

Electronic Supplementary Information for

Theoretical study on molecular packing and electronic structure of bi-1,3,4-oxadiazole derivative

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Contents

Figure S1 The UV-vis absorption spectrum of BOXD-NP in CHL solution ($\sim 10^{-5}$ M).

Figure S2 Evolution of the Oscillation strength (INDO/6-31G**) of the lowest two excited states of BOXD-NP dimer over y -displacement (with x -displacement fixed at 0 Å).

Table S1 Electronic process of BOXD-NP calculated with different methods.

Table S2 The single point energies of BOXD-NP dimers (M062x/6-31G** method).

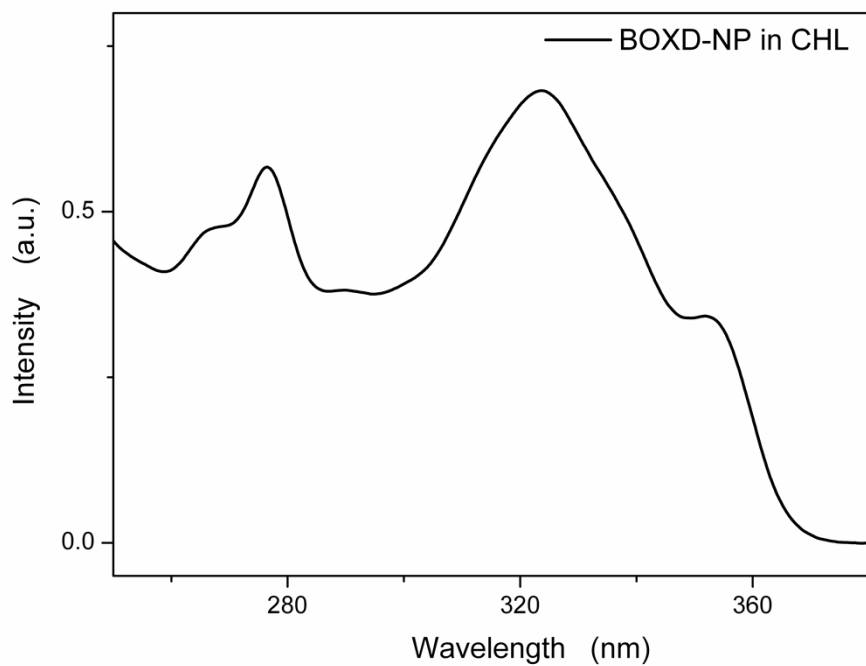


Figure S1 The UV-vis absorption spectrum of BOXD-NP in CHL solution ($\sim 10^{-5}$ M).

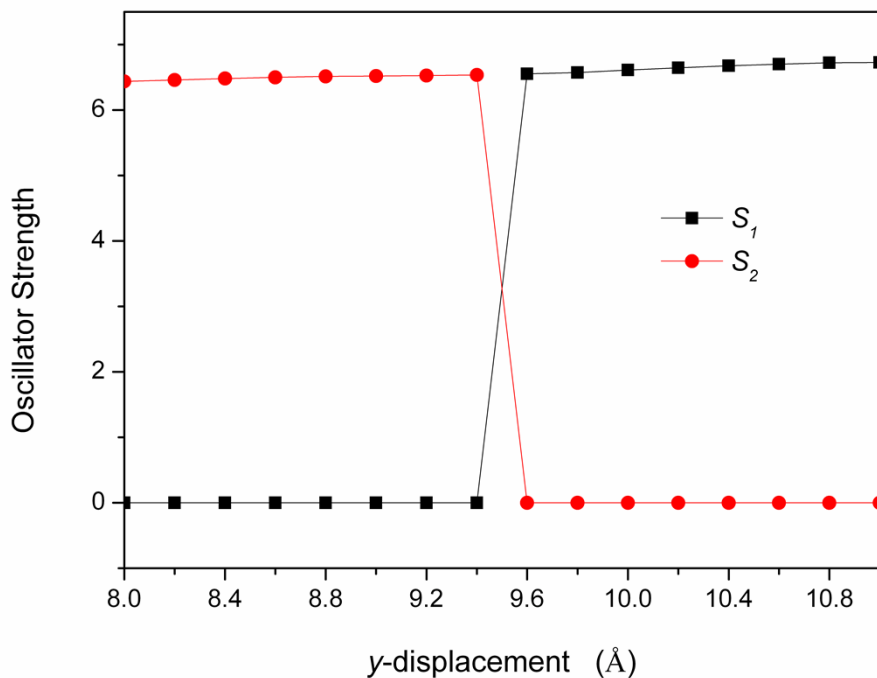


Figure S2 Evolution of the Oscillation strength (INDO/6-31G**) of the lowest two excited states of BOXD-NP dimer over y -displacement (with x -displacement fixed at 0 Å).

Table S1 Electronic process of BOXD-NP calculated with different methods.

	B3LYP/6-311+G**				M062x/6-311+G**				CAM-B3LYP			
	GAS		CHL		GAS		CHL		GAS		CHL	
S ₁	3.3910 eV	365.63 nm	3.2519 eV	381.27 nm	4.1205 eV	300.89 nm	4.0216 eV	308.30 nm	4.0719 eV	304.48 nm	3.9698 eV	312.32 nm
	(1.0632)		(1.1159)		(1.3170)		(1.5043)		f=1.3203		f=1.5063	
	101->102	0.69731	101->102	0.69640	99->104	-0.12001	99->102	0.11694	99->104	-0.12437	99->102	0.13705
					100->103		99->104	-0.10409	100->103	0.29476	99->104	0.10338
					0.28292		100->103	-0.28522	101->102	0.59262	100->103	-0.29482
				101->102		101->102	0.59952			101->102	0.58618	
				0.60297								
S ₂	3.5976 eV	344.63 nm	3.4599 eV	358.35 nm	4.3021 eV	288.20 nm	4.2171 eV	294.01 nm	4.2609 eV	290.98 nm	4.1732 eV	297.10 nm
	(0)		(0)		(0)		(0)		f=0.0000		f=0.0000	
	99->103	-0.14678	99->103	0.11231	98->102	-0.12821	98->104	0.13658	98->102	-0.11012	98->104	-0.13585
	100->102	0.67043	100->102	0.68722	98->104	-0.17032	99->103	0.20483	98->104	-0.17413	99->103	0.19911
					99->103	-0.27219	100->102	0.49525	99->103	-0.26626	100->102	0.47923
					100->102	0.47011	100->106	0.12558	100->102	0.46029	100->104	-0.11763
					100->106	0.13873	101->103	-0.35841	100->106	0.14483	100->106	0.12516
					101->103	0.28630	101->105	-0.15763	101->103	0.30725	101->103	-0.37181
				101->105	0.20617			101->105	0.19037	101->105	-0.14259	
S ₃	3.8500 eV	322.04 nm	3.7724 eV	328.66 nm	4.4222 eV	280.37 nm	4.3963 eV	282.02 nm	4.3824 eV	282.91 nm	4.3499 eV	285.03 nm
	(0.3296)		(0.4787)		(0.2955)		(0.4064)		f=0.2833		f=0.3833	
	98->103	0.17182	98->103	0.15569	98->103	0.33715	98->103	0.33333	97->104	-0.10385	98->103	0.33441
	99->102	0.61365	99->102	0.65542	99->102	0.45347	99->102	0.47918	98->103	0.34131	99->102	0.46880
	100->103	-0.12511	100->103	0.10444	100->105	-0.24241	99->104	0.13786	99->102	0.44807	99->104	-0.15989
100->105	-0.13231	101->104	0.11164	101->104	0.18985	100->103	0.14386	99->104	0.12264	100->103	0.15958	

	101->104	-0.20424			101->106	-0.18047	100->105	0.20562	100->103	-0.10390	100->105	0.19800
							101->104	0.10457	100->105	-0.23737	101->106	-0.19943
							101->106	-0.19067	101->104	0.15833		
									101->106	-0.19544		
S₄	3.9210 eV	316.20 nm	3.8669 eV	320.63 nm	4.5273 eV	273.86 nm	4.5073 eV	275.08 nm	4.4911 eV	276.07 nm	4.4672 eV	277.55 nm
	(0)		(0)		(0)		(0)		f=0.0000		f=0.0000	
	101->103	0.68331	100->104	-0.10921	98->102	0.27365	98->102	0.30811	98->102	0.28503	98->102	0.31402
			101->103	0.68460	99->103	0.20517	98->104	0.14654	98->104	0.11243	98->104	-0.16578
					99->105	0.10831	99->103	0.28221	99->103	0.21899	99->103	0.29260
					100->102	0.12677	100->104	-0.27027	99->105	0.11551	100->104	0.25287
					100->104	0.30112	100->106	0.15662	100->102	0.10566	100->106	0.18144
					100->106	-0.12013	101->103	0.33031	100->104	0.29561	101->103	0.29969
					101->103	0.40316	101->105	-0.26318	100->106	-0.14604	101->105	-0.26566
					101->105	-0.24064			101->103	0.37071		
									101->105	-0.24846		
S₅	4.0765 eV	304.14 nm	3.9900 eV	310.74 nm	4.7644 eV	260.23 nm	4.7004 eV	263.77 nm	4.7336 eV	261.92 nm	4.6693 eV	265.53 nm
	(0.0860)		(0.0889)		(0.6256)		(0.5227)		f=0.5951		f=0.4829	
	99->102	0.17433	99->102	-0.12503	97->102	-0.15098	97->102	-0.15170	97->102	-0.16701	97->102	0.16607
	99->104	0.12251	99->104	0.11811	99->102	-0.22239	99->102	-0.15598	99->102	-0.20804	99->102	0.14496
	100->103	0.66003	100->103	0.66271	99->106	0.10210	99->106	0.10168	99->106	0.11883	99->106	-0.11631
					100->103	0.37132	100->103	-0.35411	100->103	0.34870	100->103	0.33026
					100->105	-0.22340	100->105	0.26189	100->105	-0.24253	100->105	-0.27777
					101->104	0.46181	101->104	0.48118	101->104	0.46087	101->104	0.47209
S₆	4.1291 eV	300.27 nm	4.0780 eV	304.03 nm	5.2767 eV	234.96 nm	5.1174 eV	242.28 nm	5.2909 eV	234.33 nm	5.1081 eV	242.72 nm
	(0)		(0)		(0)		(0)		f=0.0000		f=0.0000	
	98->102	0.42293	98->102	0.54328	98->102	0.30216	98->102	0.33802	98->102	0.35468	98->102	-0.33388

	99->103	0.27088	99->103	0.23398	99->103	0.14999	99->103	0.27284	99->103	0.25091	99->103	-0.26908
	100->102	0.18792	100->102	-0.12341	100->102	0.43083	100->102	-0.29525	100->102	0.31587	100->102	0.26747
	100->104	-0.18973	100->104	-0.14314	100->104	-0.24466	100->104	0.36228	100->104	-0.35270	100->104	0.36796
	100->106	-0.16817	100->106	-0.15438	100->106	-0.13224	101->103	-0.16906	101->103	-0.13401	101->103	0.11599
	101->105	-0.35498	101->105	-0.27129	101->103	-0.30366	101->105	0.18746	101->105	0.17019	101->105	-0.23263
S₇	4.2203 eV	293.78 nm	4.1822 eV	296.45 nm	5.3495 eV	231.77 nm	5.2607 eV	235.68 nm	5.3948 eV	229.82 nm	5.3113 eV	233.44 nm
	(0.2270)		(0.1257)		(0)		(0)		f=0.0000		f=0.0000	
	99->102	0.24852	99->102	-0.16043	97->103	0.12280	97->103	0.12700	97->103	0.15677	97->103	0.13121
	100->105	0.12479	100->105	0.14076	98->102	0.19928	99->103	0.17393	99->103	0.20934	99->103	0.15604
	101->104	0.63006	101->104	0.65420	99->103	0.30314	100->102	0.35457	100->102	-0.33263	100->102	0.38540
					100->102	-0.15079	100->106	-0.24118	100->106	0.23061	100->106	-0.26813
					100->104	-0.27134	101->103	0.34283	101->103	0.33179	101->103	0.31965
					100->106	0.15016	101->105	0.35176	101->105	0.34668	101->105	0.32439
					101->103	0.24878						
					101->105	0.38456						

Table S2 The single point energies of BOXD-NP dimers (M062x/6-31G** method).

y \ x	0	0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6	1.8	2.0
0	1.04792	0.31423	-1.63234	-4.27983	-7.10833	-9.58959	-11.35867	-12.45107	-12.9014	-12.60609	-11.88555
0.2	0.1964	-0.45828	-2.2594	-4.75599	-7.43227	-9.71107	-11.29831	-12.2982	-12.71848	-12.48338	-11.81341
0.4	-2.00812	-2.53387	-4.06025	-6.21474	-8.49706	-10.38966	-11.65813	-12.42008	-12.64887	-12.31931	-11.64
0.6	-4.94085	-5.34884	-6.54704	-8.23843	-9.98913	-11.40906	-12.28459	-12.67726	-12.61032	-12.09897	-11.36824
0.8	-7.92772	-8.23405	-9.09036	-10.28794	-11.5263	-12.42191	-12.86144	-12.88273	-12.48297	-11.80006	-11.00851
1.0	-10.34273	-10.53255	-11.08499	-11.93637	-12.74217	-13.15601	-13.16093	-12.8244	-12.18519	-11.37137	-10.55005
1.2	-11.83473	-11.97763	-12.3572	-12.97316	-13.50261	-13.58011	-13.22567	-12.58427	-11.78053	-10.8895	-10.07758
1.4	-12.42932	-12.65849	-13.02309	-13.50059	-13.83674	-13.70786	-13.11673	-12.29805	-11.40565	-10.51969	-9.74805
1.6	-12.3389	-12.76665	-13.19815	-13.63547	-13.84848	-13.59966	-12.96743	-12.12109	-11.23068	-10.36552	-9.6099
1.8	-11.70382	-12.38494	-12.99111	-13.45356	-13.64539	-13.43576	-12.8966	-12.15078	-11.33443	-10.52039	-9.79467
2.0	-10.94087	-11.86082	-12.63706	-13.1824	-13.42617	-13.34333	-12.96665	-12.37377	-11.6895	-10.96116	-10.25954
2.2	-10.50221	-11.56967	-12.4607	-13.06054	-13.38318	-13.43278	-13.20936	-12.75975	-12.19421	-11.53674	-10.84521
2.4	-10.54961	-11.66934	-12.57918	-13.15257	-13.45473	-13.59508	-13.49703	-13.16435	-12.71737	-12.11332	-11.42164
2.6	-11.02581	-12.09629	-12.9404	-13.40369	-13.63918	-13.76639	-13.73302	-13.46873	-13.06664	-12.53323	-11.85769
2.8	-11.80884	-12.72472	-13.41707	-13.7282	-13.83735	-13.8816	-13.76759	-13.50066	-13.14968	-12.6915	-12.08508
3.0	-12.65964	-13.35254	-13.81318	-13.97279	-13.92501	-13.77981	-13.52192	-13.1972	-12.88829	-12.51187	-12.00751
3.2	-13.32496	-13.78343	-13.98982	-13.92139	-13.6928	-13.34438	-12.94723	-12.57672	-12.26884	-11.98665	-11.61477
3.4	-13.69468	-13.94894	-13.90096	-13.57987	-13.12081	-12.59075	-12.11266	-11.72344	-11.4411	-11.25382	-10.98818
3.6	-13.81902	-13.87897	-13.62805	-13.09229	-12.43391	-11.78213	-11.24236	-10.85497	-10.61137	-10.48668	-10.27195
3.8	-13.71467	-13.64145	-13.27031	-12.618	-11.87759	-11.16207	-10.57822	-10.19558	-9.988	-9.85498	-9.64765
4.0	-13.49038	-13.37856	-12.97277	-12.33335	-11.61925	-10.8919	-10.29714	-9.90459	-9.68373	-9.51327	-9.27495
4.2	-13.25785	-13.14367	-12.80478	-12.2887	-11.68612	-11.0547	-10.49973	-10.08869	-9.78067	-9.52512	-9.17794
4.4	-13.0624	-13.01827	-12.80267	-12.45355	-12.01831	-11.54626	-11.07343	-10.64453	-10.25694	-9.85918	-9.34572

4.6	-12.98481	-13.02888	-12.94914	-12.75884	-12.51154	-12.198	-11.79277	-11.37435	-10.90652	-10.33743	-9.65688
4.8	-13.04072	-13.12701	-13.14073	-13.10424	-13.00103	-12.79918	-12.47179	-12.01573	-11.435	-10.73214	-9.91405
5.0	-13.20418	-13.27379	-13.32165	-13.36172	-13.34553	-13.19795	-12.88846	-12.41155	-11.77465	-10.96828	-10.04098
5.2	-13.40637	-13.40915	-13.42553	-13.45705	-13.45218	-13.33044	-13.03919	-12.57393	-11.90752	-11.02491	-10.02098
5.4	-13.54794	-13.45503	-13.39348	-13.36031	-13.29789	-13.13936	-12.88037	-12.44535	-11.79664	-10.89731	-9.85278
5.6	-13.57938	-13.33157	-13.16938	-13.05992	-12.94806	-12.77682	-12.53181	-12.13337	-11.4949	-10.61441	-9.55525
5.8	-13.48994	-13.09509	-12.83225	-12.67367	-12.55522	-12.40185	-12.18854	-11.80507	-11.16038	-10.28221	-9.21374
6.0	-13.32087	-12.85923	-12.55751	-12.39755	-12.30601	-12.18487	-11.98319	-11.60359	-10.94008	-10.03931	-8.94029
6.2	-13.08344	-12.65719	-12.40298	-12.30192	-12.27745	-12.21748	-12.03789	-11.63974	-10.94873	-9.99495	-8.84454
6.4	-12.79651	-12.50986	-12.38999	-12.41268	-12.49435	-12.50362	-12.35152	-11.93283	-11.20009	-10.16854	-8.94629
6.6	-12.52898	-12.42275	-12.46615	-12.65621	-12.88436	-12.97603	-12.83875	-12.38638	-11.6067	-10.48834	-9.18553
6.8	-12.3009	-12.37271	-12.60689	-12.96635	-13.30618	-13.46417	-13.34592	-12.85007	-12.00768	-10.81889	-9.43255
7.0	-12.14789	-12.3646	-12.75613	-13.23003	-13.63547	-13.82446	-13.68385	-13.14361	-12.25023	-11.02905	-9.61019
7.2	-12.12669	-12.4283	-12.8689	-13.36493	-13.76409	-13.89979	-13.69019	-13.12846	-12.22933	-11.01478	-9.62223
7.4	-12.22847	-12.50907	-12.91587	-13.33389	-13.61601	-13.66971	-13.41977	-12.83853	-11.93393	-10.7633	-9.42492
7.6	-12.40387	-12.59765	-12.87852	-13.14956	-13.28324	-13.24409	-12.9371	-12.30618	-11.42549	-10.32727	-9.0745
7.8	-12.54162	-12.62301	-12.74346	-12.8382	-12.83866	-12.67973	-12.28572	-11.64427	-10.78755	-9.75555	-8.62047
8.0	-12.5214	-12.52592	-12.51942	-12.4637	-12.32073	-12.0262	-11.56953	-10.91517	-10.0838	-9.14437	-8.1137
8.2	-12.37285	-12.32325	-12.2475	-12.08166	-11.80887	-11.40656	-10.88727	-10.21127	-9.42216	-8.55486	-7.61008
8.4	-12.11926	-12.09262	-11.9871	-11.74625	-11.38603	-10.9058	-10.32384	-9.63781	-8.88755	-8.078	-7.21351
8.6	-11.78331	-11.82238	-11.75003	-11.51211	-11.1246	-10.59931	-9.97873	-9.28013	-8.54307	-7.76983	-6.95007
8.8	-11.43669	-11.57754	-11.5742	-11.3837	-10.99787	-10.46413	-9.84616	-9.14094	-8.38904	-7.62057	-6.82069
9.0	-11.09917	-11.38034	-11.47715	-11.35237	-10.99272	-10.47004	-9.85509	-9.14097	-8.36139	-7.57884	-6.78433
9.2	-10.8915	-11.25718	-11.41691	-11.34854	-11.03208	-10.54032	-9.92313	-9.18173	-8.3875	-7.59352	-6.80943
9.4	-10.79415	-11.19206	-11.3522	-11.28585	-10.9966	-10.53086	-9.91619	-9.1908	-8.42431	-7.64546	-6.86243

9.6	-10.80193	-11.15816	-11.27548	-11.14998	-10.84721	-10.39527	-9.78976	-9.09251	-8.36393	-7.6327	-6.90601
9.8	-10.84902	-11.09739	-11.12249	-10.9472	-10.5887	-10.10743	-9.52688	-8.54274	-8.18718	-7.53597	-6.89044
10.0	-10.85074	-10.95615	-10.85781	-10.57606	-10.14306	-9.64006	-9.1027	-8.29861	-7.96313	-7.40689	-6.84852
10.2	-10.73278	-10.67852	-10.43776	-10.02852	-9.53862	-9.02869	-8.55315	-8.12704	-7.69443	-7.24677	-6.80649
10.4	-10.47219	-10.25962	-9.88182	-9.37145	-8.83475	-8.33171	-7.95514	-7.66932	-7.38423	-7.07608	-6.74374
10.6	-10.1176	-9.77304	-9.26888	-8.68619	-8.13025	-7.69332	-7.4097	-7.23643	-7.09301	-6.91437	-6.66907
10.8	-9.74405	-9.33105	-8.75786	-8.13754	-7.60393	-7.24294	-7.03723	-6.9436	-6.89997	-6.79036	-6.58537
11.0	-9.44368	-9.02653	-8.46286	-7.87907	-7.38799	-7.05932	-6.89705	-6.83694	-6.81414	-6.70931	-6.50674