

## Supporting Information

# Facile Charge Transfer between Barbituric Acid and Chloranilic Acid over g-C<sub>3</sub>N<sub>4</sub>: Synthesis, Characterization and DFT Study

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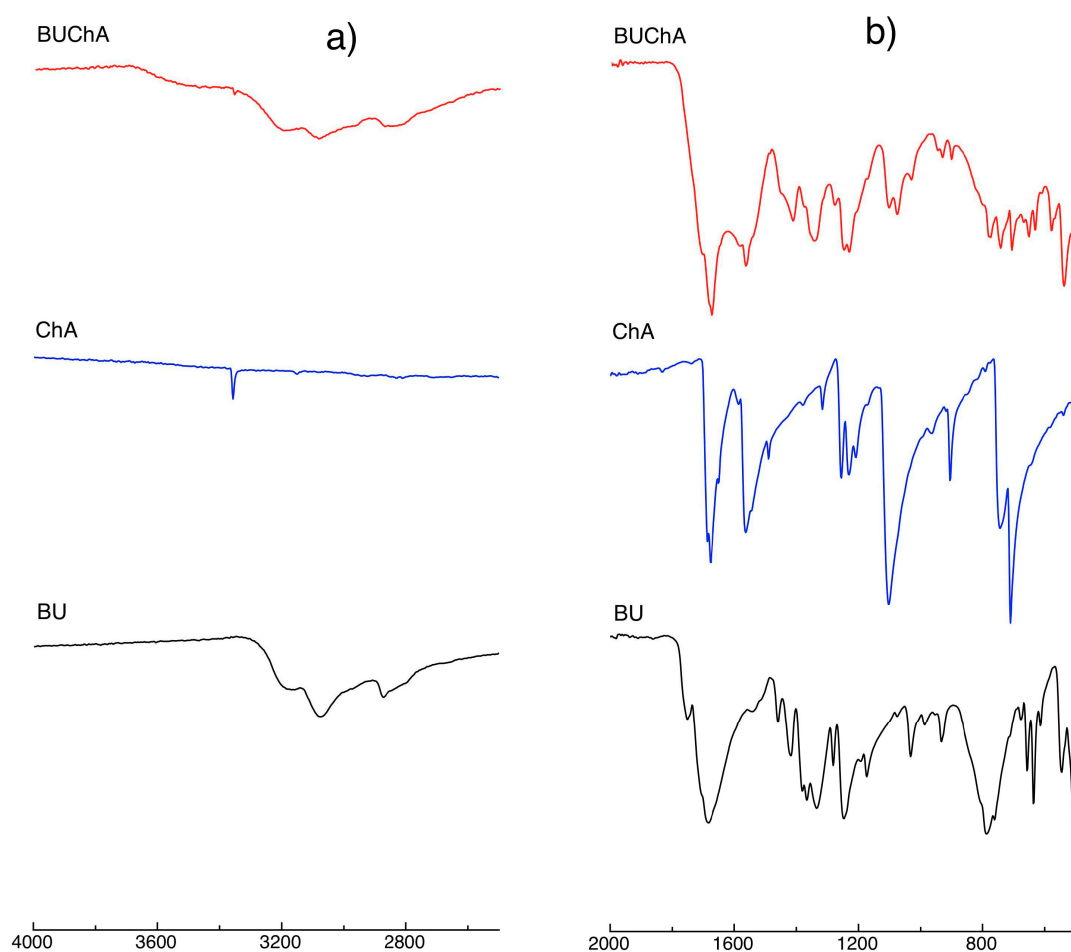


Figure S1: the selected area of FTIR of BU and ChA a) 2500-4000  $\text{cm}^{-1}$  and b) a) 500-2000  $\text{cm}^{-1}$ .

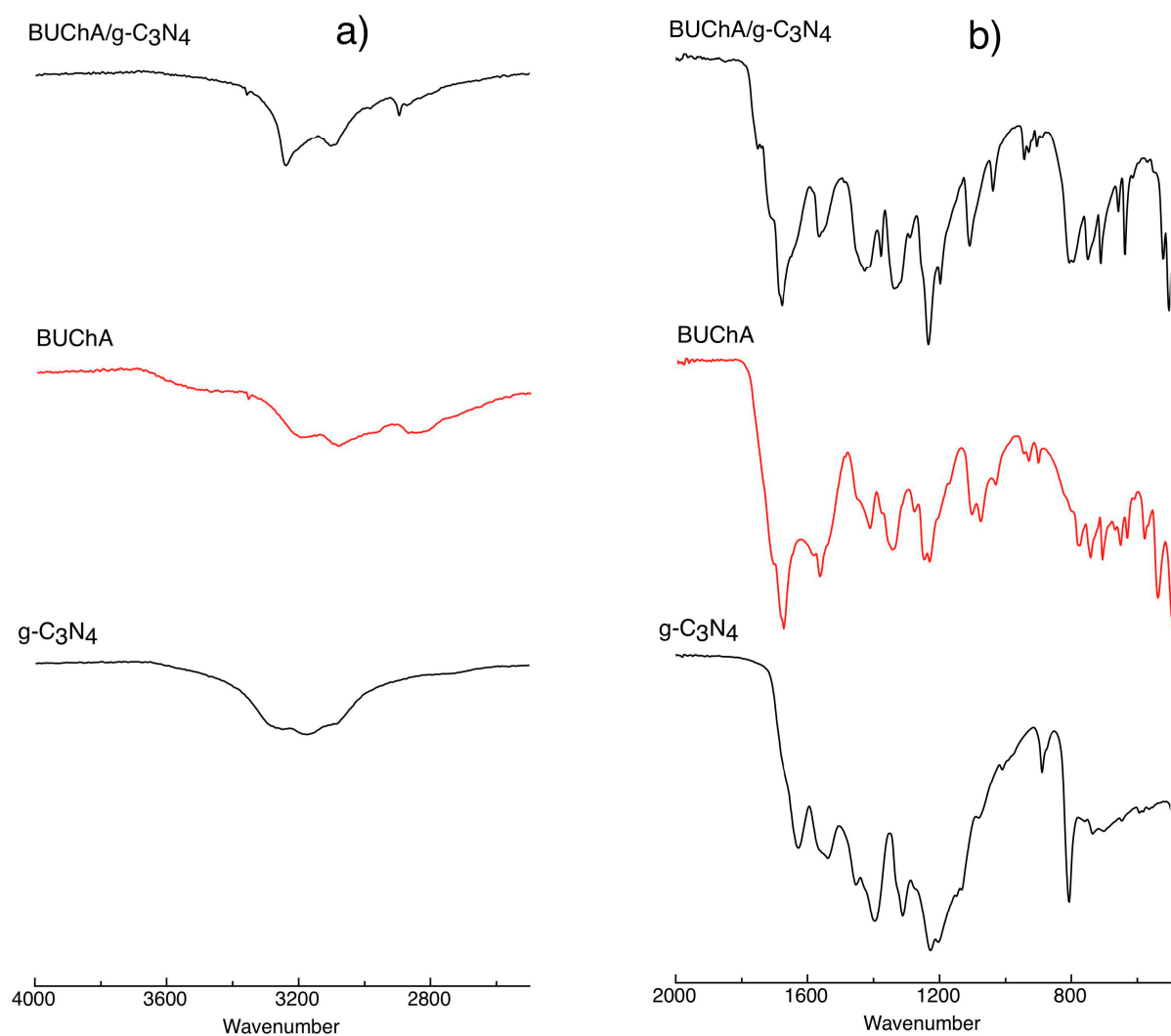


Figure S2: FTIR of BUCHA over g-C<sub>3</sub>N<sub>4</sub> nanosheet a) 2500-4000  $\text{cm}^{-1}$  and b) a) 500-2000  $\text{cm}^{-1}$ .

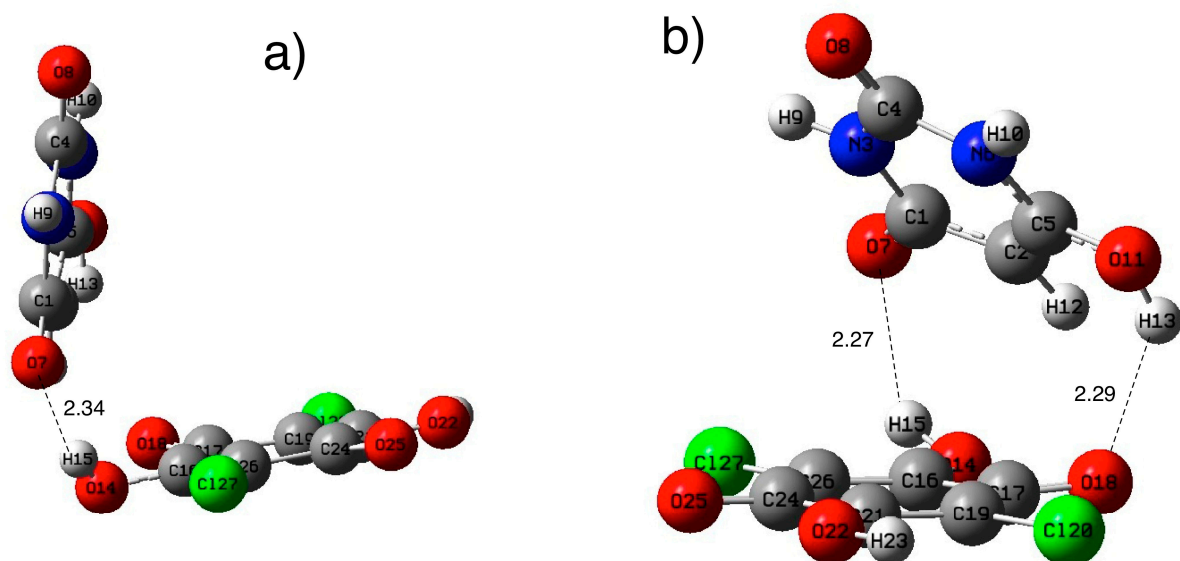


Figure S3: optimized structure of a) T-shaped BUCChA-III and b)  $\pi$ - $\pi$  stacking BUCChA-IV in the gas phase calculated at wB97XD/def2tzvpp level of theory.

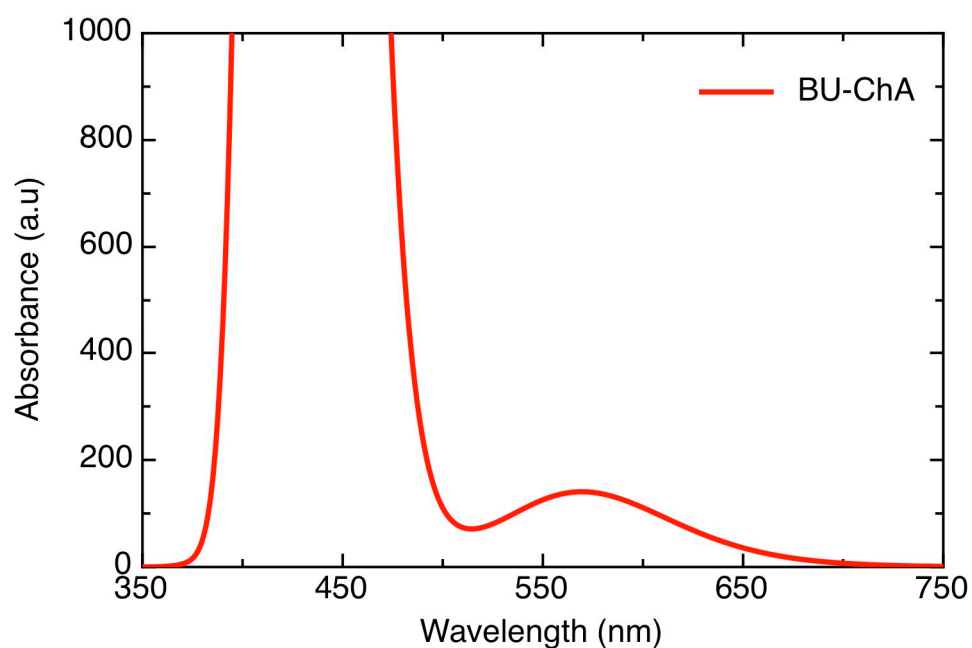


Figure S4: Calculated electronic spectra of BU-ChA complex in methanol using TD-DFT method.

Table S1: the optimized structure of BU

C	-1.00731	-1.08886	0.00003
C	0.41257	-1.35641	-0.00000
N	-1.33692	0.27572	0.00001
C	-0.47657	1.34269	-0.00002
C	1.28079	-0.32580	0.00004

N	0.85921	0.97058	0.00001
O	-1.88588	-1.91990	-0.00002
O	-0.82138	2.49746	-0.00001
H	-2.31919	0.49977	0.00001
H	1.53421	1.71611	-0.00001
O	2.61323	-0.40971	-0.00003
H	0.74218	-2.38293	-0.00006
H	2.88212	-1.32960	0.00009

Table S2: Calculated Frequencies of BU

	1	2	3
	A	A	A
Frequencies --	146.5391	166.8201	202.2129
Red. masses --	11.0274	6.0208	6.1740
Frc consts --	0.1395	0.0987	0.1487
IR Inten --	0.3733	2.0470	2.0535

Table S3: the optimized structure of CHL

O	-1.51041	2.29570	0.00009
H	-2.45901	2.12060	0.00001
C	-0.85754	1.14745	0.00006
C	0.64366	1.30863	0.00008
O	1.13429	2.40477	-0.00019
C	1.42912	0.06853	0.00003
Cl	3.14535	0.21311	0.00002
C	0.85754	-1.14745	0.00001
O	1.51041	-2.29570	0.00003
H	2.45901	-2.12060	0.00003
C	-0.64366	-1.30863	-0.00012
O	-1.13429	-2.40477	-0.00003
C	-1.42912	-0.06853	-0.00000
Cl	-3.14535	-0.21311	-0.00000

Table S4: Calculated Frequencies of ChA

	1	2	3
	A	A	A
Frequencies --	61.4173	88.0910	100.9299
Red. masses --	16.4706	11.8960	12.5045
Frc consts --	0.0366	0.0544	0.0751

IR Inten	--	4.3501	2.4452	0.0000
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Table S5: the optimized structure of BUChA-I

C	2.51308	0.79793	-0.58677
C	2.06539	-0.51451	-0.94841
N	3.43734	0.84066	0.44959
C	3.89966	-0.22517	1.18851
C	2.46915	-1.57653	-0.21851
N	3.35925	-1.44275	0.80110
O	2.14039	1.84838	-1.09776
O	4.68804	-0.12640	2.09197
H	3.76775	1.75195	0.72778
H	3.64820	-2.25315	1.32562
O	2.06563	-2.83310	-0.38553
H	1.37309	-0.63209	-1.76308
H	1.37092	-2.86739	-1.04970
O	-0.20232	1.04463	-2.14103
H	0.53235	1.64273	-1.87206
C	-0.99118	0.75369	-1.12571
C	-1.39378	-0.70390	-1.06679
O	-0.88658	-1.50706	-1.81357
C	-2.36300	-1.09096	-0.04307
Cl	-2.89034	-2.73410	-0.01090
C	-2.78997	-0.22575	0.89232
O	-3.62413	-0.51433	1.87304
H	-3.88975	-1.43990	1.80553
C	-2.31034	1.20878	0.90840
O	-2.68792	1.95219	1.77354
C	-1.39919	1.61435	-0.17245
Cl	-0.90510	3.25589	-0.18318

Table S6: Calculated Frequencies of BUChA-I

	1	2	3
	A	A	A
Frequencies --	9.4597	21.9665	34.5317
Red. masses --	10.7729	14.6050	8.7418
Frc consts --	0.0006	0.0042	0.0061
IR Inten --	0.2221	0.0421	3.6470

Table S7: the optimized structure of BUChA-II

C	-5.28425	-0.71235	0.40225
C	-4.90153	0.41340	1.22144
N	-4.28425	-1.13409	-0.49843
C	-3.04369	-0.60022	-0.65505
C	-3.67797	0.95759	1.07130
N	-2.77698	0.46735	0.16827
O	-6.34268	-1.29136	0.43039
O	-2.22875	-1.02351	-1.45523
H	-4.50935	-1.92527	-1.08114
H	-1.89139	0.93641	0.03691
O	-3.17924	1.99654	1.73934
H	-5.61332	0.78964	1.93836
H	-3.82676	2.33224	2.36142
O	0.33736	-1.48388	-0.91049
H	-0.49708	-1.06772	-1.22135
C	1.30871	-0.66938	-0.60080
C	2.50269	-1.40372	-0.00917
O	2.46555	-2.59595	0.12459
C	3.65885	-0.58854	0.37763
Cl	5.02346	-1.40187	1.04559
C	3.67680	0.74617	0.23490
O	4.68187	1.53541	0.57080
H	5.39725	0.99852	0.93166
C	2.49665	1.48423	-0.34685
O	2.53782	2.68086	-0.46058
C	1.34410	0.67180	-0.74514
Cl	0.01840	1.53508	-1.43785

Table S8: Calculated Frequencies of BUChA-II

	1	2	3
	A	A	A
Frequencies --	9.3896	18.5772	28.0200
Red. masses --	11.7153	11.3813	8.6716
Frc consts --	0.0006	0.0023	0.0040
IR Inten --	0.6383	1.1820	1.9145

Table S9: the optimized structure of BUChA-I/g-C3N4

C	4.46809	1.06974	2.69570
C	3.24106	0.43121	3.08909
N	5.62394	0.30774	2.96934

C	5.66739	-0.98890	3.39098
C	3.26611	-0.82452	3.57286
N	4.44609	-1.50044	3.75159
O	4.57435	2.16118	2.17520
O	6.68946	-1.64943	3.45135
H	6.46985	0.64366	2.53621
H	4.42138	-2.46547	4.03165
O	2.21543	-1.54093	3.93558
H	2.30656	0.92964	2.90842
H	1.39055	-1.09108	3.66882
O	-0.60933	-2.89211	2.95228
H	-0.93890	-3.79494	2.86988
C	-1.63664	-2.06100	2.86747
C	-1.24883	-0.60982	2.93256
O	-0.11110	-0.26889	3.18338
C	-2.30736	0.36019	2.73204
Cl	-1.87166	2.02778	2.73318
C	-3.59696	0.00052	2.60869
O	-4.60433	0.84109	2.51370
H	-4.25189	1.73385	2.39083
C	-4.01373	-1.45307	2.62981
O	-5.17439	-1.76012	2.57500
C	-2.92109	-2.42959	2.74251
Cl	-3.33386	-4.09852	2.65302
N	-5.81424	3.09149	-1.27131
C	-6.56850	2.01335	-1.46935
N	-7.76816	2.08978	-1.99541
C	-8.40752	0.92845	-2.20849
N	-9.63916	1.02213	-2.71413
H	-10.02763	1.92755	-2.89617
H	-10.15747	0.18521	-2.90078
N	-7.94527	-0.31216	-1.99911
C	-6.74071	-0.41251	-1.47744
N	-6.15503	-1.58623	-1.27977
C	-4.96167	-1.56111	-0.69154
N	-4.34453	-0.51651	-0.17799
C	-4.84409	0.66671	-0.47029
N	-4.20119	1.76180	-0.14246
N	-4.30967	-2.78234	-0.66461
H	-4.84214	-3.53009	-1.08348
C	-2.94410	-2.96423	-0.76098
N	-2.58680	-4.10206	-1.35554
C	-1.30615	-4.22968	-1.66701

N	-0.44246	-3.15779	-1.43460
C	0.88558	-3.20896	-1.85870
N	1.63060	-2.11869	-1.73895
C	1.09220	-1.10023	-1.08587
N	-0.05951	-1.08458	-0.41515
N	1.80855	0.07292	-1.08271
C	3.21292	0.04240	-1.36102
N	3.55471	0.52952	-2.53527
C	4.85785	0.54119	-2.80194
N	5.31721	1.00537	-3.94069
C	6.64249	0.94675	-4.11916
N	7.10162	1.39568	-5.29235
H	6.45452	1.75414	-5.96762
H	8.08795	1.38616	-5.46633
N	7.56195	0.49143	-3.26093
C	7.12319	0.04829	-2.09946
N	7.94996	-0.37915	-1.16622
C	7.41259	-0.81534	-0.02490
N	6.09908	-0.90016	0.26313
C	5.26884	-0.45222	-0.64023
N	8.24231	-1.20323	0.93985
H	9.22902	-1.13131	0.78075
H	7.86821	-1.49264	1.83624
N	5.74580	0.04009	-1.85129
N	3.96122	-0.44010	-0.40813
C	1.23457	1.32174	-0.86930
N	-0.03449	1.46011	-1.21679
C	-0.61046	2.58401	-0.85601
N	-1.90290	2.77933	-1.05374
C	-2.42344	3.86396	-0.51088
N	-1.78677	4.88648	0.05322
C	-0.46042	4.78611	0.11966
N	0.28644	5.77084	0.56123
C	1.61022	5.54880	0.61423
N	2.36547	6.57004	1.02138
H	1.92754	7.43082	1.28727
H	3.35362	6.43250	1.11966
N	2.26093	4.41914	0.31102
C	1.52822	3.41883	-0.10420
N	-3.80574	3.97083	-0.54950
H	-4.20315	4.89362	-0.59590
N	0.14601	3.58597	-0.26185
N	2.05546	2.22710	-0.36798



N	1.34687	-4.31418	-2.39760
C	0.47166	-5.32300	-2.53355
N	0.95921	-6.45603	-3.04591
H	1.91936	-6.49076	-3.33019
H	0.34231	-7.23044	-3.19939
C	-0.88658	-2.06922	-0.69411
N	-0.82943	-5.32577	-2.21741
N	-2.14310	-2.02007	-0.30183
N	-6.04368	0.75452	-1.15400
C	-4.64737	2.89045	-0.67283