Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Phase Transition Induced by External Electric Field as a Buffer to Facilitate the Initial Decomposition of Series of Catenated Nitrogen Energetic Systems: A First-Principles Study

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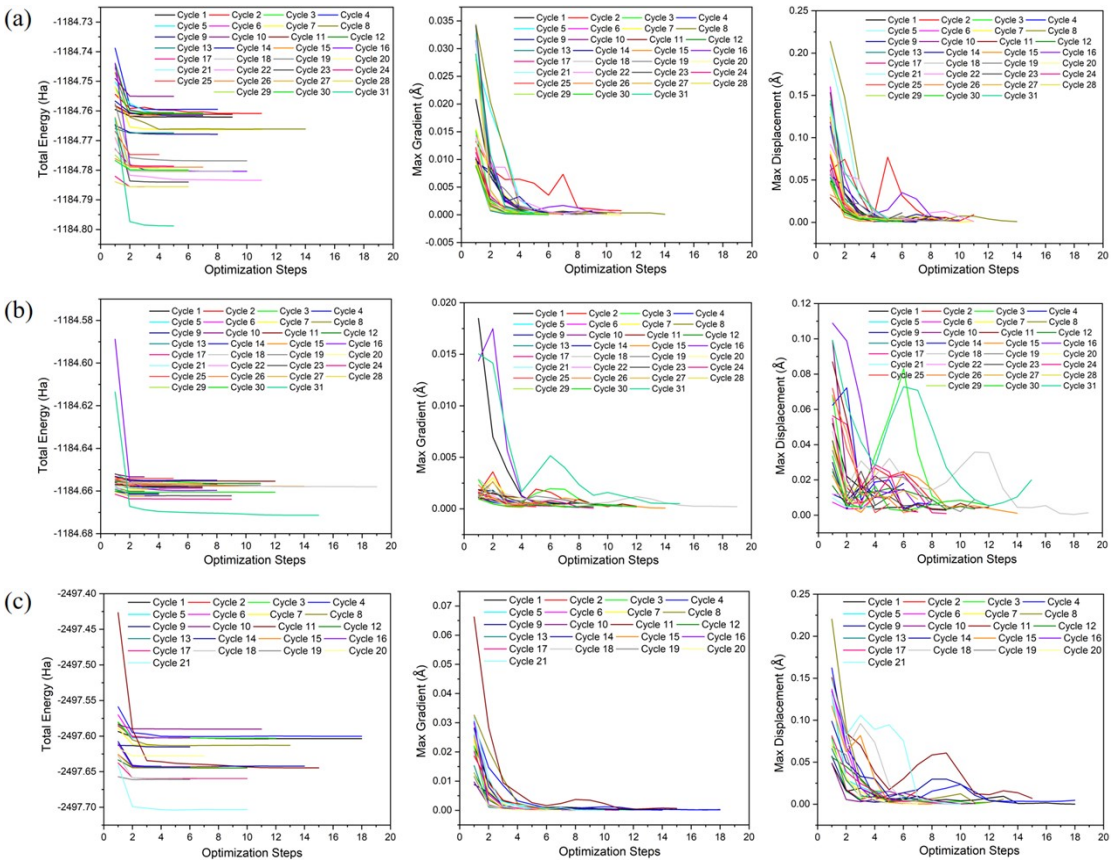

Fig. S1. Converged process of (a) N_4, (b) N_8, and (c) N_{10} during the cell optimization under the external electric field strength of 0.01 a.u..

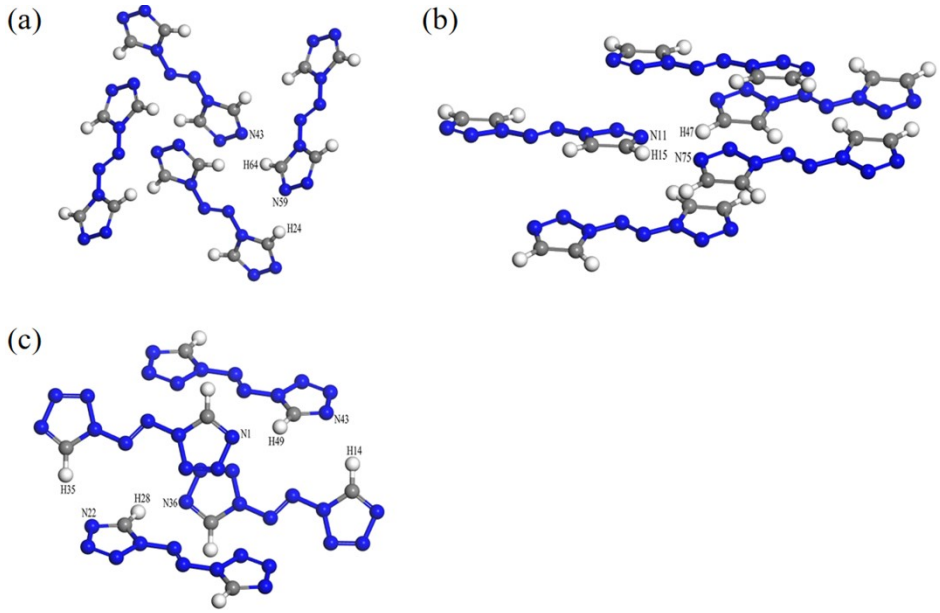

Fig. S2. Selected clusters from crystals (a) N_4, (b) N_8, and (c) N_{10}.

Table S1. The deviations between the calculated and experimental lattice constants of N_4, N_8, and N_{10}.

	N_4			N_8			N_{10}		
	calc.	expt.	deviation	calc.	expt.	deviation	calc.	expt.	deviation
a	4.885	5.032	2.92%	7.321	7.488	2.23%	8.352	8.177	2.14%
b	6.497	6.498	0.02%	5.234	5.266	0.61%	6.672	6.835	2.38%
c	9.813	10.301	4.73%	8.674	9.131	5.00%	10.786	11.130	3.09%
β	94.514	91.56	3.22%	110.053	112.604	2.27%	90.000	90.000	0.00%

Table S2. C_{ij} (GPa) of N_4 with intensity of external electric field ranging from 0-0.01 a.u..

	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{23}
0	32.67	38.02	23.77	26.81	13.56	9.5	18.51	16.75	21.13
0.001	31.39	34.98	21.72	25.53	12.88	9.16	18.22	15.76	19.32
0.002	31.15	33.89	20.94	25.06	12.68	8.95	18.3	15.48	18.68
0.003	30.6	31.9	19.5	24.16	12.26	8.68	18.36	14.97	17.45
0.004	29.54	29.03	17.18	22.48	11.53	8.36	18.35	14.24	15.44
0.005	27.37	25.14	13.98	19.52	10.43	8.17	17.54	13.23	12.43
0.006	23.41	21.25	10.91	14.83	8.69	8.07	16.05	11.85	8.76
0.007	21.41	19.8	9.7	13.18	7.94	7.54	14.86	10.85	7.62
0.008	19.83	19.49	8.91	12.55	7.39	6.92	14.08	10.24	7.06
0.009	20.92	20.19	9.46	13.12	7.69	7.22	15.33	11.27	8
0.01	19.75	18.14	8.73	12.5	7.1	7.06	13.01	9.2	6.95

Table S3. C_{ij} (GPa) of N_8 with intensity of external electric field ranging from 0-0.01 a.u..

	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{23}
0	48.15	32.17	21.34	-2.21	8.38	4.77	23.23	19.05	11.38
0.001	45.9	30.69	18.52	-2.25	7.54	4.43	22.77	17.64	10.99
0.002	44.73	30.85	18.12	-2.06	7.36	4.54	22.59	17.21	10.85
0.003	44.76	29.19	16.11	-2.98	7.17	3.56	22.25	16.87	10.7
0.004	43.42	28.8	14.79	-2.99	7.19	3.47	22.1	16.31	10.41
0.005	40.78	28.14	12.5	-3.01	6.7	3.2	21.7	15.41	9.84
0.006	38.26	27.1	10	-2.71	6.51	3.06	21.28	14.09	9.07
0.007	34.07	24.66	6.34	-2.86	6.3	2.38	19.59	12.48	6.33
0.008	28.49	26.17	3.48	-1.26	6.8	2.54	17.04	11.6	8.48
0.009	26.03	26.65	2.87	-0.83	6.86	2.58	16.39	10.99	6.09
0.01	31.55	29.21	6.95	-2.03	7.1	2.58	19.27	13.22	9.26

Table S4. C_{ij} (GPa) of N_{10} with intensity of external electric field ranging from 0-0.01 a.u..

	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{23}
0	17.25	25.35	24.62	15.34	8.55	10.78	12.17	14.74	19.34
0.001	17.65	25.12	24.31	15.28	8.73	10.95	12.73	15.13	19
0.002	17.67	24.51	23.33	15.04	8.57	10.94	13.17	15.14	18.37
0.003	18.06	23.35	20.95	14.25	8.16	10.85	14.32	15.29	16.99
0.004	16.91	21.32	17.26	12.91	7.27	10.42	14.12	14.08	14.52
0.005	19.67	19.04	11.69	10.92	6.52	10.25	16.35	14.17	10.56
0.006	18.96	19.05	10.77	10.3	5.68	9.99	16.08	13.26	10.47
0.007	17.1	17.54	9.29	9.27	4.95	9.16	14.91	11.85	9.5
0.008	19.45	18.88	10.63	10.37	5.85	10.01	16.65	13.46	10.18
0.009	17.49	17.28	9.52	9.42	5.31	9.23	15.14	12.25	9.27
0.01	18.31	17.35	10.75	10.45	6.6	9.4	15.94	13.3	9.05