Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Molecular dynamics simulation on HMX/HA·BTO cocrystal

Pengfei Zhai[ab], Chengying Shi[a] and Shengxiang Zhao*[b],

Zongshu Mei[a] and Yinguang Pan[a]

([a]Xi'an High-tech Research Institute, Xi'an 710025, People's Republic of China;

[b]Xi'an Modern Chemistry Research Institute, Xi'an 710065, People's Republic of China)

Table of contents

Table 1 Dominant crystal facets of HA·BTO predicted by Grow Morphology method with PCFF

Facet	Multiplicity	d_{hkl}/ Å	E_{att} (total) (kJ·mol^{-1})	E_{att} (vdW) (kJ·mol^{-1})	E_{att} (electrostatic) (kJ·mol^{-1})	E_{att} (H-bond) (kJ·mol^{-1})	Total facet percentage (%)
[0 1 -1]	2	4.13	-18.58	-10.556	-8.02	0	42.47
[1 0 1]	2	3.70	-23.42	-10.399	-13.02	0	27.75
[1 -1 0]	2	3.96	-29.69	-9.002	-20.69	0	18.69
[0 1 1]	2	4.33	-41.68	-7.025	-34.66	0	9.16
[1 0 -1]	2	3.61	-40.61	-9.374	-31.23	0	1.94

Table 2 Mechanical moduli of HMX, HA·BTO and HMX/HA·BTO

		Mechanical moduli					
Materials	T/K	E/GPa	K/GPa	G/GPa	ν	K/G	C12-C44
HMX	198	27.64	17.74	11.14	0.24	1.59	-12.16
	248	27.31	16.33	11.18	0.22	1.46	-12.77
	298	27.10	16.31	11.08	0.22	1.47	-12.27
	348	24.64	14.57	10.11	0.22	1.44	-11.24
	398	23.81	13.33	9.90	0.20	1.35	-12.16
HA·BTO	198	28.95	19.42	11.57	0.25	1.68	17.67
	248	28.73	19.18	11.49	0.25	1.67	17.89
	298	29.05	18.97	11.67	0.24	1.63	17.25
	348	26.90	17.86	10.77	0.25	1.66	16.57
	398	26.11	17.31	10.46	0.25	1.66	17.16
HMX/HA·BTO	198	12.44	15.56	4.55	0.37	3.42	9.02
	248	12.26	15.81	4.47	0.37	3.54	9.18
	298	11.54	13.95	4.23	0.36	3.29	7.74
	348	11.52	14.45	4.21	0.37	3.43	8.23
	398	11.45	13.50	4.21	0.36	3.21	8.93

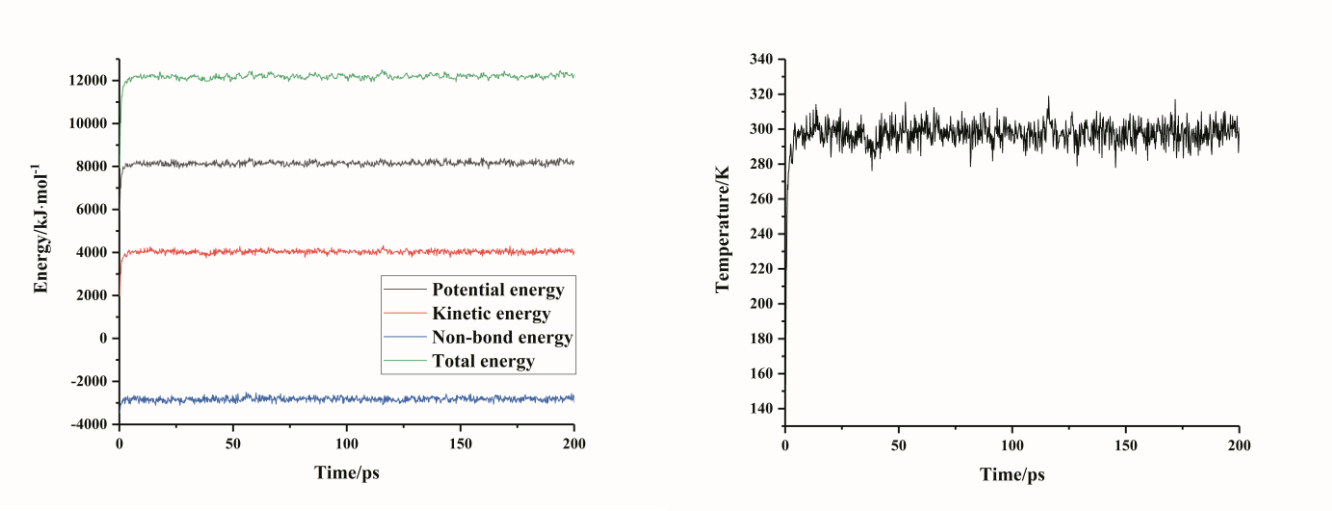

Fig. S1 Convergence characteristic of equilibrium structure of HMX/HA·BTO cocrystal model

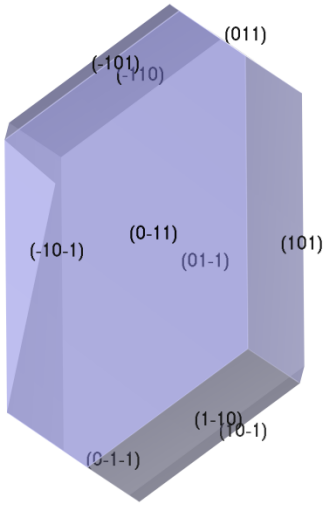

Fig. S2 Crystal morphology of HA·BTO predicted by Growth Morphology method with PCFF

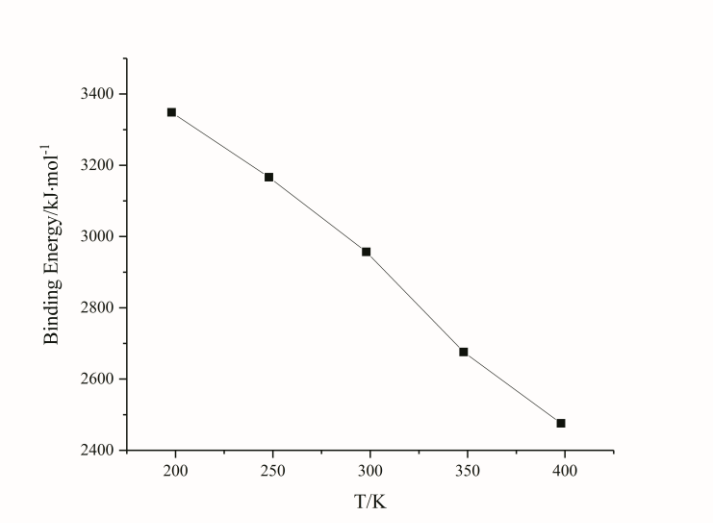

Fig. S3 Binding energy of HMX/HA·BTO