Formation and growth mechanisms of natural metastable twin boundary in crystalline β-octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine: A computational study

Zhichao Liu, Qiong Wu, Weihua Zhu,* Heming Xiao
Institute for Computation in Molecular and Materials Science and Department of Chemistry, Nanjing University of Science and Technology, Nanjing 210094, China

Keywords HMX, twin boundary, SCC-DFTB, dispersion correction, metastability

* Corresponding author. E-mail: zhuwh@njust.edu.cn

Table S1. Comparison of theoretical and experimental lattice parameters of several typical high explosives by using SCC-DFTB-D methods.

		a	*b*	*c*	*β*	*V*	*ρ*
	Expt.[a]	**6.54**	**11.05**	**8.70**	**124.30**	**519.39**	**1.89**
β-HMX	pbc	6.43(-1.68)[g]	11.08(0.27)	8.68(-0.23)	123.6(-0.56)	515.26(-0.80)	1.91(1.05)
	CHNO	6.45(-1.38)	11.01(-0.36)	8.71(0.11)	123.9(-0.32)	513.19(-1.19)	1.92(1.59)
	Expt.[b]	**11.4**	**10.6**	**13.1**	**90.0**	**1588.5**	**1.86**
RDX	pbc	11.39	10.52	13.44	90.0	1610.56	1.83
	CHNO	11.41	10.54	13.38	90.0	1609.49	1.83
	Expt.[c]	**8.85**	**12.56**	**13.39**	**106.82**	**1424.15**	**2.04**
ε-CL-20	pbc	8.76	12.27	13.61	109.17	1382.32	2.11
	CHNO	8.77	12.28	13.80	110.34	1392.43	2.09
	Expt.[d]	**9.01**	**9.03**	**6.81**	**91.82**	**442.52**	**1.94**
TATB	pbc	9.04	9.04	6.65	94.25	442.02	1.94
	CHNO	9.02	9.02	6.75	94.56	441.39	1.94
	Expt.[e]	**9.28**	**9.28**	**6.61**	**90.0**	**568.97**	**1.85**
PETN	pbc	9.20	9.20	6.53	90.0	552.75	1.90
	CHNO	9.19	9.19	6.56	90.0	554.06	1.89

[a-e]The experimental data are taken from references 27-31, respectively.

[f] The values in parentheses correspond to the percentage differences relative to the experimental data.