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

Theoretical Analysis of the Intermolecular Interactions in Naphthalene Diimide and Pyrene Complexes

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Table S1 Binding energies for selected configurations of the pyrene (Py), naphthalene diimide (NDI) and NDI-Py dimers. Results are calculated at CP-corrected M06-2X functional at various basis sets.

	S		**SP-L**		**SP-S**	
	R	E	R	E	R	E
Py dimer						
6-31G(d)	3.69	-2.08	3.42	-7.77	3.35	-6.95
6-31G(d,p)	3.69	-2.10	3.42	-7.75	3.35	-6.93
6-31++G(d,p)	3.70	-5.13	3.43	-11.21	3.36	-10.19
6-311++G(d,p)	3.70	-5.76	3.42 (3.43)[a]	-11.51(-11.82)[a]	3.35	-10.75
NDI dimer						
6-31G(d)	3.79	-1.27	3.36	-9.53	3.35	-8.67
6-31G(d,p)	3.79	-1.31	3.36	-9.65	3.35	-8.74
6-31++G(d,p)	3.76	-2.98	3.38	-11.92	3.37	-11.07
6-311++G(d,p)	3.77	-3.30	3.38	-12.10	3.37	-11.29
NDI-Py dimer						
6-31G(d)	3.39	-11.41	3.35	-12.02	3.30	-12.53
6-31G(d,p)	3.39	-11.37	3.36	-12.00	3.30	-12.50
6-31++G(d,p)	3.41	-14.51	3.37	-15.10	3.31	-15.60
6-311++G(d,p)	3.41	-14.89	3.36	-15.43	3.30	-15.95

[a] ref. 34. R is the interplanar distance (in Å): it is the interplane distance for the stacked configurations. E is the binding energy in kcal·mol^{-1}. The symbols S, SP-L and SP-S, denote the angular configurations of the parallel sandwich, slipped parallel with a shift along the long monomer's axis and slipped parallel with a shift along the short monomer's axis, respectively.

Table S2 Binding energies of NDI-Py dimers in the S, SP-L and SP-S configurations as a function of rotation angles of Py monomer along its z axis. Results are presented for CP-corrected M06-2X/6-311++G(d,p).

Rotation angle (degree)	S configuration (kcal·mol^{-1})	SP-L configuration (kcal·mol^{-1})	SP-S configuration (kcal·mol^{-1})
0 (180)	-14.89	-15.43	-15.95
10 (170)	-14.93	-15.32	-16.01
20 (160)	-14.91	-14.72	-16.29
30 (150)	-14.75	-14.32	-16.26
40 (140)	-15.32	-13.76	-15.14
50 (130)	-16.40	-12.76	-14.30
60 (120)	-16.78	-12.64	-14.48
70 (110)	-16.90	-13.34	-14.84
80 (100)	-16.77	-13.67	-15.37
90	-16.44	-13.79	-15.54

Table S3 The NBO atomic charges (e) of NDI and Py calculated by the M06-2X method with 6-311++G(d,p) basis set.

	NDI		Py
C1	-0.12584	C1	-0.17057
C2	-0.14252	C2	-0.17057
C3	-0.14077	C3	-0.10238
C4	0.05883	C4	0.05445
C5	0.05883	C5	0.05445
C6	-0.15241	C6	-0.10238
C7	-0.15241	C7	-0.10238
C8	-0.12585	C8	-0.17057
C9	-0.14252	C9	-0.17057
C10	-0.14077	C10	-0.10238
C11	0.70798	C11	-0.1737
N12	-0.53414	C12	-0.21462
C13	0.72088	C13	-0.1737
C14	0.70798	C14	-0.1737
N15	-0.53414	C15	-0.21462
C16	0.72088	C16	-0.1737
O17	-0.58637	H17	0.21044
O18	-0.59193	H18	0.21044
O19	-0.58637	H19	0.21044
O20	-0.59193	H20	0.21044
C21	-0.37027	H21	0.20981
C22	-0.37027	H22	0.21298
H23	0.24653	H23	0.20981
H24	0.24687	H24	0.20981
H25	0.24653	H25	0.21298
H26	0.24687	H26	0.20981
H27	0.21387		
H28	0.21387		
H29	0.23543		
H30	0.21387		
H31	0.21387		
H32	0.23543		

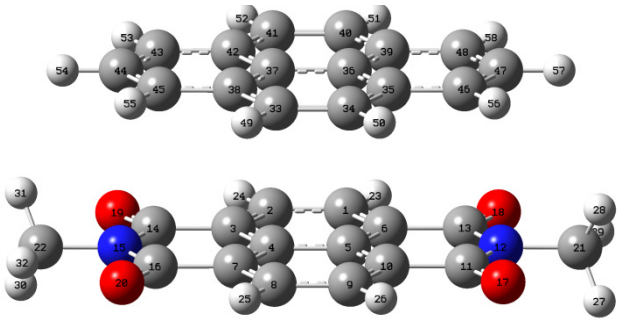

Table S4 The NBO atomic charges (e) of NDI-Py dimers in the sandwich (S) configuration with various rotation angles calculated by the M06-2X method with 6-311++G(d,p) basis set.

	0 (180)	10 (170)	20 (160)	30 (150)	40 (140)	50 (130)	55 (125)	60 (120)	65 (115)	70 (110)
C1	-0.13047	-0.13036	-0.13218	-0.13042	-0.13397	-0.14059	-0.14052	-0.13272	-0.13917	-0.13861
C2	-0.1426	-0.14036	-0.13249	-0.14111	-0.13404	-0.13203	-0.13258	-0.13464	-0.13247	-0.13229
C3	-0.11851	-0.11365	-0.11443	-0.10904	-0.12019	-0.10865	-0.12292	-0.12571	-0.12595	-0.12648
C4	0.01305	0.01346	0.01279	0.01205	0.01214	-0.03078	0.01274	0.01257	0.0126	0.01247
C5	0.01292	0.01339	0.01259	0.01213	0.01203	0.02031	0.01206	0.01275	0.01255	0.01249
C6	-0.11928	-0.12368	-0.12269	-0.12175	-0.11665	-0.1157	-0.1171	-0.11902	-0.11625	-0.11602
C7	-0.11927	-0.12372	-0.12268	-0.12229	-0.1159	-0.10744	-0.11877	-0.11631	-0.11982	-0.11966
C8	-0.13035	-0.13195	-0.1309	-0.13213	-0.1408	-0.13278	-0.13279	-0.1397	-0.13157	-0.13109
C9	-0.14261	-0.13237	-0.1407	-0.13327	-0.13175	-0.13365	-0.13415	-0.13254	-0.13397	-0.13379
C10	-0.11844	-0.1162	-0.11194	-0.11178	-0.1165	-0.11859	-0.12421	-0.1242	-0.12605	-0.12666
C11	0.71896	0.71422	0.71345	0.71253	0.71314	0.71849	0.71867	0.71935	0.71974	0.71979
N12	-0.53647	-0.53537	-0.53523	-0.53531	-0.535	-0.53787	-0.53743	-0.53684	-0.53637	-0.53606
C13	0.71841	0.72343	0.72372	0.7238	0.71913	0.72311	0.71785	0.71744	0.71714	0.71663
C14	0.71897	0.71431	0.7133	0.71271	0.71699	0.71877	0.71881	0.71943	0.71962	0.7197
N15	-0.53639	-0.5352	-0.53522	-0.53523	-0.53737	-0.53723	-0.53687	-0.53659	-0.53696	-0.53663
C16	0.71825	0.72335	0.7236	0.72358	0.7234	0.72329	0.71772	0.71754	0.71655	0.71604
O17	-0.59663	-0.59574	-0.59435	-0.59367	-0.59433	-0.59572	-0.59626	-0.59641	-0.59648	-0.5964
O18	-0.60099	-0.60071	-0.59917	-0.59776	-0.59785	-0.5988	-0.59898	-0.59924	-0.59922	-0.59909
O19	-0.5966	-0.59568	-0.59441	-0.59359	-0.59463	-0.59574	-0.59614	-0.59645	-0.59646	-0.59637
O20	-0.60108	-0.60076	-0.59928	-0.59789	-0.59803	-0.59904	-0.59913	-0.59922	-0.59943	-0.5993
C21	-0.3695	-0.36946	-0.36941	-0.36926	-0.36893	-0.36901	-0.36902	-0.36911	-0.3692	-0.36927
C22	-0.36956	-0.36949	-0.3695	-0.36928	-0.36916	-0.36914	-0.36908	-0.36916	-0.36928	-0.36936
H23	0.24352	0.24348	0.24353	0.24414	0.24465	0.2456	0.24567	0.24512	0.24567	0.24563
H24	0.24368	0.24391	0.24345	0.24409	0.2433	0.24296	0.2429	0.24284	0.24303	0.24331
H25	0.24347	0.24335	0.24356	0.24403	0.24517	0.24496	0.24503	0.24564	0.24505	0.24501
H26	0.24366	0.2433	0.24402	0.24347	0.24336	0.2429	0.24281	0.24288	0.24296	0.24323

H27	0.21398	0.21403	0.21396	0.21397	0.21395	0.21394	0.21393	0.21393	0.21393	0.21392
H28	0.21004	0.20986	0.20966	0.20932	0.20906	0.2091	0.20916	0.20925	0.20938	0.20952
H29	0.23429	0.23439	0.23445	0.23457	0.23452	0.23438	0.23428	0.23421	0.23413	0.23406
H30	0.21398	0.21402	0.21397	0.21397	0.21395	0.21394	0.21393	0.21394	0.21392	0.21392
H31	0.21004	0.20986	0.20966	0.20933	0.20907	0.20912	0.20917	0.20926	0.20937	0.20952
H32	0.23435	0.23445	0.23452	0.23463	0.23458	0.23448	0.23437	0.23426	0.23419	0.23411
C33	-0.17523	-0.17247	-0.19009	-0.18255	-0.16822	-0.17708	-0.17051	-0.17049	-0.17272	-0.17511
C34	-0.19266	-0.17939	-0.18574	-0.17649	-0.19014	-0.18142	-0.20364	-0.18594	-0.18551	-0.18495
C35	0.00097	-0.07808	-0.07266	-0.07189	-0.06395	-0.08023	-0.00367	-0.07542	-0.07312	-0.07249
C36	-0.01046	0.01298	0.01178	0.01279	-0.05551	0.01306	-0.00911	-0.0107	0.00705	0.00732
C37	-0.01052	-0.03297	-0.05459	-0.03374	0.01171	-0.03193	0.00624	0.00654	-0.00852	-0.00841
C38	-0.07696	-0.05926	0.01071	-0.05818	-0.0759	-0.05767	-0.07147	-0.06874	-0.07107	-0.07105
C39	-0.07694	-0.06907	-0.06718	-0.07599	0.01358	-0.06595	-0.07074	0.00782	-0.07133	-0.07125
C40	-0.17516	-0.17257	-0.17311	-0.17068	-0.18887	-0.17748	-0.16967	-0.19931	-0.17341	-0.17584
C41	-0.19265	-0.18187	-0.18377	-0.18645	-0.18325	-0.18228	-0.18557	-0.18463	-0.20405	-0.20369
C42	0.00102	-0.06151	-0.06472	-0.06359	-0.0726	-0.06208	-0.07394	-0.0743	-0.0017	-0.00044
C43	-0.20946	-0.18459	-0.18705	-0.18756	-0.19377	-0.1883	-0.18769	-0.18614	-0.20446	-0.20426
C44	-0.21038	-0.20993	-0.20849	-0.2059	-0.20103	-0.20089	-0.19984	-0.20103	-0.2034	-0.20443
C45	-0.19003	-0.18316	-0.20193	-0.17641	-0.17686	-0.17726	-0.18721	-0.1856	-0.18643	-0.18646
C46	-0.20941	-0.18352	-0.18714	-0.19485	-0.18627	-0.18034	-0.20655	-0.18676	-0.18505	-0.18461
C47	-0.21035	-0.2127	-0.20792	-0.20393	-0.2012	-0.20352	-0.20068	-0.20205	-0.20237	-0.2034
C48	-0.19008	-0.17633	-0.18318	-0.17562	-0.20574	-0.17735	-0.18684	-0.20618	-0.18649	-0.18653
H49	0.21508	0.21403	0.21237	0.21381	0.21448	0.21645	0.21685	0.2177	0.21841	0.21888
H50	0.21394	0.2168	0.21789	0.21786	0.21766	0.21603	0.21409	0.2147	0.21449	0.21457
H51	0.21503	0.21399	0.21333	0.21341	0.21322	0.21643	0.2168	0.21747	0.21836	0.21883
H52	0.2139	0.2167	0.21775	0.21821	0.21718	0.21593	0.21513	0.2148	0.2134	0.21348
H53	0.21832	0.2172	0.2146	0.21293	0.21354	0.21473	0.21554	0.21634	0.21635	0.21686
H54	0.21636	0.21735	0.21886	0.21984	0.22015	0.2194	0.21886	0.21827	0.21775	0.21719
H55	0.2191	0.21808	0.21524	0.21356	0.21278	0.2127	0.21337	0.21362	0.21396	0.21442
H56	0.21831	0.21727	0.21461	0.21339	0.21304	0.21435	0.2148	0.21632	0.21709	0.2176
H57	0.21634	0.21733	0.21877	0.21984	0.22017	0.21938	0.21891	0.21831	0.21765	0.21709
H58	0.21909	0.21761	0.21602	0.21363	0.21245	0.21273	0.21339	0.21288	0.21395	0.21441

	75 (105)	80 (100)	90
C1	-0.13832	-0.13073	-0.13882
C2	-0.13206	-0.13315	-0.12989
C3	-0.12643	-0.12554	-0.1121
C4	0.01224	0.01239	-0.03166
C5	0.01227	0.01253	0.01994

C6	-0.11568	-0.11765	-0.11545
C7	-0.11948	-0.11492	-0.10773
C8	-0.13087	-0.13798	-0.13123
C9	-0.13356	-0.13162	-0.13153
C10	-0.1267	-0.12523	-0.12185
C11	0.7196	0.71913	0.71823
N12	-0.53591	-0.53595	-0.53716
C13	0.71635	0.71632	0.72214
C14	0.7195	0.71928	0.71842
N15	-0.53644	-0.5357	-0.53654
C16	0.71577	0.71632	0.72233
O17	-0.59615	-0.59588	-0.59518
O18	-0.59893	-0.59905	-0.5997
O19	-0.59616	-0.59581	-0.59523
O20	-0.59916	-0.59906	-0.59988
C21	-0.36931	-0.36931	-0.36917
C22	-0.3694	-0.36936	-0.36927
H23	0.24558	0.24488	0.24517
H24	0.24366	0.24391	0.24436
H25	0.24494	0.24538	0.24454
H26	0.24358	0.24394	0.24432
H27	0.21389	0.21387	0.21377
H28	0.20963	0.20968	0.2095
H29	0.23403	0.23403	0.23413
H30	0.21389	0.21387	0.21377
H31	0.20963	0.20968	0.20951
H32	0.23409	0.2341	0.23421
C33	-0.17753	-0.17909	-0.18026
C34	-0.18421	-0.18266	-0.18089
C35	-0.07163	-0.06809	-0.05836
C36	0.00749	0.01505	-0.03093
C37	-0.00841	-0.03197	0.0153
C38	-0.07096	-0.05946	-0.07736
C39	-0.07111	-0.0773	-0.05978
C40	-0.17831	-0.17748	-0.18164
C41	-0.20312	-0.18268	-0.18074
C42	0.00103	-0.05949	-0.06652
C43	-0.20467	-0.18437	-0.18545

C44	-0.20526	-0.20706	-0.20751
C45	-0.1866	-0.17685	-0.17587
C46	-0.18479	-0.18495	-0.18475
C47	-0.20423	-0.2073	-0.20725
C48	-0.18668	-0.17573	-0.17707
H49	0.21894	0.21856	0.21695
H50	0.21494	0.21567	0.2174
H51	0.21889	0.21863	0.21677
H52	0.21386	0.21559	0.21739
H53	0.21709	0.21786	0.21695
H54	0.21678	0.21637	0.21607
H55	0.21495	0.21501	0.21641
H56	0.21784	0.21789	0.21689
H57	0.21668	0.21636	0.21603
H58	0.21494	0.21512	0.2163

Table S5 The NBO atomic charges (e) of NDI-Py dimers in the slipped-parallel L (SP-L) configuration with various rotation angles calculated by the M06-2X method with 6-311++G(d,p) basis set.

	0 (180)	10 (170)	20 (160)	30 (150)	40 (140)	50 (130)	60 (120)	70 (110)	80 (100)	90
C1	-0.13507	-0.12633	-0.12866	-0.13175	-0.13341	-0.14266	-0.13948	-0.13711	-0.1373	-0.138
C2	-0.13832	-0.13666	-0.13244	-0.12843	-0.12588	-0.12453	-0.12568	-0.12781	-0.12954	-0.13009
C3	-0.09814	-0.11912	-0.12245	-0.12557	-0.12652	-0.11355	-0.11098	-0.10956	-0.10955	-0.11035
C4	-0.03349	0.02235	0.0244	0.02642	0.02736	-0.02748	-0.02867	-0.02982	-0.03089	-0.03006
C5	0.02452	-0.02819	-0.03113	-0.03354	-0.03522	0.0192	0.02142	0.02292	0.02307	0.02331
C6	-0.11587	-0.10856	-0.10727	-0.10416	-0.102	-0.11208	-0.11431	-0.11624	-0.11699	-0.11473
C7	-0.10123	-0.10864	-0.10974	-0.11125	-0.11213	-0.10374	-0.10341	-0.10308	-0.10295	-0.1035
C8	-0.13895	-0.14722	-0.14526	-0.14273	-0.14156	-0.13247	-0.1326	-0.13294	-0.13307	-0.13309
C9	-0.1276	-0.12887	-0.13306	-0.13634	-0.13762	-0.13764	-0.13561	-0.13418	-0.13344	-0.13339
C10	-0.12187	-0.10985	-0.10759	-0.10614	-0.10004	-0.1179	-0.11872	-0.11925	-0.11904	-0.11858
C11	0.71801	0.71865	0.71917	0.71974	0.71609	0.71958	0.71823	0.71659	0.7152	0.71513
N12	-0.53708	-0.5363	-0.5363	-0.53715	-0.53746	-0.5383	-0.53695	-0.5367	-0.53697	-0.53671
C13	0.72239	0.72236	0.72118	0.72061	0.72025	0.72022	0.72132	0.723	0.72422	0.72458
C14	0.71258	0.71729	0.71735	0.71667	0.71567	0.71555	0.71635	0.71787	0.71955	0.72099
N15	-0.53484	-0.53686	-0.53714	-0.5369	-0.53646	-0.53542	-0.53582	-0.53633	-0.53641	-0.53613
C16	0.72151	0.72123	0.7214	0.72151	0.72114	0.72124	0.72101	0.72068	0.72005	0.7194
O17	-0.59581	-0.59428	-0.59383	-0.59499	-0.59522	-0.59475	-0.59463	-0.59461	-0.59419	-0.59359
O18	-0.59979	-0.59898	-0.59484	-0.59118	-0.59125	-0.59326	-0.59487	-0.59623	-0.59746	-0.59734

O19	-0.59253	-0.59342	-0.59421	-0.59461	-0.59415	-0.59312	-0.59227	-0.59197	-0.5924	-0.59293
O20	-0.59747	-0.59731	-0.59779	-0.59825	-0.59831	-0.59795	-0.59753	-0.59755	-0.59785	-0.59827
C21	-0.37029	-0.36926	-0.36903	-0.36911	-0.36928	-0.36957	-0.36962	-0.3695	-0.3694	-0.36946
C22	-0.36948	-0.36966	-0.36959	-0.36952	-0.36954	-0.36965	-0.36961	-0.36949	-0.3694	-0.36939
H23	0.24552	0.24522	0.24522	0.24547	0.24647	0.2482	0.24904	0.24919	0.24906	0.24848
H24	0.24275	0.24295	0.24335	0.24378	0.24417	0.24466	0.24506	0.2455	0.24647	0.24766
H25	0.24293	0.24359	0.24359	0.24364	0.24367	0.24301	0.24305	0.2431	0.24311	0.24314
H26	0.24473	0.24429	0.2437	0.24324	0.24295	0.24285	0.24284	0.2429	0.2429	0.24294
H27	0.21093	0.21136	0.21257	0.21368	0.21409	0.2143	0.21427	0.21412	0.21404	0.21408
H28	0.21731	0.21436	0.21142	0.209	0.20879	0.20919	0.20957	0.20986	0.20999	0.21011
H29	0.23354	0.23466	0.23538	0.2355	0.2349	0.23432	0.23402	0.23403	0.23425	0.23449
H30	0.21399	0.21393	0.21382	0.21376	0.21381	0.21391	0.21399	0.21402	0.21401	0.21401
H31	0.2106	0.21083	0.21087	0.2107	0.2105	0.21047	0.21048	0.21039	0.21024	0.21016
H32	0.23466	0.23464	0.23458	0.23459	0.23465	0.23477	0.2348	0.23475	0.23464	0.23451
C33	-0.17256	-0.17482	-0.1858	-0.17426	-0.1798	-0.18621	-0.19564	-0.19622	-0.1915	-0.1977
C34	-0.1802	-0.18023	-0.17354	-0.18641	-0.17744	-0.17584	-0.17177	-0.17063	-0.19124	-0.16595
C35	-0.06028	-0.06397	-0.0664	-0.0666	-0.06843	-0.07926	-0.08446	-0.08148	0.01764	-0.08013
C36	-0.03811	-0.03766	-0.05966	-0.0601	-0.03407	-0.00027	0.02095	0.02255	-0.05031	0.0241
C37	0.01545	0.01505	0.01336	0.01311	0.01263	-0.03753	-0.03465	-0.03507	0.0101	-0.03541
C38	-0.07839	-0.0775	-0.06734	-0.06696	-0.06684	-0.05983	-0.05885	-0.06027	-0.07095	-0.06163
C39	-0.06032	-0.06063	0.0149	0.01843	-0.05831	0.00343	-0.07061	-0.07052	-0.06176	-0.06935
C40	-0.17167	-0.18128	-0.19259	-0.19502	-0.17455	-0.2047	-0.18265	-0.17978	-0.17736	-0.17791
C41	-0.17478	-0.17372	-0.17706	-0.17664	-0.18455	-0.17689	-0.17935	-0.18285	-0.18649	-0.18863
C42	-0.07903	-0.0703	-0.07056	-0.07029	-0.06827	-0.0604	-0.0598	-0.06058	-0.0692	-0.06137
C43	-0.17992	-0.18613	-0.1974	-0.19928	-0.1938	-0.20093	-0.19939	-0.19672	-0.1948	-0.19116
C44	-0.22151	-0.22095	-0.21658	-0.21169	-0.21014	-0.20678	-0.20506	-0.20465	-0.20278	-0.20465
C45	-0.18	-0.17832	-0.17899	-0.1862	-0.18759	-0.18116	-0.18153	-0.18174	-0.19065	-0.1843
C46	-0.17515	-0.18172	-0.19033	-0.18211	-0.17365	-0.17357	-0.15956	-0.16381	-0.20211	-0.17276
C47	-0.21379	-0.21234	-0.20253	-0.19613	-0.19365	-0.20258	-0.20894	-0.21184	-0.21012	-0.21317
C48	-0.17983	-0.16302	-0.19067	-0.19685	-0.17953	-0.19248	-0.17463	-0.17623	-0.17629	-0.17391
H49	0.2139	0.21388	0.21496	0.21598	0.21769	0.21877	0.21878	0.21676	0.21445	0.21409
H50	0.21706	0.21868	0.21859	0.21759	0.21467	0.21348	0.21414	0.21566	0.21619	0.21808
H51	0.21649	0.21516	0.21226	0.21166	0.21278	0.21301	0.21482	0.21631	0.21765	0.21824
H52	0.21373	0.21431	0.21513	0.2161	0.21729	0.21674	0.21565	0.21431	0.21355	0.21389
H53	0.21673	0.21678	0.21644	0.21508	0.21356	0.21363	0.21414	0.21515	0.2161	0.21651
H54	0.217	0.2176	0.21881	0.22018	0.22055	0.21981	0.21867	0.21753	0.21658	0.21614
H55	0.21685	0.21598	0.2149	0.21452	0.21407	0.21364	0.21433	0.21511	0.2162	0.21588
H56	0.21681	0.21523	0.21267	0.21115	0.21116	0.21255	0.21359	0.21484	0.21463	0.21422

H57	0.21637	0.21592	0.21602	0.21605	0.21588	0.21581	0.21558	0.21551	0.2155	0.21536
H58	0.21704	0.21576	0.21373	0.21199	0.21187	0.21017	0.21153	0.21216	0.21302	0.21415

Table S6 The NBO atomic charges (e) of NDI-Py dimers in the slipped-parallel S (SP-S) configuration with various rotation angles calculated by the M06-2X method with 6-311++G(d,p) basis set.

	0 (180)	10 (170)	20 (160)	30 (150)	40 (140)	50 (130)	60 (120)	70 (110)	80 (100)	90
C1	-0.12976	-0.12698	-0.12981	-0.12837	-0.12753	-0.12766	-0.12721	-0.12622	-0.12742	-0.13921
C2	-0.1301	-0.13886	-0.13365	-0.13988	-0.13823	-0.13085	-0.13184	-0.13272	-0.13298	-0.1307
C3	-0.1105	-0.11218	-0.11446	-0.11332	-0.1146	-0.1066	-0.10476	-0.10365	-0.10379	-0.10904
C4	-0.03053	0.021	0.01989	0.01903	0.01953	-0.03196	-0.03175	-0.03233	-0.03412	-0.03446
C5	0.02272	-0.02839	-0.02866	-0.02829	-0.02989	0.02566	0.02621	0.02783	0.02889	0.02919
C6	-0.11463	-0.11192	-0.10815	-0.11253	-0.11315	-0.12346	-0.12663	-0.12813	-0.12921	-0.11964
C7	-0.10349	-0.11737	-0.11556	-0.11473	-0.11472	-0.10013	-0.10797	-0.10976	-0.10479	-0.1047
C8	-0.13505	-0.13602	-0.13637	-0.13932	-0.13843	-0.13398	-0.13046	-0.1288	-0.1292	-0.13194
C9	-0.1354	-0.13523	-0.14372	-0.1357	-0.1369	-0.1477	-0.14836	-0.1475	-0.14445	-0.13153
C10	-0.11891	-0.1033	-0.10211	-0.10412	-0.10351	-0.11067	-0.1105	-0.11184	-0.11514	-0.12674
C11	0.71614	0.71547	0.71507	0.71565	0.71585	0.71549	0.71553	0.71596	0.71642	0.71623
N12	-0.53533	-0.53584	-0.53708	-0.53678	-0.53665	-0.53655	-0.53625	-0.53597	-0.53633	-0.53644
C13	0.72007	0.72462	0.7245	0.72308	0.72142	0.71922	0.71816	0.71863	0.71953	0.72026
C14	0.72052	0.7203	0.72002	0.71972	0.71915	0.71852	0.71875	0.71965	0.71926	0.7188
N15	-0.53553	-0.53608	-0.53656	-0.53637	-0.53628	-0.53557	-0.53646	-0.5363	-0.53482	-0.53508
C16	0.72043	0.72159	0.72306	0.72393	0.72396	0.72024	0.72303	0.72266	0.71918	0.72269
O17	-0.59418	-0.59426	-0.59406	-0.59368	-0.59306	-0.59243	-0.59241	-0.59298	-0.59369	-0.5942
O18	-0.59635	-0.59676	-0.59753	-0.59694	-0.59636	-0.59627	-0.5969	-0.59787	-0.59862	-0.59867
O19	-0.59182	-0.59239	-0.59343	-0.59316	-0.59241	-0.59282	-0.59413	-0.59431	-0.59413	-0.59432
O20	-0.59887	-0.59869	-0.59906	-0.59949	-0.59932	-0.5983	-0.59773	-0.59797	-0.59886	-0.59902
C21	-0.36977	-0.36977	-0.36977	-0.36987	-0.36991	-0.36988	-0.36997	-0.37002	-0.36999	-0.3698
C22	-0.36939	-0.36949	-0.36957	-0.36968	-0.36937	-0.36904	-0.36958	-0.37016	-0.36998	-0.36957
H23	0.24658	0.24642	0.24651	0.24701	0.24695	0.24667	0.24615	0.24525	0.24432	0.24411
H24	0.24626	0.24721	0.24699	0.24749	0.24692	0.24606	0.2463	0.24655	0.24652	0.24652
H25	0.24353	0.24364	0.24369	0.24365	0.24375	0.24415	0.24488	0.24562	0.24625	0.24666
H26	0.24331	0.24315	0.24364	0.24294	0.2429	0.24356	0.24351	0.2434	0.24339	0.24322
H27	0.21443	0.21433	0.21423	0.21418	0.2141	0.21402	0.21396	0.21387	0.2137	0.21362
H28	0.2099	0.20989	0.20997	0.21041	0.21085	0.21111	0.2113	0.21143	0.21145	0.21133
H29	0.23453	0.23447	0.2345	0.23458	0.23455	0.23452	0.23451	0.23452	0.23451	0.2345
H30	0.21413	0.21411	0.21416	0.2141	0.21417	0.21444	0.21443	0.21424	0.21405	0.21387
H31	0.21021	0.211	0.21109	0.21091	0.20995	0.20863	0.20934	0.21094	0.2114	0.21095

H32	0.23429	0.23421	0.23425	0.23441	0.23463	0.23474	0.23443	0.23405	0.23385	0.23405
C33	-0.18105	-0.18559	-0.18369	-0.18244	-0.18388	-0.17326	-0.1748	-0.17474	-0.17933	-0.18386
C34	-0.19545	-0.17991	-0.18073	-0.18102	-0.19764	-0.18587	-0.20391	-0.19645	-0.18599	-0.18358
C35	-0.0034	-0.06178	-0.06102	-0.05947	0.00307	-0.06027	0.004	-0.06811	-0.07832	-0.0686
C36	-0.05002	-0.03272	-0.03531	-0.03459	-0.05259	-0.03223	-0.04956	0.01418	0.01283	0.01219
C37	0.01428	0.01476	0.0129	0.01138	0.00906	0.00759	0.00565	-0.03499	-0.03292	-0.03243
C38	-0.07353	-0.07297	-0.07166	-0.07028	-0.07015	-0.07769	-0.07813	-0.06225	-0.0617	-0.06222
C39	-0.05922	-0.05524	-0.05389	-0.05288	-0.05416	-0.05507	-0.05905	-0.07532	-0.06922	-0.0812
C40	-0.1848	-0.18701	-0.18802	-0.18744	-0.18589	-0.17831	-0.1708	-0.17114	-0.17308	-0.17883
C41	-0.17182	-0.16801	-0.16543	-0.16231	-0.16242	-0.1704	-0.18082	-0.18462	-0.19093	-0.17784
C42	-0.07741	-0.07778	-0.0677	-0.06976	-0.07299	-0.07342	-0.07101	-0.06478	-0.06665	-0.06311
C43	-0.16802	-0.17123	-0.18834	-0.19299	-0.19438	-0.18757	-0.19005	-0.18024	-0.16584	-0.17531
C44	-0.21036	-0.2169	-0.21337	-0.20999	-0.2059	-0.20201	-0.1968	-0.2001	-0.20519	-0.20737
C45	-0.19872	-0.18951	-0.18777	-0.18344	-0.18054	-0.18064	-0.1808	-0.17887	-0.18432	-0.17751
C46	-0.21558	-0.19985	-0.19365	-0.19635	-0.21041	-0.18987	-0.2046	-0.17909	-0.17795	-0.18568
C47	-0.20941	-0.20103	-0.19793	-0.19652	-0.20151	-0.20549	-0.20954	-0.21229	-0.21168	-0.2076
C48	-0.16964	-0.17296	-0.1777	-0.18063	-0.18294	-0.18171	-0.17922	-0.17512	-0.1731	-0.16662
H49	0.21631	0.21632	0.21591	0.21575	0.21598	0.21593	0.2164	0.21652	0.21627	0.21559
H50	0.21521	0.21665	0.21653	0.21593	0.21394	0.21371	0.21249	0.21433	0.2149	0.21587
H51	0.21445	0.21379	0.21357	0.21369	0.21421	0.21532	0.21705	0.21853	0.21744	0.21507
H52	0.21403	0.21528	0.21658	0.21744	0.21695	0.21511	0.21318	0.21287	0.21483	0.21624
H53	0.21604	0.21727	0.21709	0.21478	0.21292	0.21262	0.21429	0.21581	0.21657	0.2172
H54	0.21564	0.21541	0.21706	0.21902	0.22049	0.22062	0.21934	0.21774	0.21658	0.216
H55	0.21688	0.21825	0.21863	0.21729	0.21514	0.21354	0.21274	0.21276	0.21406	0.21462
H56	0.21543	0.21419	0.21309	0.21353	0.21366	0.21578	0.21618	0.2166	0.21592	0.21527
H57	0.21686	0.21834	0.21959	0.21984	0.21921	0.2179	0.21689	0.21611	0.21582	0.21599
H58	0.21588	0.21434	0.21324	0.21261	0.2124	0.21258	0.21328	0.21461	0.21583	0.21675

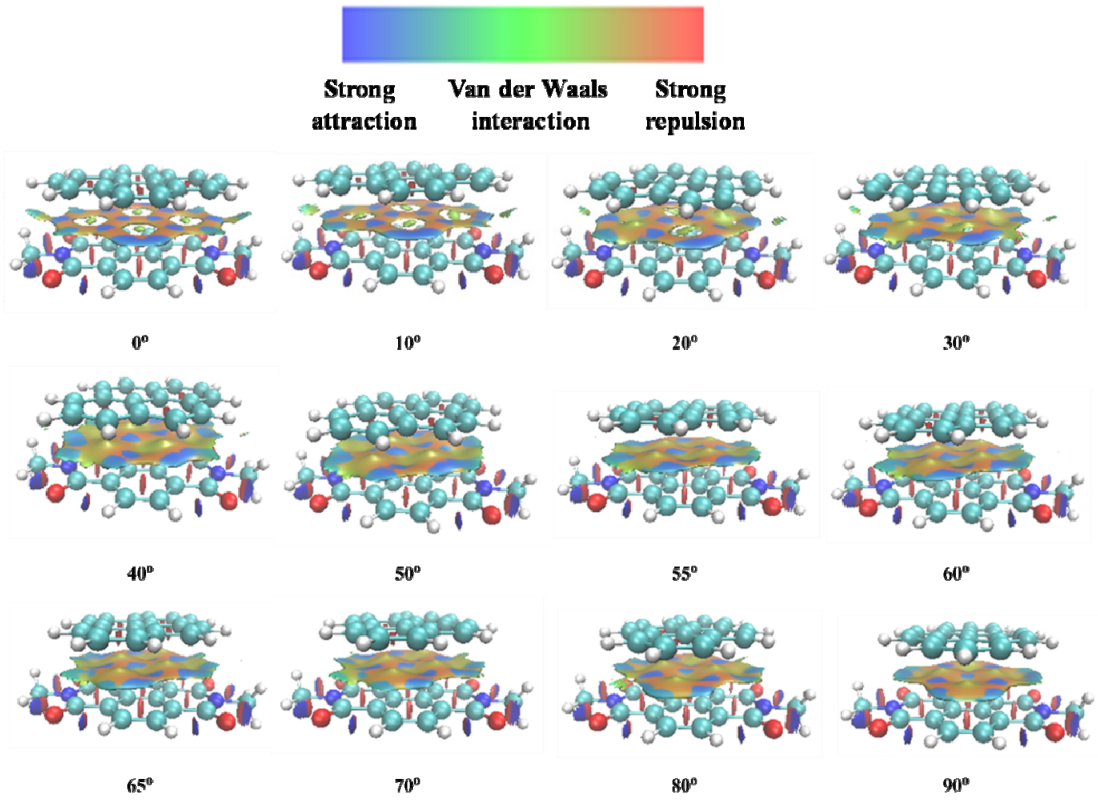

Fig. S1 Visualization of the weak interactions for NDI-Py dimers in the S configuration (side view) in real space. The scale runs from -0.008 (min) to 0.008 (max).

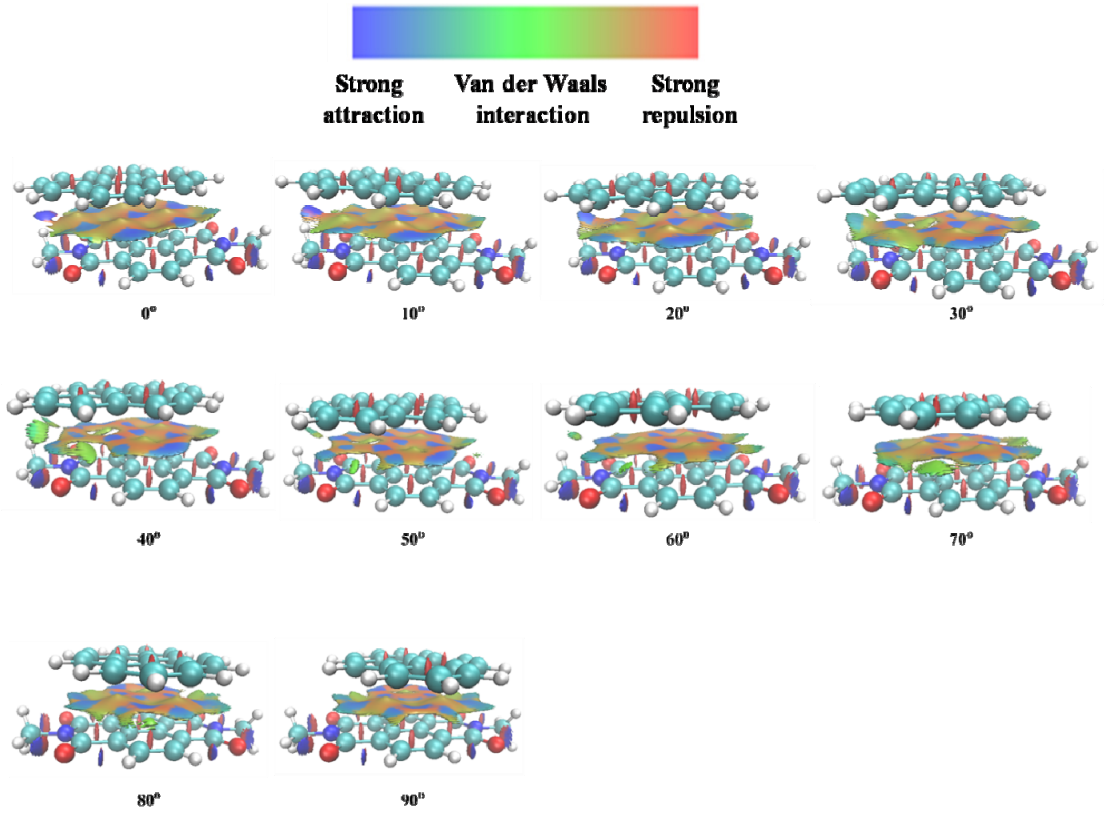

Fig. S2 Visualization of the weak interactions for NDI-Py dimers in the SP-L configuration (side view) in real space. The scale runs from -0.008 (min) to 0.008 (max).

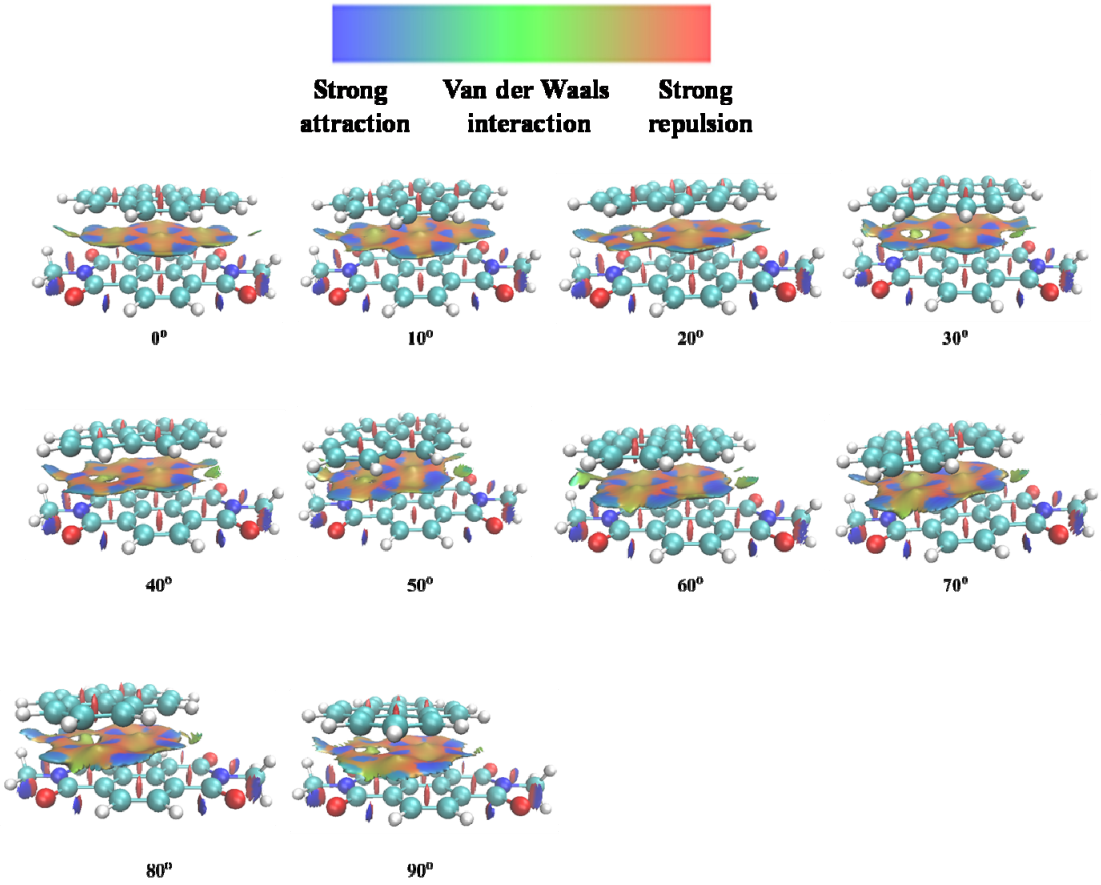

Fig. S3 Visualization of the weak interactions for NDI-Py dimers in the SP-S configuration (side view) in real space. The scale runs from -0.008 (min) to 0.008 (max).