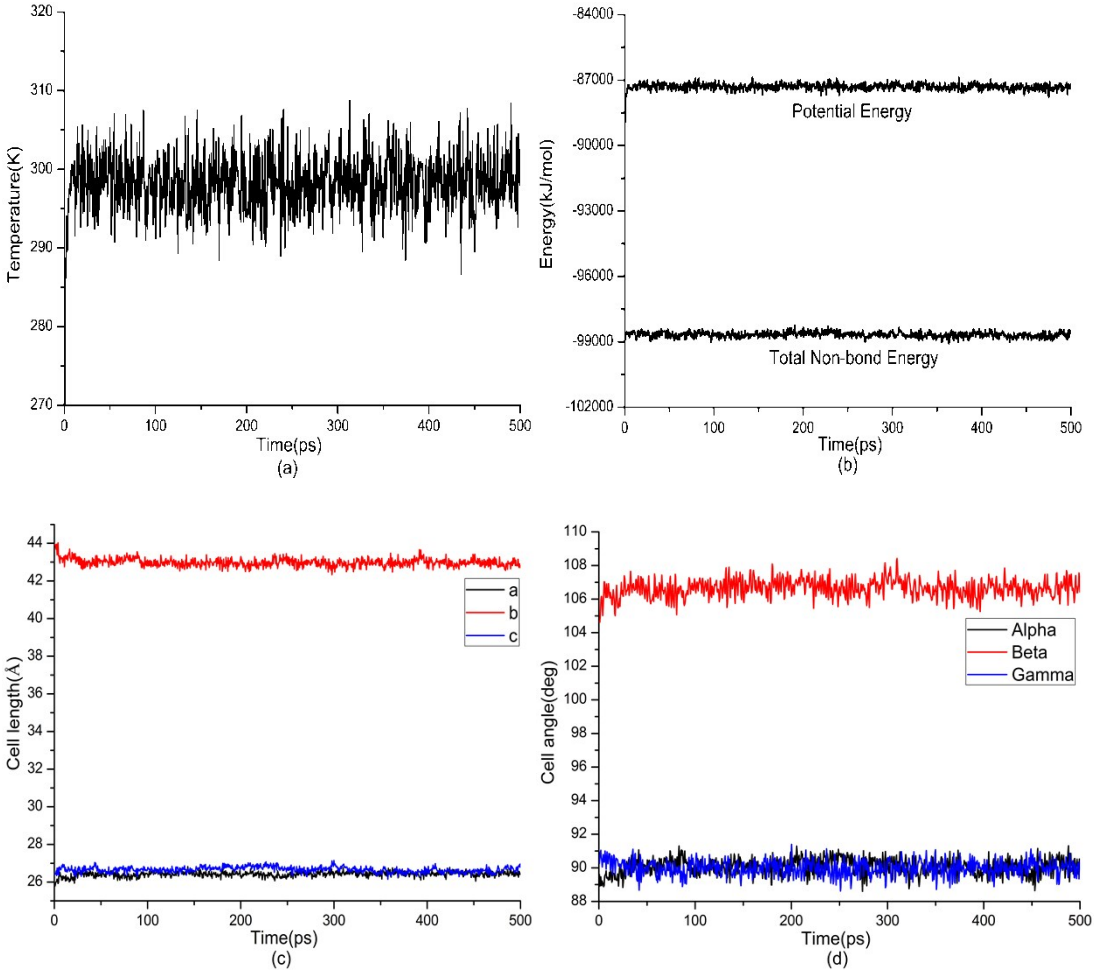

Fig. S1 The balanced parameters of CL-20/DNDAP cocrystal at 298 K

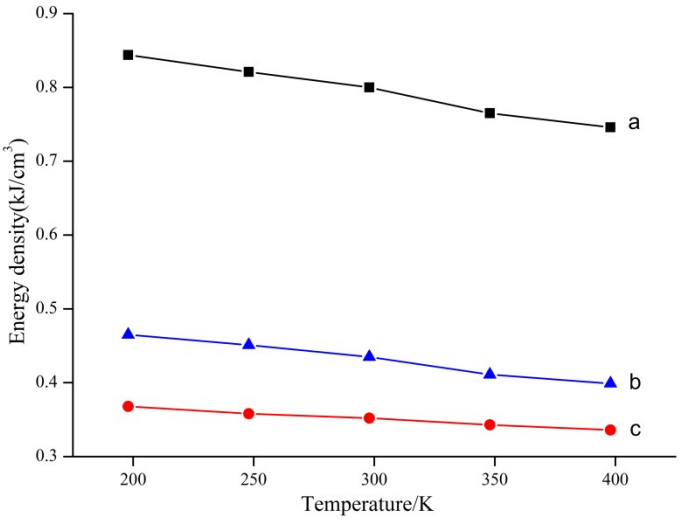

Fig. S2 (a) CED, (b) Electrostatic energy and (c) vdW energy of CL-20/DNDAP cocrystal *vs*. temperature

References

1 N. Liu, B. H. Duan, X. M. Lu, H. C. Mo, M. H. Xu, Q. Zhang and B. Z. Wang, *CrystEngComm*, 2018, **20**, 2060-2067.