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

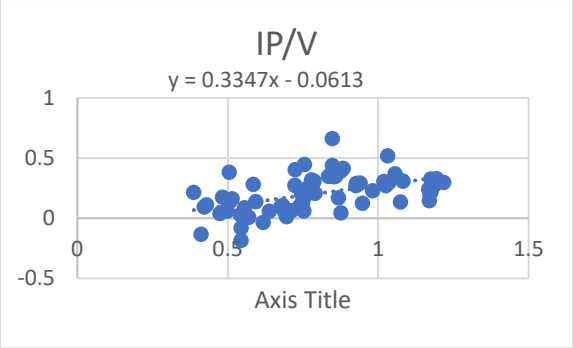
Supporting Information

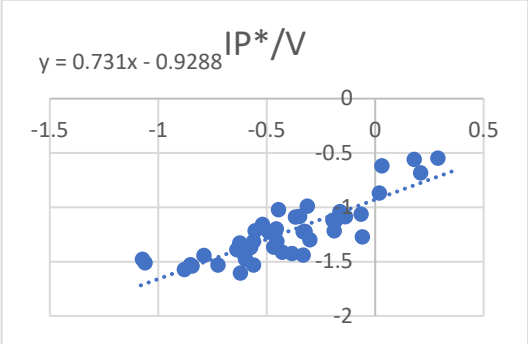
Screening potential dye sensitizers for water splitting photocatalysts using a Genetic Algorithm

Tao Liu*[a], Linjiang Chen*[b], Xiaoyan Wang[a], and Andrew I. Cooper*[a]

[a]*Department of Chemistry and Materials Innovation Factory, Leverhulme Research Centre for Functional Materials Design, University of Liverpool, 51 Oxford Street, Liverpool, L7 3NY, UK.*
Email: T. Liu tao.liu@liverpool.ac.uk
Email: A.I. Cooper *aicooper@liverpool.ac.uk*

[b]*School of Chemistry and School of Computer Science, University of Birmingham, Birmingham, B15 2TT UK*
Email: L. Chen l.j.chen@bham.ac.uk





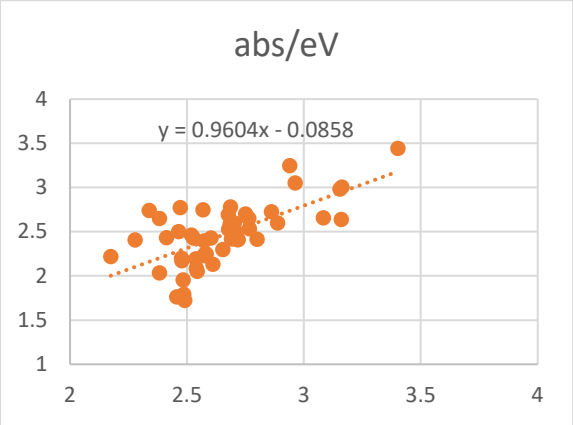


Figure S1. Calibration of IP, IP*, and absorption of GNF-xTB (x axis) on TD-DFT (y axis) level.

Binding energy

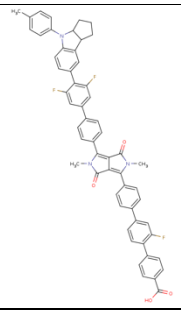
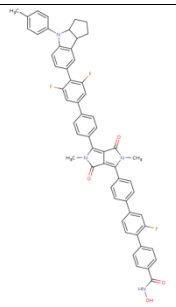
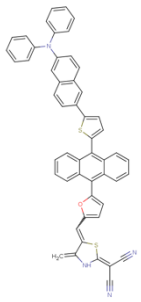
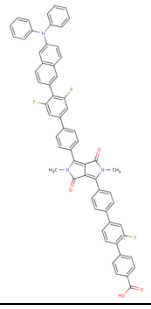
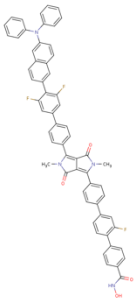
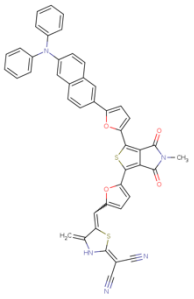
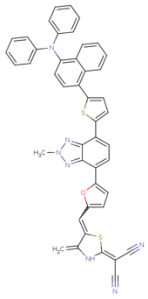
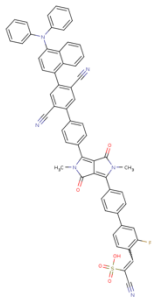
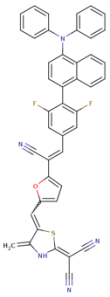
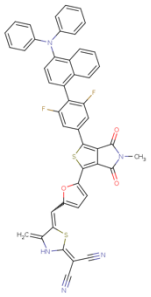
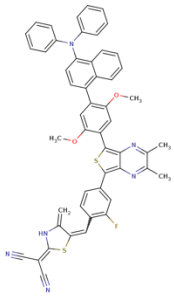
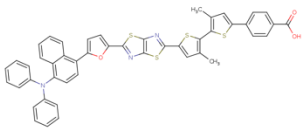
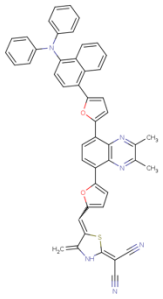
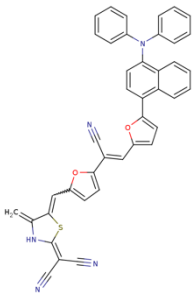
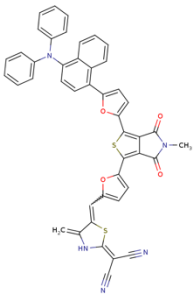
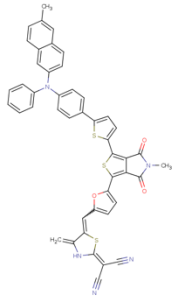
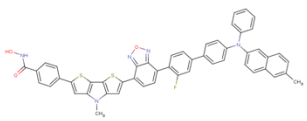
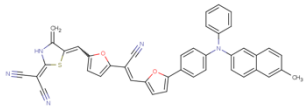
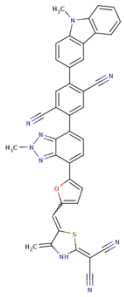
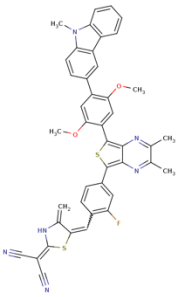
The binding energy quantifies the interaction strength between the dye and FS-COF; a more negative value indicates a stronger interaction. To assess this, we conducted binding energy calculations employing a semiempirical free energy force field, which has been implemented in AutoDock4.[1,2] This calculation involves the evaluation of energies for both the bound and unbound states, and also incorporates a new charge-based desolvation method utilizing a standard set of atom types and charges.[3] Through calibration with over 100 complexes of known structures and binding energies, the standard error was found to be less than 3 kcal/mol. The model used for this binding energy calculation consists of eight layers of FS-COF forming a single channel as the receptor, with a dye molecule serving as the ligand.

$E_{binding} = E_{dye\_COF} - E_{COF} - E_{dye}$

1 G. M. Morris, D. S. Goodsell, R. S. Halliday, R. Huey, W. E. Hart, R. K. Belew and A. J. Olson, Automated docking using a Lamarckian genetic algorithm and an empirical binding free energy function, *Journal of Computational Chemistry*, 1998, **19**, 1639–1662.

2 G. M. Morris, R. Huey, W. Lindstrom, M. F. Sanner, R. K. Belew, D. S. Goodsell and A. J. Olson, AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility, *J Comput Chem*, 2009, **30**, 2785–2791.

3 R. Huey, G. M. Morris, A. J. Olson and D. S. Goodsell, A semiempirical free energy force field with charge-based desolvation, *Journal of Computational Chemistry*, 2007, **28**, 1145–1152.

0204180301	0204180305	0401231507	0404180301
			
0404180305	0415091507	0501101507	0502180312
			
0504061507	0504091507	0505130307	0515011401
			
0515031507	0515061507	0515091507	1101091507
			
1103150705	1115061507	1602101507	1605130307
			
1611091507	1614091507	1615021507	1615091507

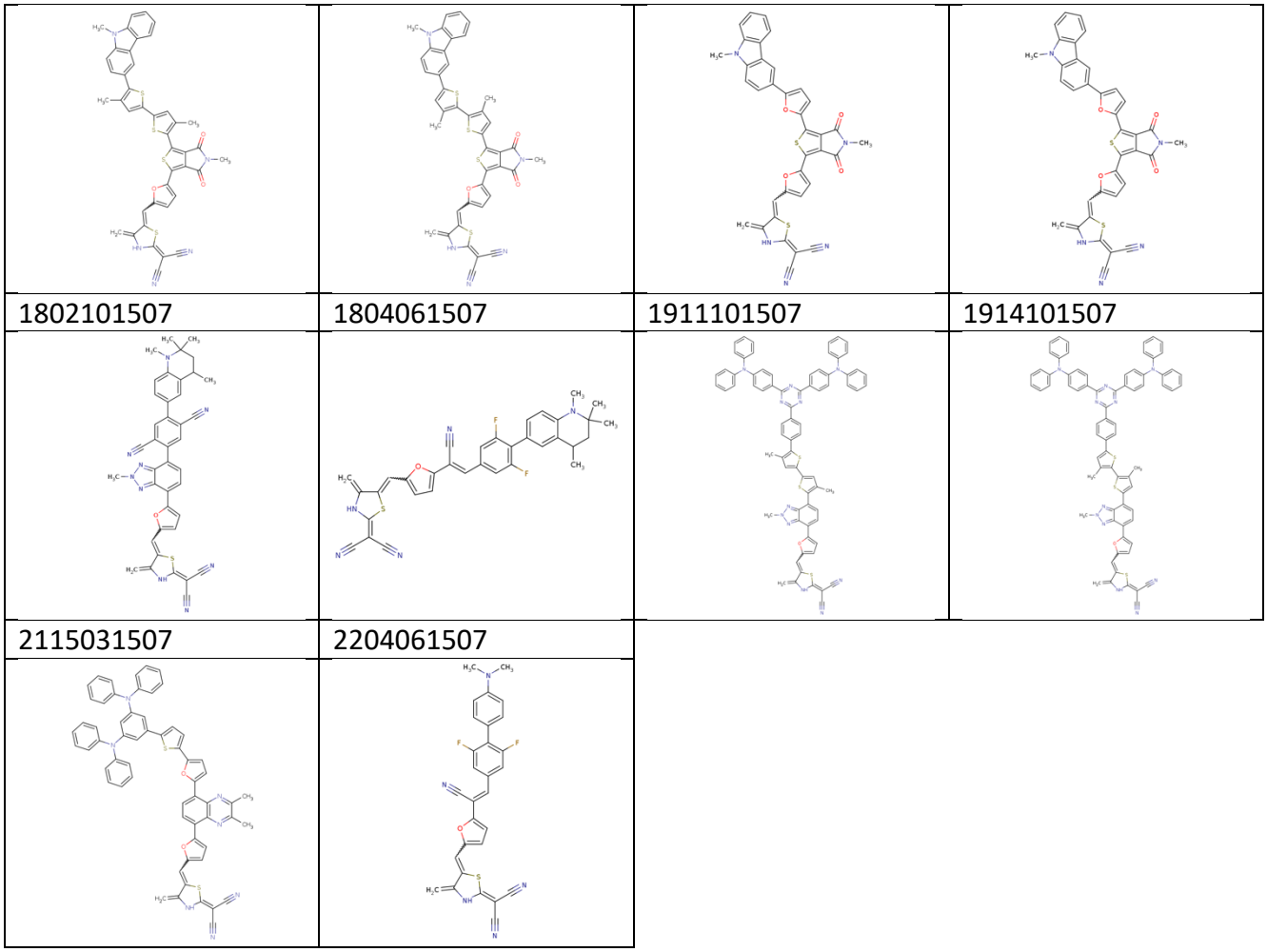


Figure S2. Structures of 30 optimized sensitizers screened by setting absorption and/or binding energy as fitness functions in GA.

Table S1. IP, IP*, E_b, E_{abs}, S_r, DM, E_c of optimized dyes.

name	ID	E_b	E_{abs}	IP*	IP	Sr	DM	Ec
WS5F. Ref.	0	-0.93	499	-1.421	0.308	0.756	41.307	3.746
1115061507	1	-2.05	531	-1.469	0.252	0.800	27.397	3.632
1911101507	2	-2.43	495	-1.433	0.327	0.822	12.908	3.413
0515011401	3	-2.13	463	-1.486	0.309	0.811	19.154	3.210
1914101507	4	-1.94	504	-1.426	0.275	0.825	12.836	3.329
1611091507	5	-10.02	501	-1.429	0.374	0.810	39.684	3.310
0515091507	6	-9.04	497	-1.417	0.380	0.811	15.950	3.581
1101091507	7	-4.03	496	-1.448	0.319	0.806	43.326	3.329
1615091507	8	-7.58	495	-1.408	0.417	0.800	31.577	3.472
1804061507	9	-4.99	481	-1.473	0.290	0.799	38.434	3.585
2204061507	10	-3.9	476	-1.413	0.414	0.810	32.778	3.716
0505130307	11	-3.85	465	-1.570	0.337	0.773	4.609	4.177
0504091507	12	-4.25	464	-1.514	0.523	0.812	44.644	3.771
1802101507	13	-4.55	457	-1.579	0.366	0.815	21.376	3.835
0501101507	14	-4.85	500	-1.520	0.272	0.822	10.728	3.393
0515031507	15	-5.36	493	-1.510	0.278	0.815	7.857	3.363
1605130307	16	-8.17	530	-1.411	0.316	0.787	27.502	3.724
0415091507	17	-6.36	508	-1.417	0.328	0.808	12.649	3.439
1614091507	18	-10.65	503	-1.426	0.284	0.806	43.876	3.311
1615021507	19	-8.33	475	-1.543	0.299	0.805	34.494	3.717
2115031507	20	-0.74	506	-1.463	0.306	0.812	9.441	3.252
0401231507	21	-5	522	-1.557	0.349	0.841	14.558	3.661
0404180305	22	-6.34	501	-1.480	0.431	0.848	21.428	4.455
0204180305	23	-5.8	501	-1.508	0.271	0.851	60.754	4.410
0204180301	24	-3.8	499	-1.503	0.273	0.853	58.991	4.411
0404180301	25	-5.67	500	-1.486	0.431	0.850	24.115	4.346
0515061507	26	-9.36	529	-1.378	0.327	0.815	8.444	3.640
0504061507	27	-6.34	472	-1.382	0.517	0.817	10.784	4.032
1103150705	28	-2.3	518	-1.371	0.349	0.763	9.386	3.745
1602101507	29	-8.16	452	-1.380	0.657	0.817	8.561	3.769
0505090701	30	-3.93	479	-1.576	0.434	0.776	7.335	3.556
1105130307	31	-0.71	477	-1.620	0.247	0.771	8.689	3.958
0500141507	32	-5.18	443	-1.575	0.468	0.794	37.842	4.007
0502221505	33	-5.16	417	-1.580	0.522	0.772	5.386	3.571
1602221505	34	-5.52	415	-1.624	0.521	0.772	13.489	3.636
1605101505	35	-5.17	415	-1.774	0.425	0.812	21.431	3.945
1602231505	36	-7.09	408	-1.611	0.610	0.861	4.213	4.213
0002221505	37	-2.84	422	-1.660	0.385	0.756	3.378	3.378
0402221505	38	-4.95	420	-1.633	0.457	0.768	6.388	3.457
0102230405	39	-4.67	410	-1.671	0.395	0.663	27.677	3.871

0202231507	40	-5.77	429	-1.782	0.350	0.838	24.178	3.717
1802230509	41	-4.02	426	-1.769	0.378	0.664	32.226	4.309
0505230509	42	-5.78	426	-1.677	0.444	0.666	18.948	4.327
0402230509	43	-5.49	425	-1.733	0.470	0.666	14.854	4.263
0504070309	44	-5.75	414	-2.140	0.511	0.764	22.338	3.750
0504231505	45	-6.75	404	-1.707	0.513	0.865	6.975	4.317