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

High Throughput Scanning of Dimer Interactions Facilitating to Confirm Molecular Stacking Mode: A Case of 1, 3, 5-Trinitrobenzene and Its Amino-derivatives

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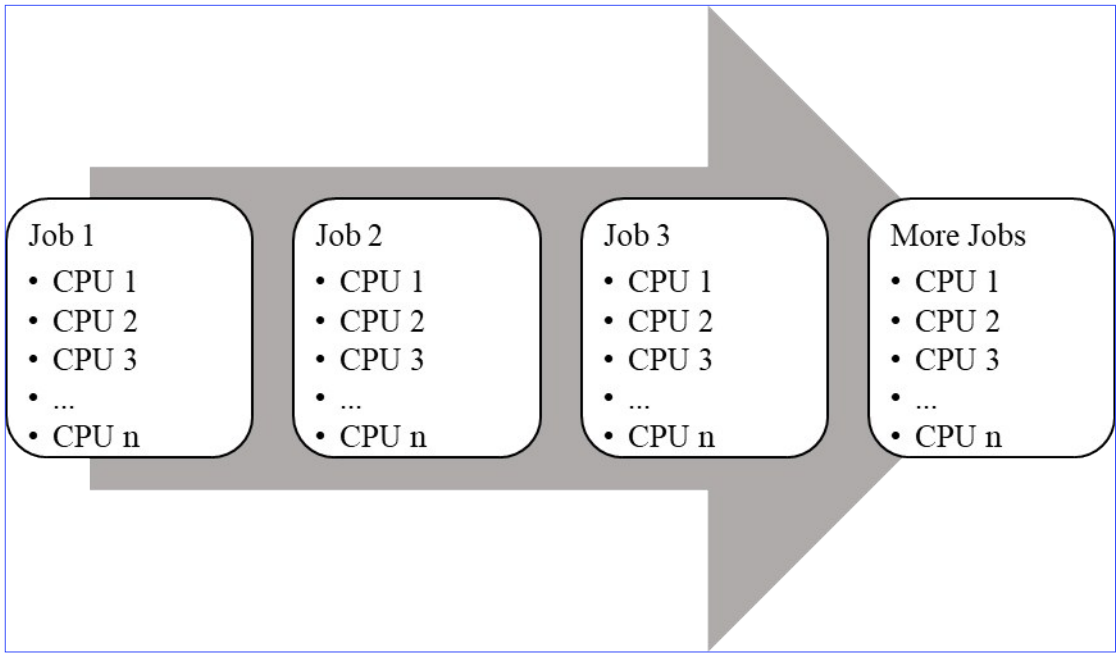
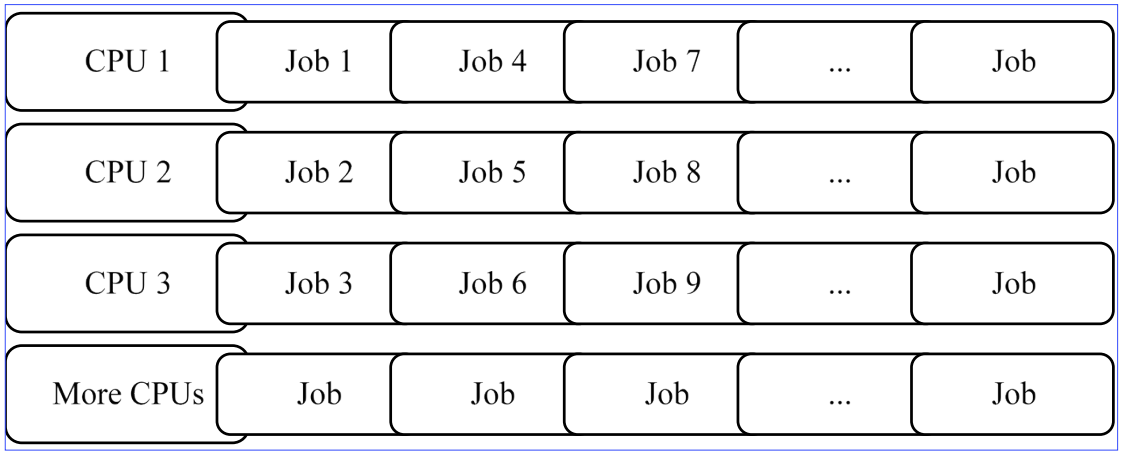


Figure S1. Model for sequential computations.



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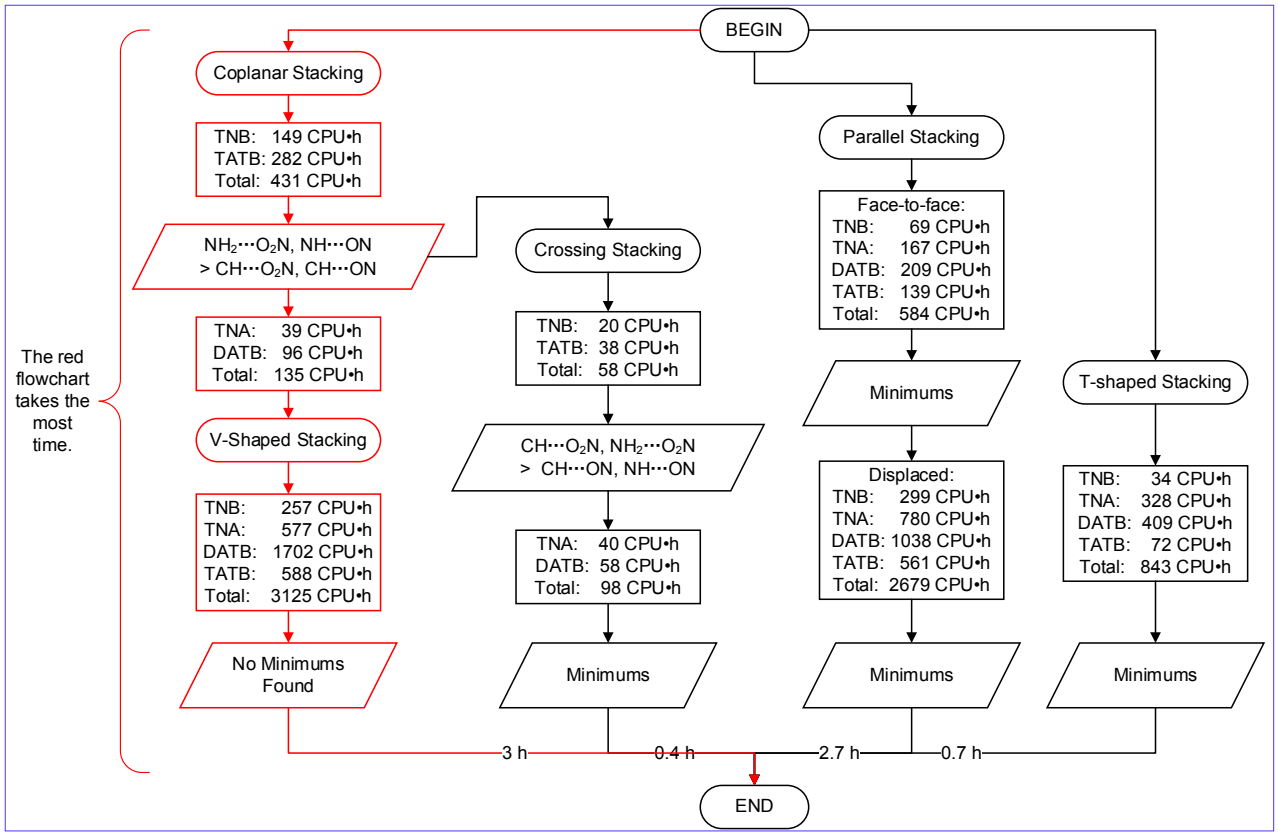

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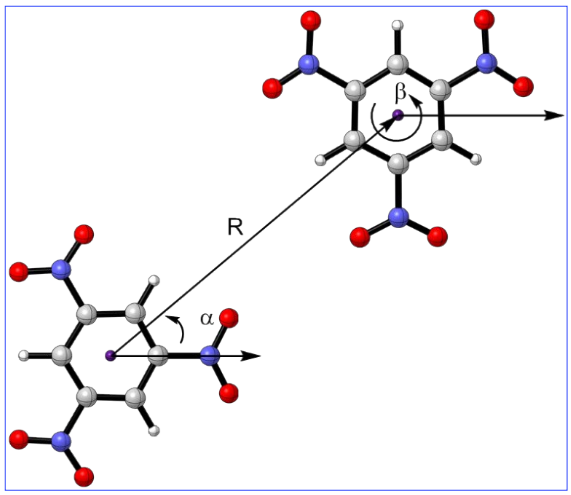
S2: PES scanning of the coplanar stacking.



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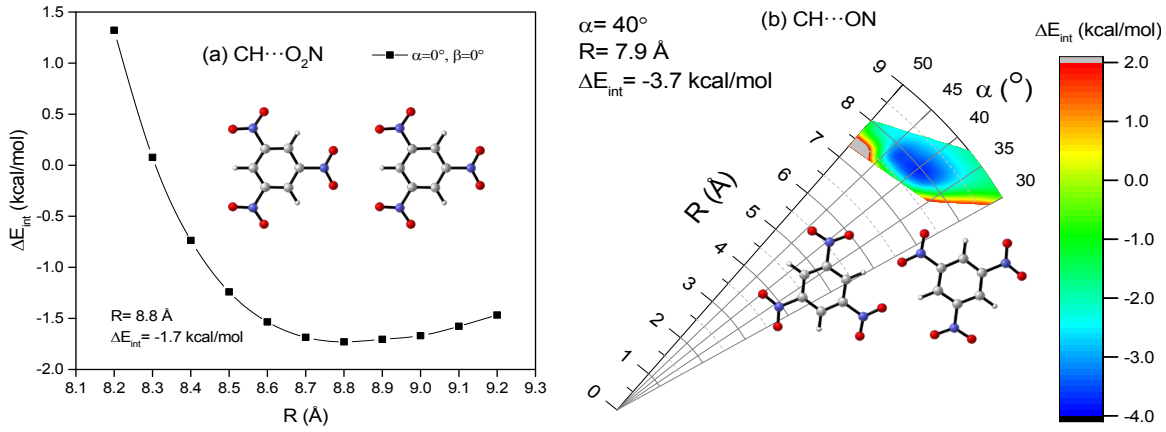

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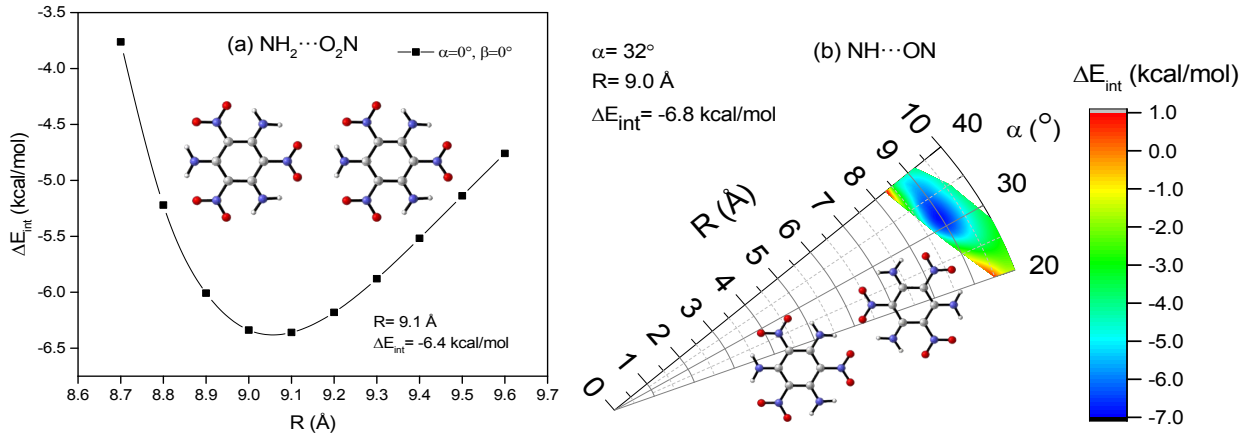

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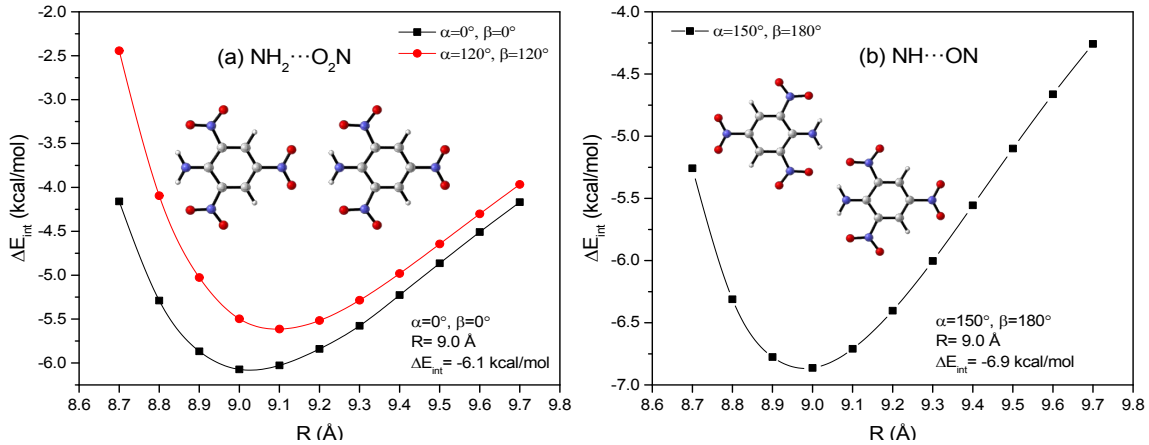

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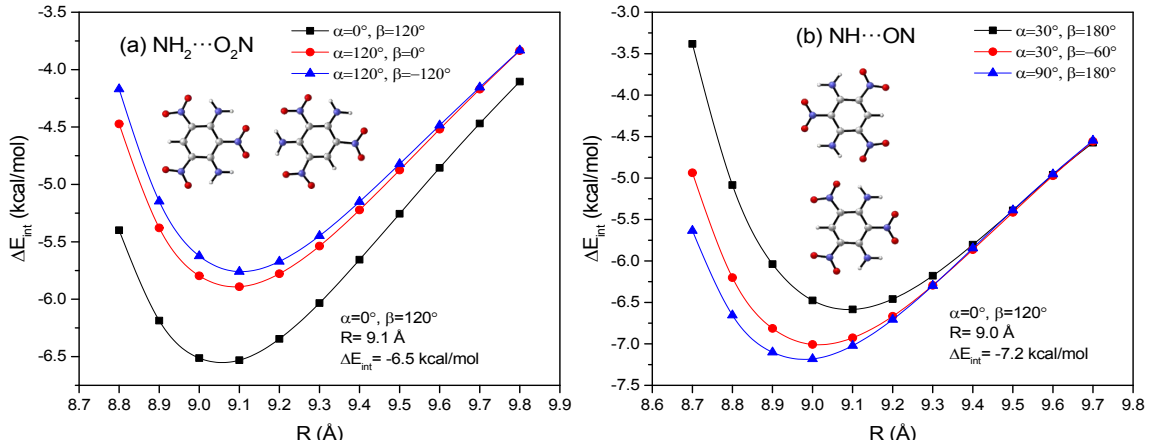

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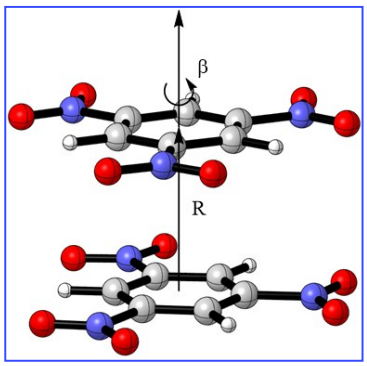

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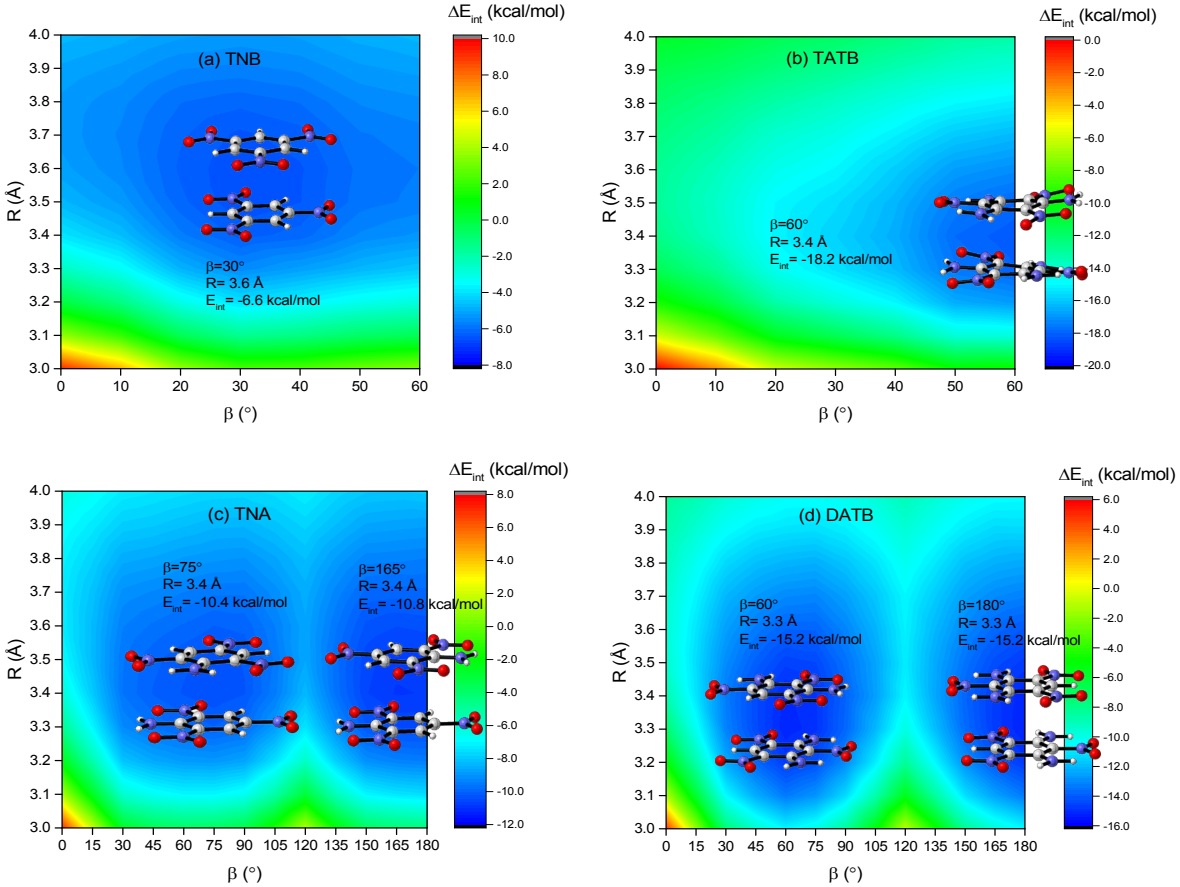

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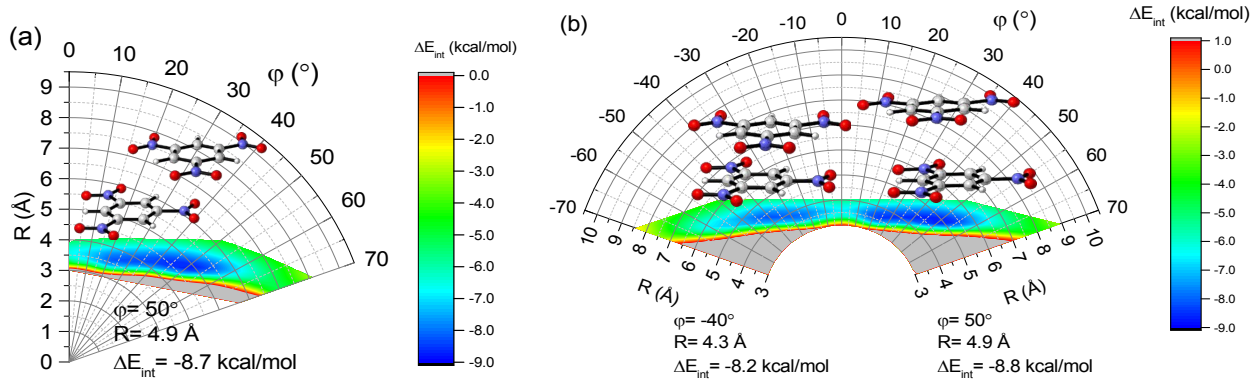

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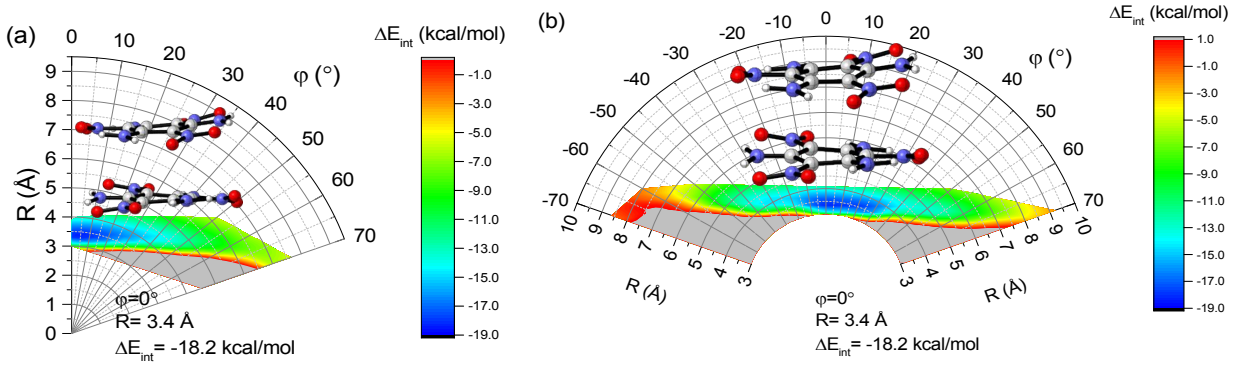

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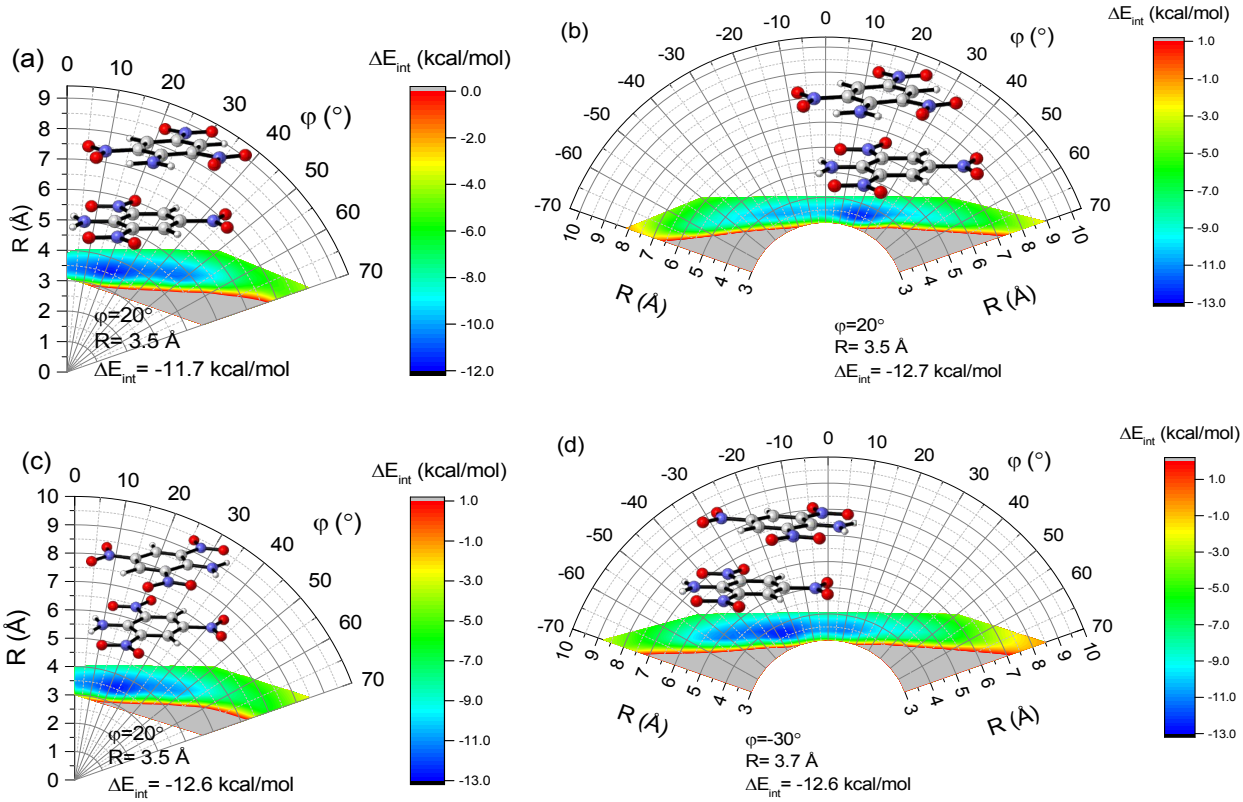

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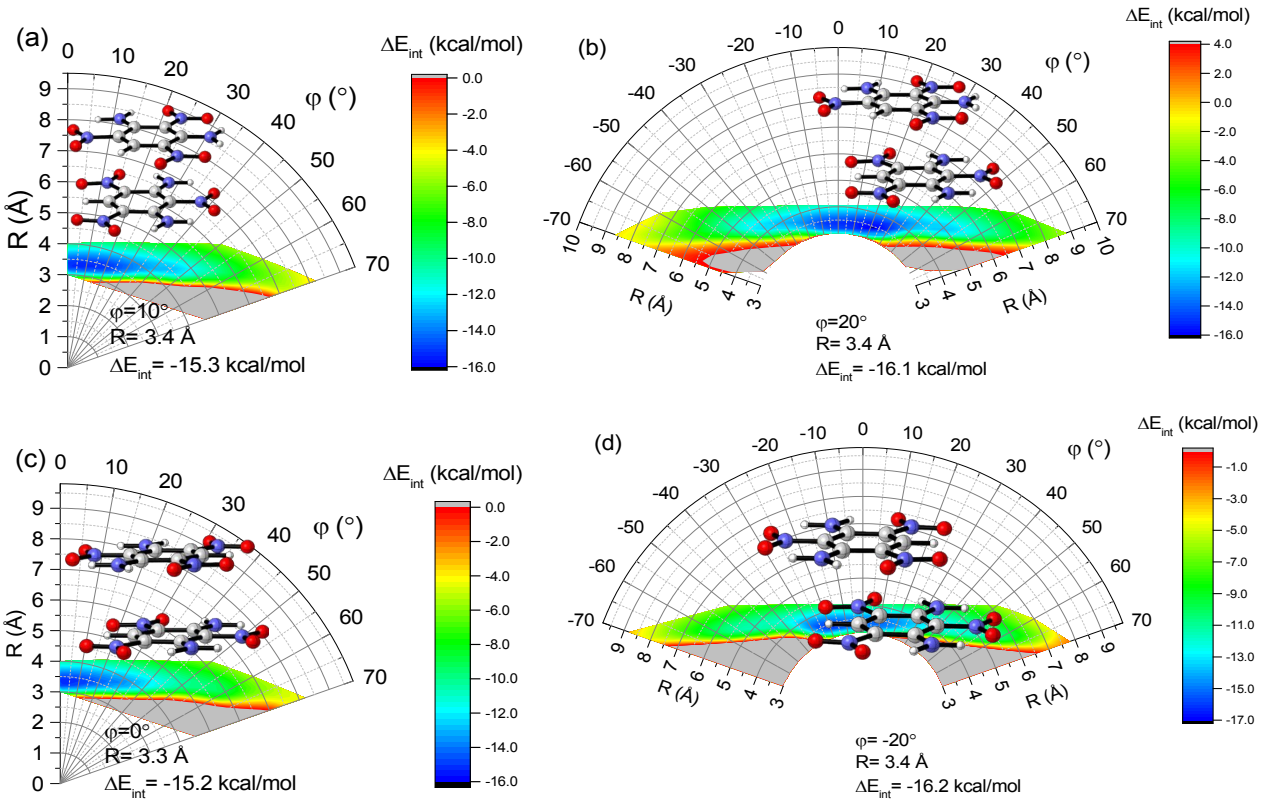

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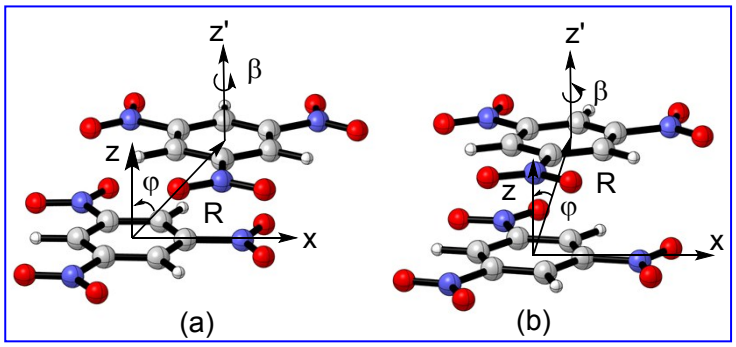

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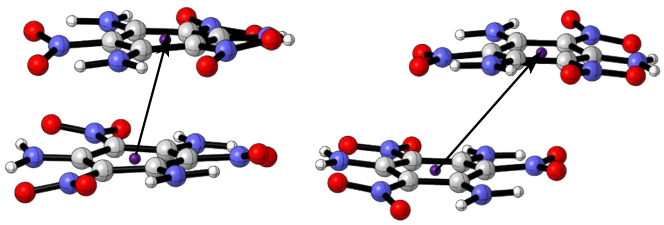

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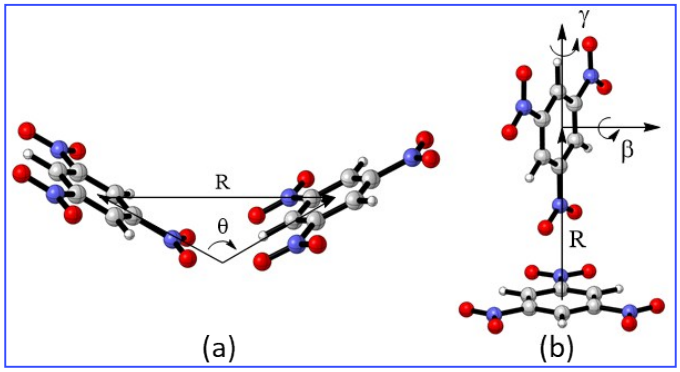

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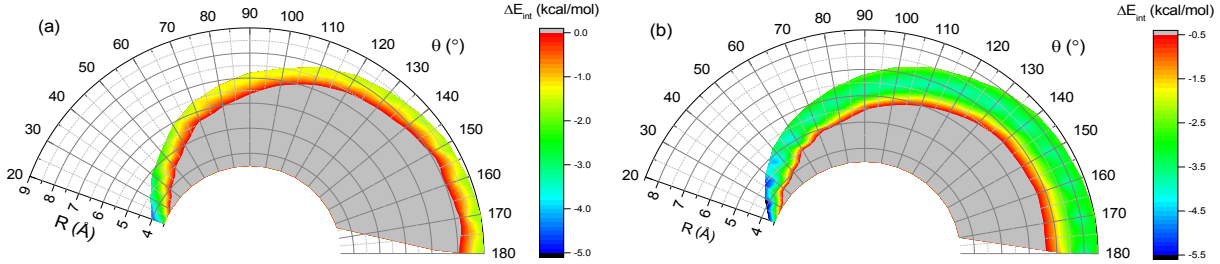

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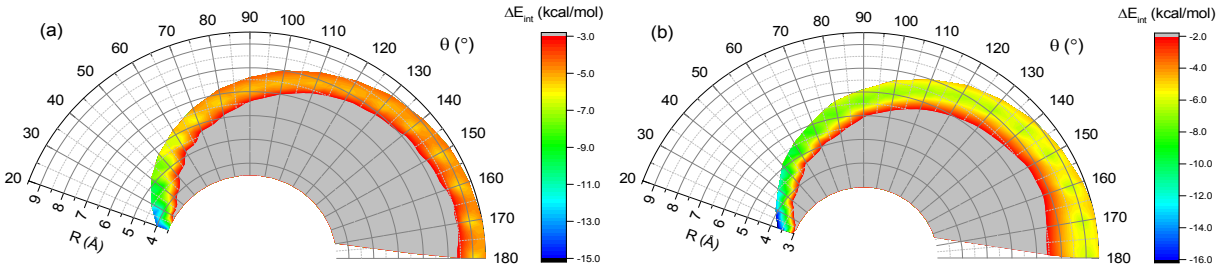

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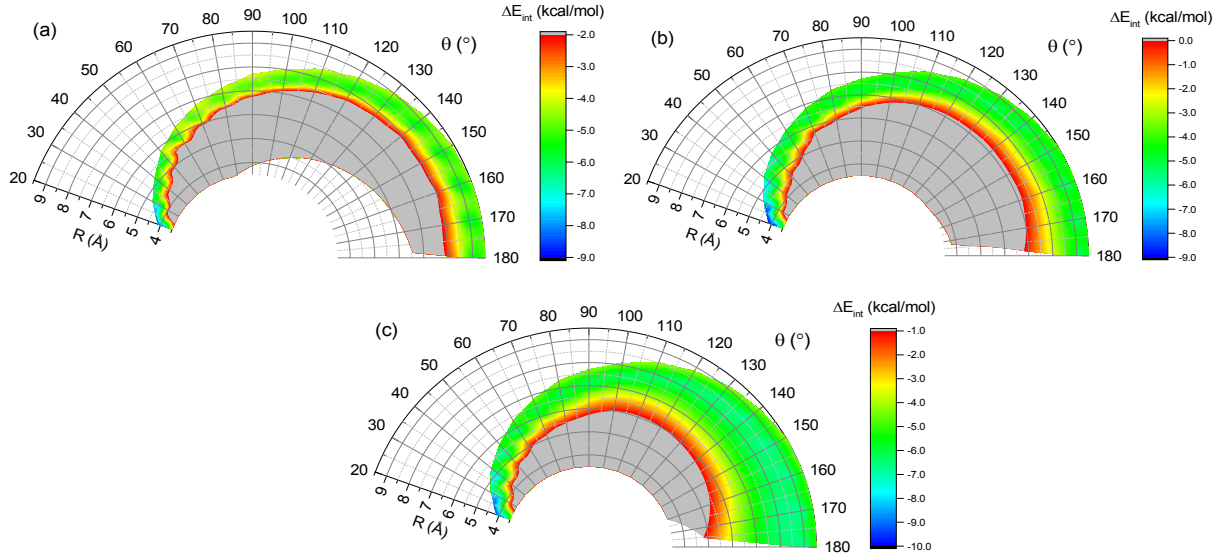

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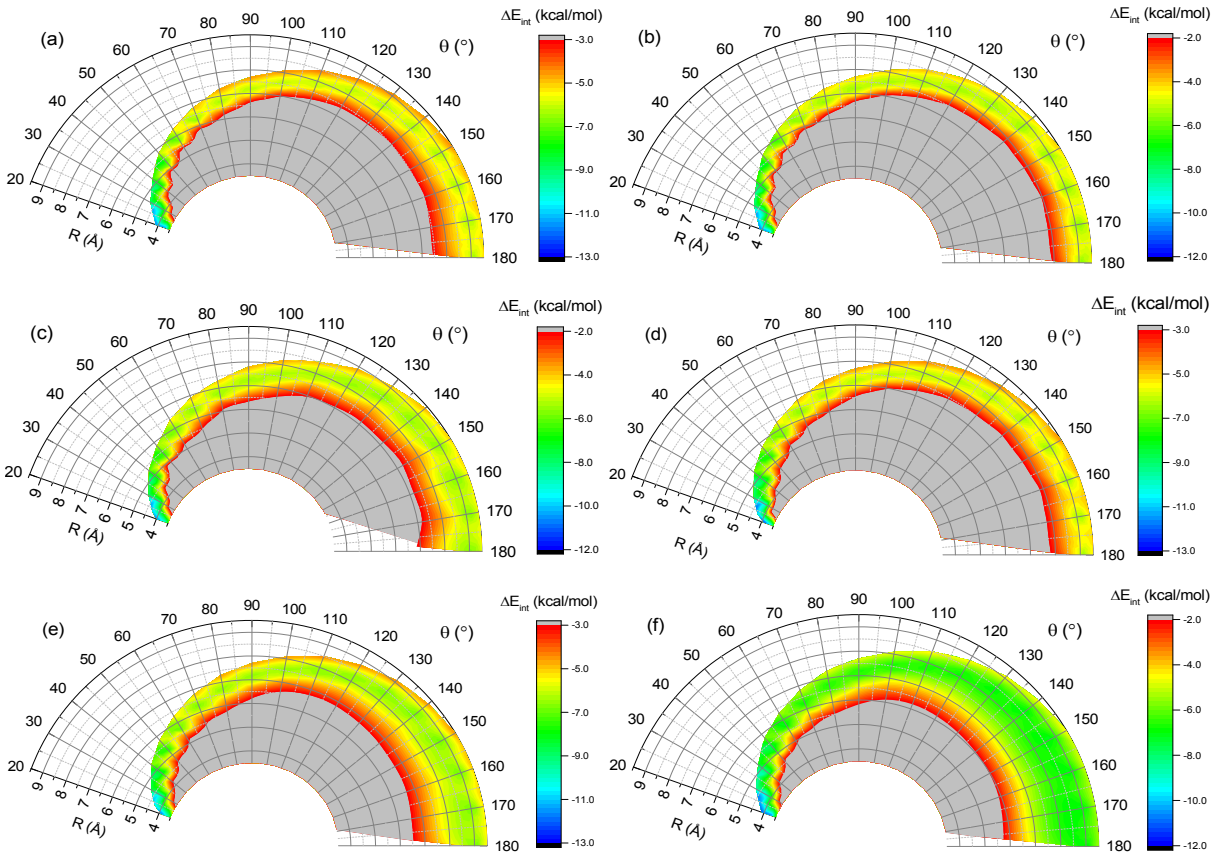

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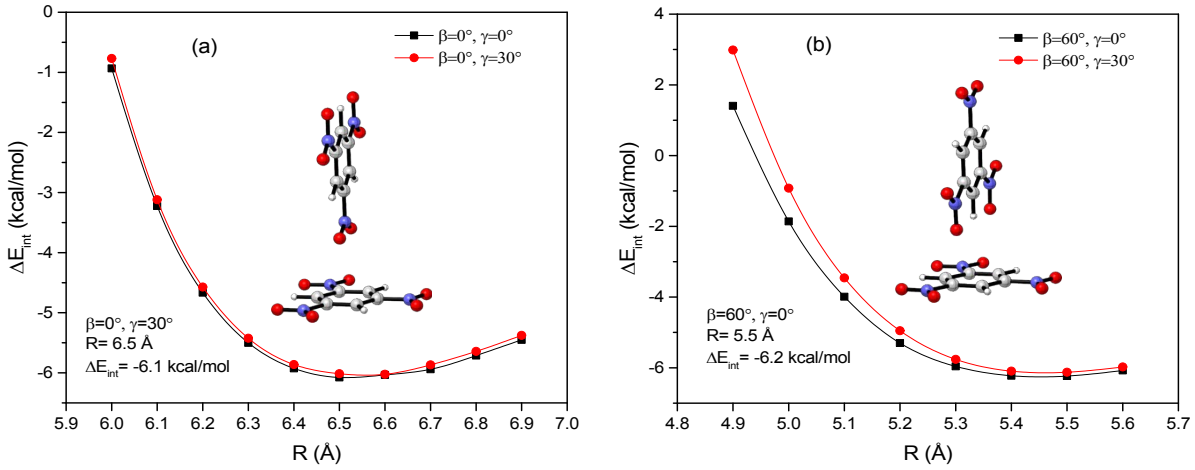

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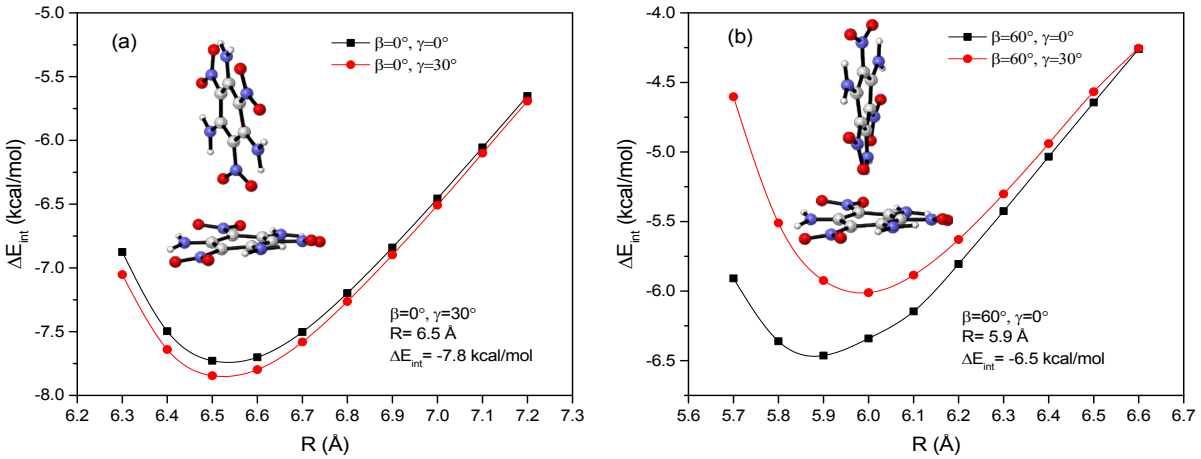

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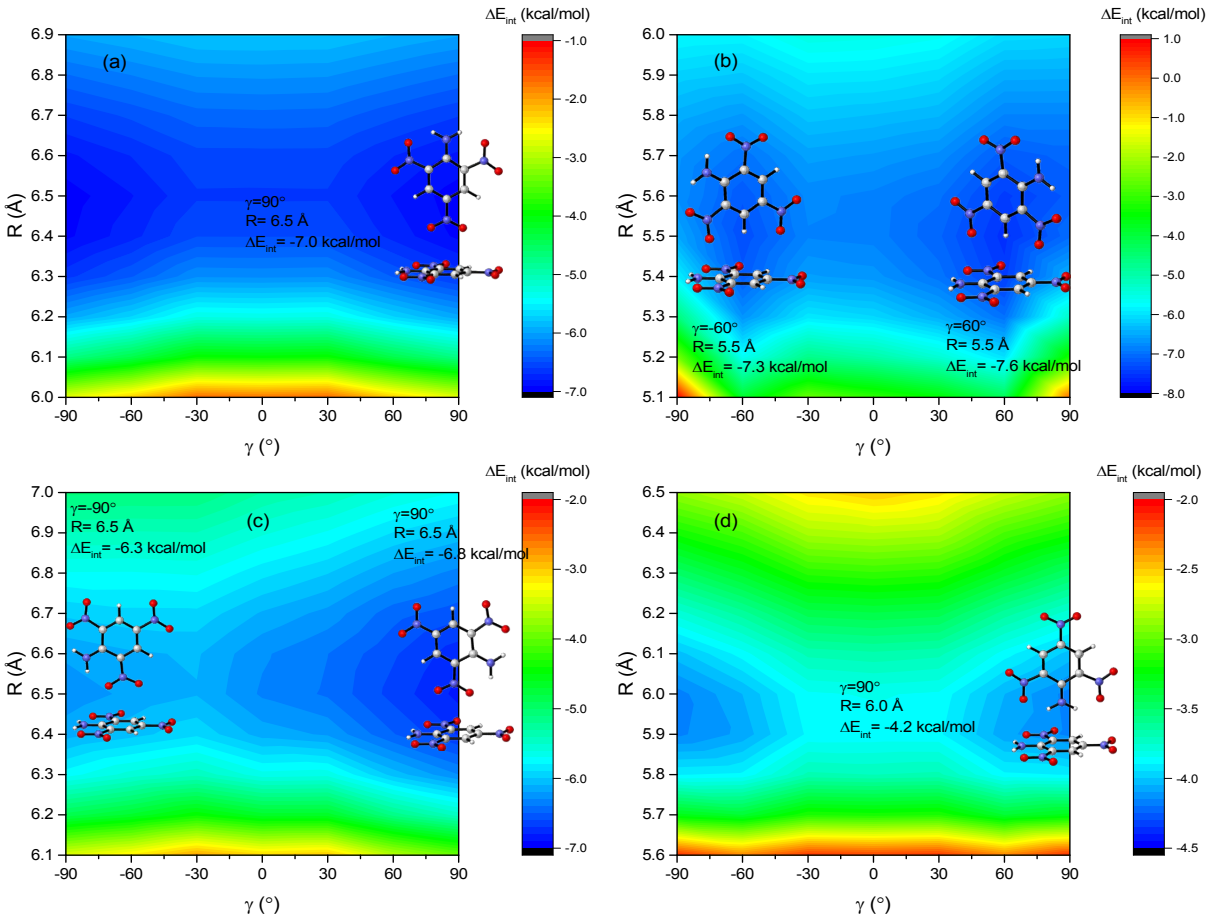

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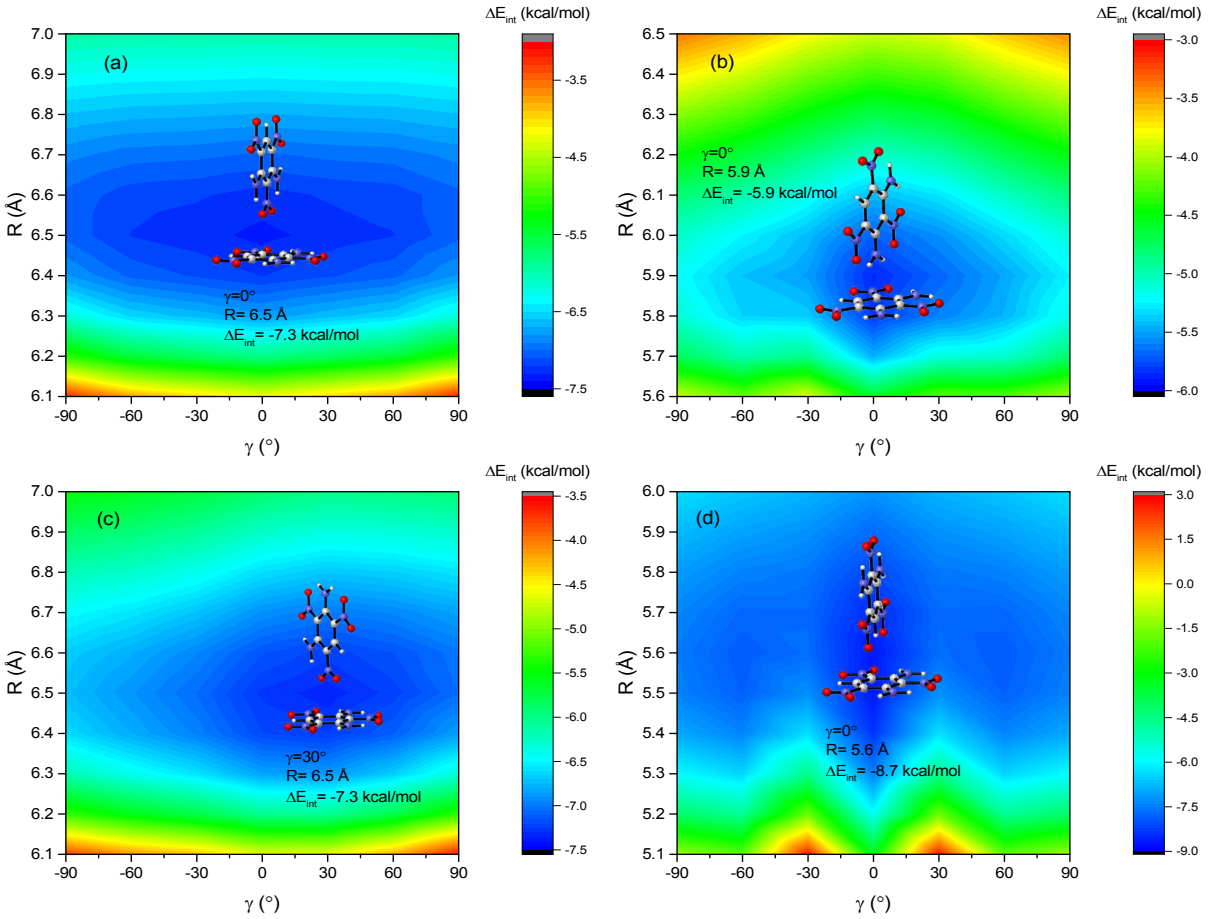

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S5: PES scanning of the crossing stacking.

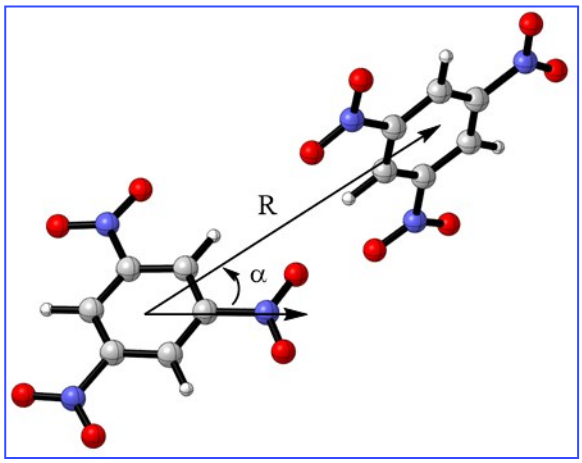
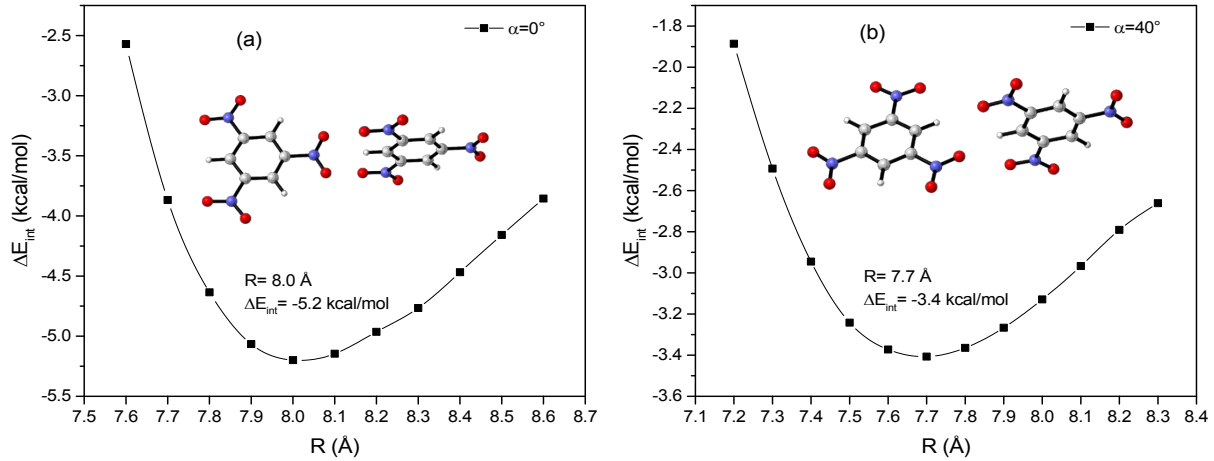


Figure S26. Degree of freedom of crossing stacking.



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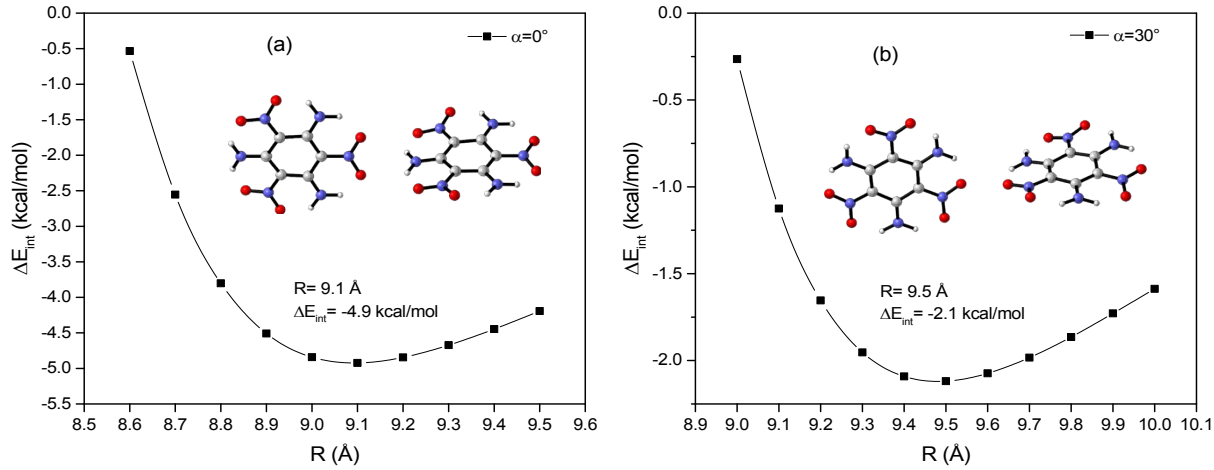

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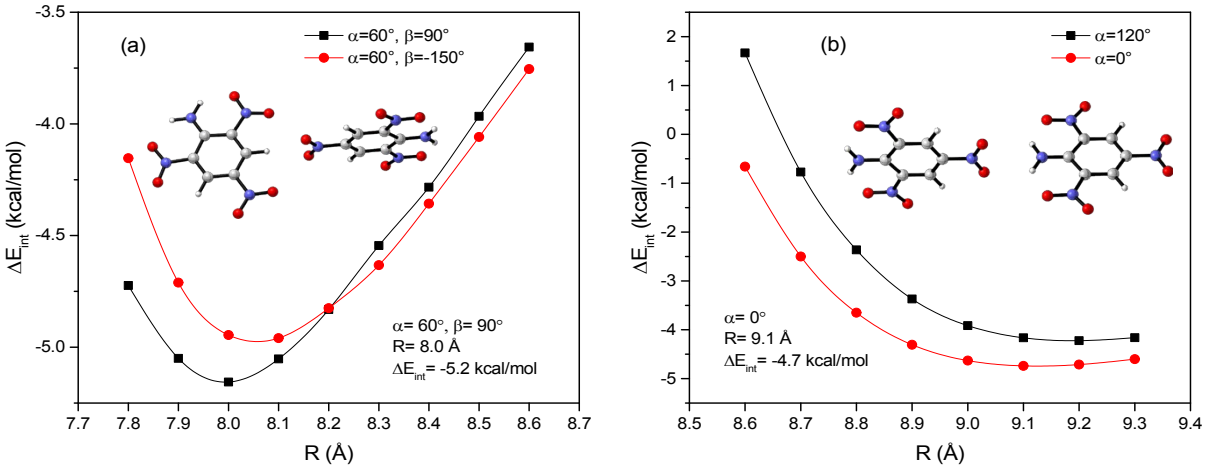

Figure S29. PESs of the crossing TNA dimers along (a) CH···NO_2 and (b) NH_2···NO_2.

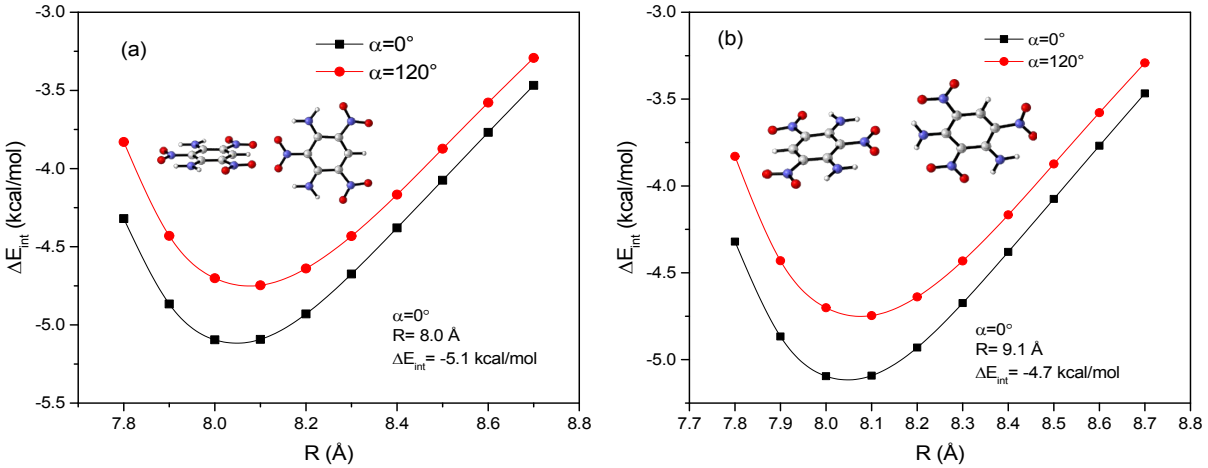

Figure S30. PESs of the crossing DATB dimers stacked along (a) CH···NO_2 and (b) NH_2···NO_2.

S6: Summary of the locally lowest points on all PESs and the related ΔE_{int}.

Table S1. Summary of the Locally Lowest Points on All PESs and the Related ΔE_{int}.

No.	Label	α (°)	β (°)	φ (°)	θ (°)	γ (°)	R (Å)	ΔE_{int} (kcal/mol)
1	TNB-C1	0	0	90	0	0	8.8	-1.7
2	TNB-C2	40	60	90	0	0	7.9	-3.7
3	TNB-P1	15	30	50	0	0	4.9	-8.7
4	TNB-P2	285	30	40	0	0	4.3	-8.2
5	TNB-P3	105	30	50	0	0	4.9	-8.8
6	TNB-P4	0	30	0	0	0	3.6	-6.6
7	TNB-T1	0	0	0	90	0	6.5	-6.1
8	TNB-T2	0	0	0	90	30	6.6	-6.0
9	TNB-T3	0	180	0	90	0	5.5	-6.2
10	TNB-T4	0	180	0	90	30	5.5	-6.1
11	TNB-X1	0	30	90	90	90	8	-5.2
12	TNB-X2	40	20	90	90	130	7.8	-3.4
13	TATB-C1	0	0	90	0	0	9.1	-6.4
14	TATB-C2	32	60	90	0	0	8.9	-6.8
15	TATB-P	0	60	0	0	0	3.4	-18.2
16	TATB-T1	0	0	0	90	0	6.5	-7.7
17	TATB-T2	0	0	0	90	30	6.5	-7.8
18	TATB-T3	0	180	0	90	0	5.9	-6.5
19	TATB-T4	0	180	0	90	30	6	-6.0
20	TATB-X1	0	30	90	90	90	9.1	-4.9
21	TATB-X2	30	0	90	90	120	9.5	-2.1
22	TNA-C1	0	0	90	0	0	9	-6.1
23	TNA-C2	120	120	90	0	0	9.1	-5.6
24	TNA-C3	150	180	90	0	0	9	-6.9
25	TNA-P1	38	75	20	0	0	3.5	-11.7
26	TNA-P2	128	75	20	0	0	3.5	-12.7
27	TNA-P3	308	75	30	0	0	3.8	-10.6
28	TNA-P4	83	165	20	0	0	3.5	-12.6
29	TNA-P5	173	165	10	0	0	3.4	-11.2
30	TNA-P6	353	165	30	0	0	3.7	-12.6
31	TNA-PV1	0	75	0	0	0	3.4	-10.4
32	TNA-PV2	0	165	0	0	0	3.4	-10.8
33	TNA-T1	0	0	0	90	90	6.5	-7.0
34	TNA-T2	0	60	0	90	60	5.5	-7.6
35	TNA-T3	0	60	0	90	-60	5.5	-7.3
36	TNA-T4	0	120	0	90	90	6.5	-6.8
37	TNA-T5	0	120	0	90	-90	6.5	-6.3
38	TNA-T6	0	180	0	90	90	6	-4.2
39	TNA-X1	60	210	90	90	150	8.1	-5.0

40	TNA-X2	60	90	90	90	150	8	-5.2
41	TNA-X3	120	270	90	90	210	9.2	-4.2
42	TNA-X4	0	270	90	90	90	9.1	-4.7
43	DATB-C1	0	120	90	0	0	9.1	-6.5
44	DATB-C2	120	0	90	0	0	9.1	-5.9
45	DATB-C3	120	240	90	0	0	9.1	-5.8
46	DATB-C4	30	180	90	0	0	9.1	-6.6
47	DATB-C5	30	300	90	0	0	9	-7.0
48	DATB-C6	90	180	90	0	0	9	-7.2
49	DATB-P1	30	60	10	0	0	3.4	-15.3
50	DATB-P2	120	60	20	0	0	3.4	-16.1
51	DATB-P3	90	180	0	0	0	3.3	-15.2
52	DATB-P4	0	180	20	0	0	3.4	-16.2
53	DATB-PV1	0	60	0	0	0	3.3	-15.2
54	DATB-PV2	0	180	0	0	0	3.3	-15.2
55	DATB-T1	0	0	0	90	0	6.5	-7.3
56	DATB-T2	0	60	0	90	0	5.9	-5.9
57	DATB-T3	0	120	0	90	30	6.5	-7.3
58	DATB-T4	0	180	0	90	0	5.6	-8.7
59	DATB-X1	120	270	90	90	210	8.1	-4.7
60	DATB-X2	0	270	90	90	90	8	-5.1
61	DATB-X3	120	30	90	90	210	9.2	-4.6
62	DATB-X4	0	30	90	90	90	9.1	-4.7