Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Title:

An Exceptional Functionalization of Doped Fullerene Observed via Theoretical Studies on the Interactions of Sulfur-Doped Fullerenes with Halogens and Halides

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Table S1. Important NBO atomic charges for all complexes

Complexes	First S	C (Av)[a]	X(1)	X(2)	Second S	C (Av)[a]	X(1)	X(2)
SF (alone)	0.859	-0.198	-	-	-	-	-	-
SF-F	0.977	-0.178	-0.731	-	-	-	-	-
SF-Cl	0.934	-0.171	-0.866	-	-	-	-	-
SF-Br	0.918	-0.173	-0.820	-	-	-	-	-
SF-D-F_2	0.871	-0.197	-0.026	-0.010	-	-	-	-
SF-D-Cl_2	0.853	-0.194	-0.028	-0.004	-	-	-	-
SF-D-Br_2	0.856	-0.196	-0.007	0.018	-	-	-	-
SF-P-F_2	0.860	-0.197	-0.003	0.006	-	-	-	-
SF-P-Cl_2	0.857	-0.196	-0.005	0.007	-	-	-	-
SF-P-Br_2	0.852	-0.197	0.000	0.013	-	-	-	-
S2F1-2F	0.946	-0.215	-0.746	-	0.962	-0.200	-0.752	-
S2F1-2Cl	0.920	-0.213	-0.872	-	0.931	-0.187	-0.901	-
S2F1-2Br	0.898	-0.221	-0.851	-	0.921	-0.197	-0.870	-
S2F1-2D-F_2	0.859	-0.241	-0.006	0.007	0.866	-0.205	-0.009	0.010
S2F1-2D-Cl_2	0.901	-0.227	-0.036	-0.454	0.924	-0.174	-0.033	-0.004
S2F1-2D-Br_2	0.896	-0.253	0.042	-0.433	0.888	-0.164	-0.026	0.015
S2F1-2P-F_2	0.860	-0.242	-0.004	0.009	0.867	-0.206	-0.006	0.011
S2F1-2P-Cl_2	0.861	-0.242	0.000	0.004	0.867	-0.206	-0.004	0.006
S2F1-2P-Br_2	0.864	-0.241	-0.011	0.150	0.864	-0.202	0.004	-0.039
S2F1-DP-F_2	0.813	-0.042	-0.301	-0.597	1.040	-0.134	-0.018	-0.124
S2F1-DP-Cl_2	0.878	-0.206	0.080	-0.289	0.974	-0.125	-0.543	-0.05
S2F1-DP-Br_2	0.880	-0.244	0.199	-0.332	0.945	-0.132	-0.462	-0.027
S2F2-2F	0.970	-0.208	-0.712	-	0.950	-0.189	-0.760	-
S2F2-2Cl	0.921	-0.190	-0.890	-	0.921	-0.181	-0.915	-
S2F2-2Br	0.905	-0.192	-0.873	-	0.903	-0.188	-0.866	-
S2F2-2D-F_2	0.874	-0.203	-0.028	-0.014	0.872	-0.198	-0.025	-0.010
S2F2-2D-Cl_2	0.858	-0.203	-0.004	0.006	0.858	-0.198	-0.005	0.008
S2F2-2D-Br_2	0.855	-0.203	-0.005	0.016	0.856	-0.198	-0.007	0.018
S2F2-2P-F_2	0.889	-0.183	-0.176	-0.278	0.866	-0.197	-0.006	0.011
S2F2-2P-Cl_2	0.857	-0.205	0.003	-0.001	0.858	-0.198	-0.007	0.010
S2F2-2P-Br_2	0.851	-0.205	0.014	0.005	0.855	-0.198	-0.007	0.018
S2F2-DP-F_2	0.919	-0.106	-0.228	-0.399	0.891	-0.178	-0.136	-0.20
S2F2-DP-Cl_2	0.866	-0.199	-0.001	0.005	0.888	-0.177	-0.066	-0.275
S2F2-DP-Br_2	0.860	-0.200	0.009	0.012	0.889	-0.177	0.004	-0.309

[a] This value is the average of atomic charges of three carbon atoms connected to the doped sulfur

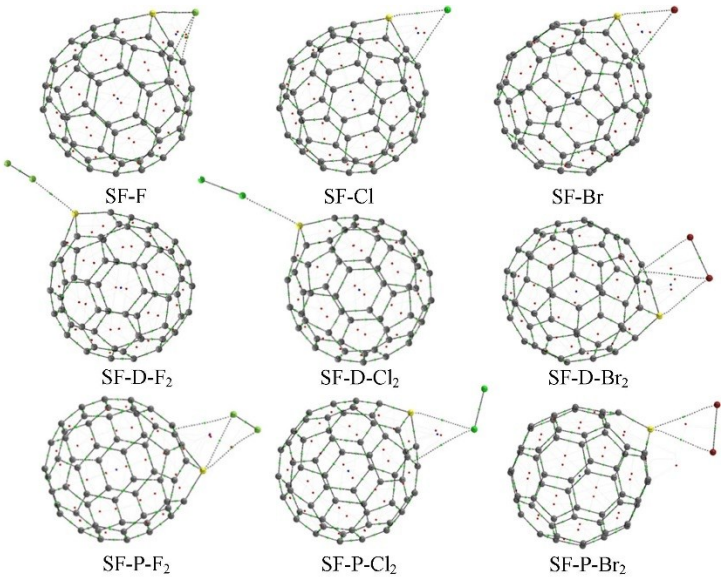

Figure S1. BCPs (green dots) and RCPs (red dots) of noncovalent interactions of SF model with halogens and halides

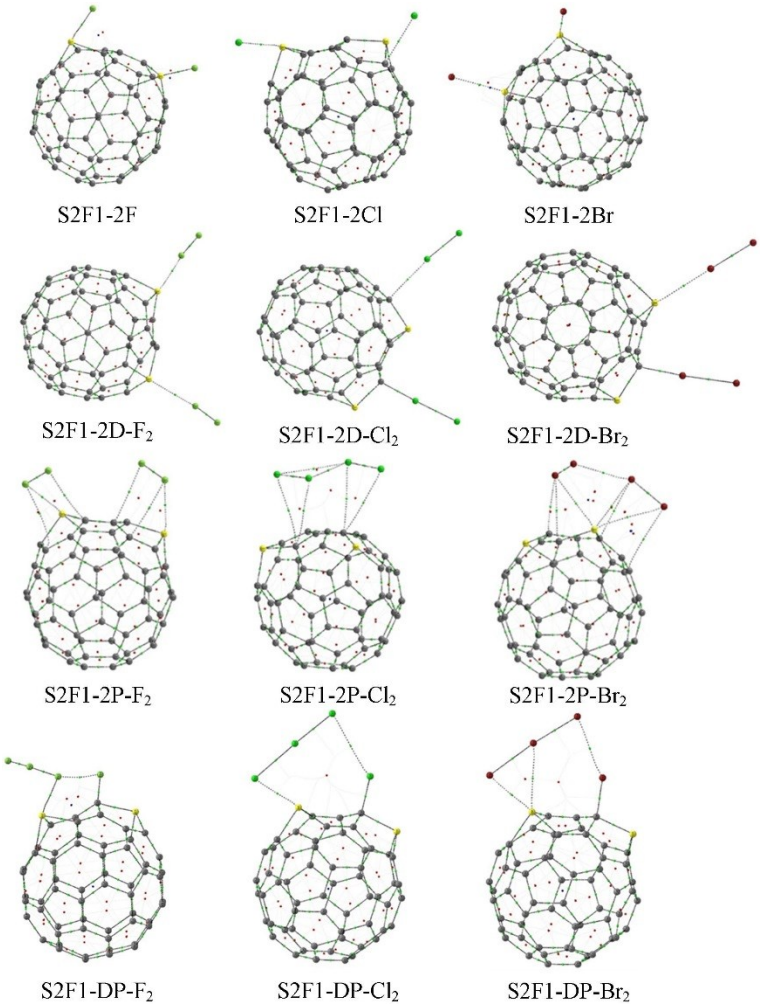

Figure S2. BCPs (green dots) and RCPs (red dots) of noncovalent interactions of S2F1 model with halogens and halides

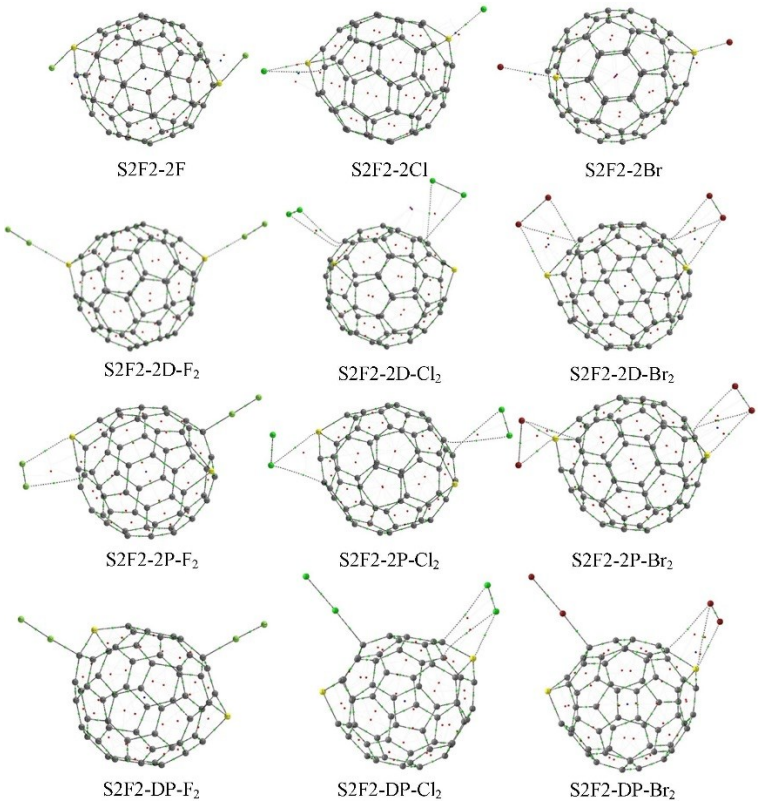

Figure S3. BCPs (green dots) and RCPs (red dots) of noncovalent interactions of S2F2 model with halogens and halides

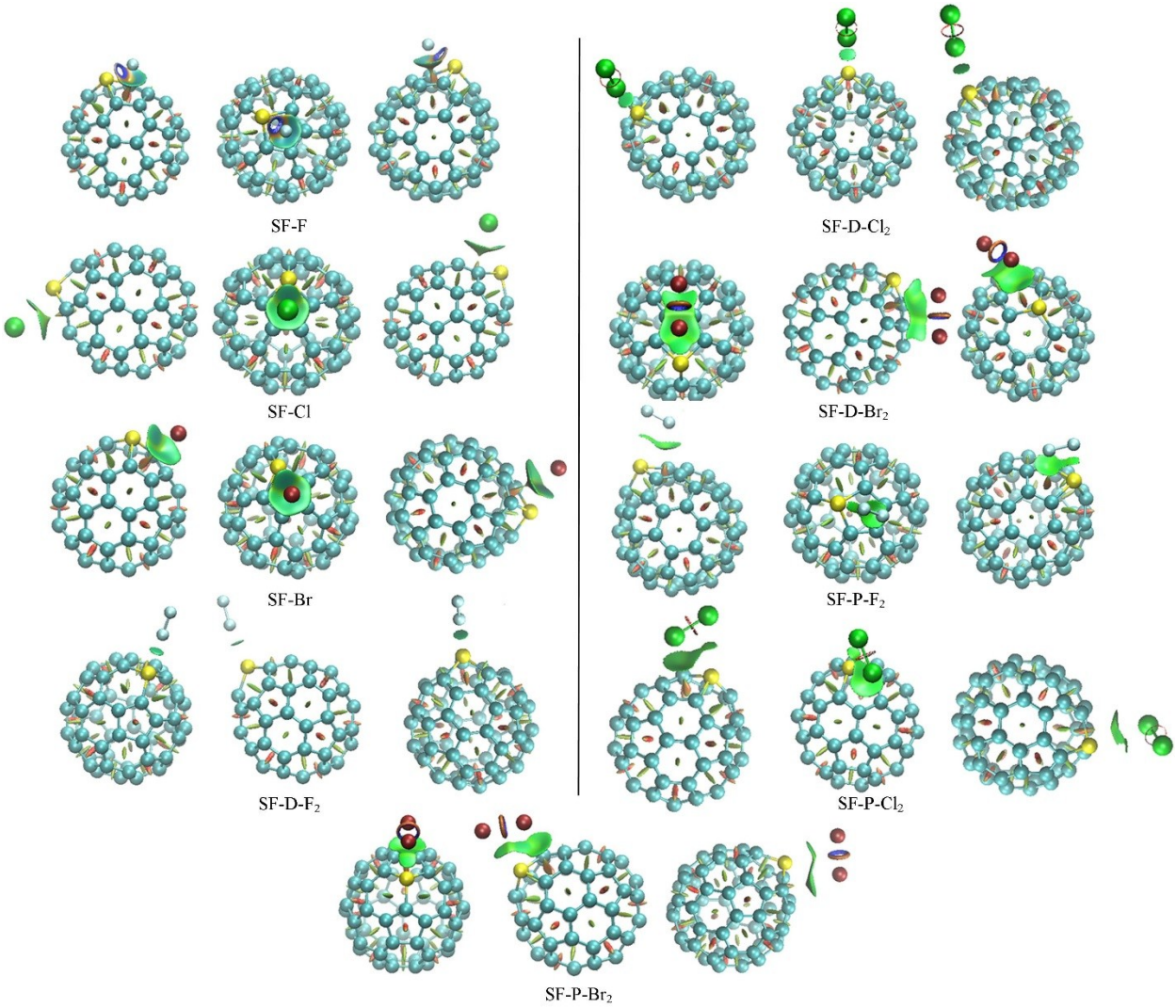

Figure S4. Noncovalent interaction isosurfaces obtained from RDG and electron density frames for SF complexes

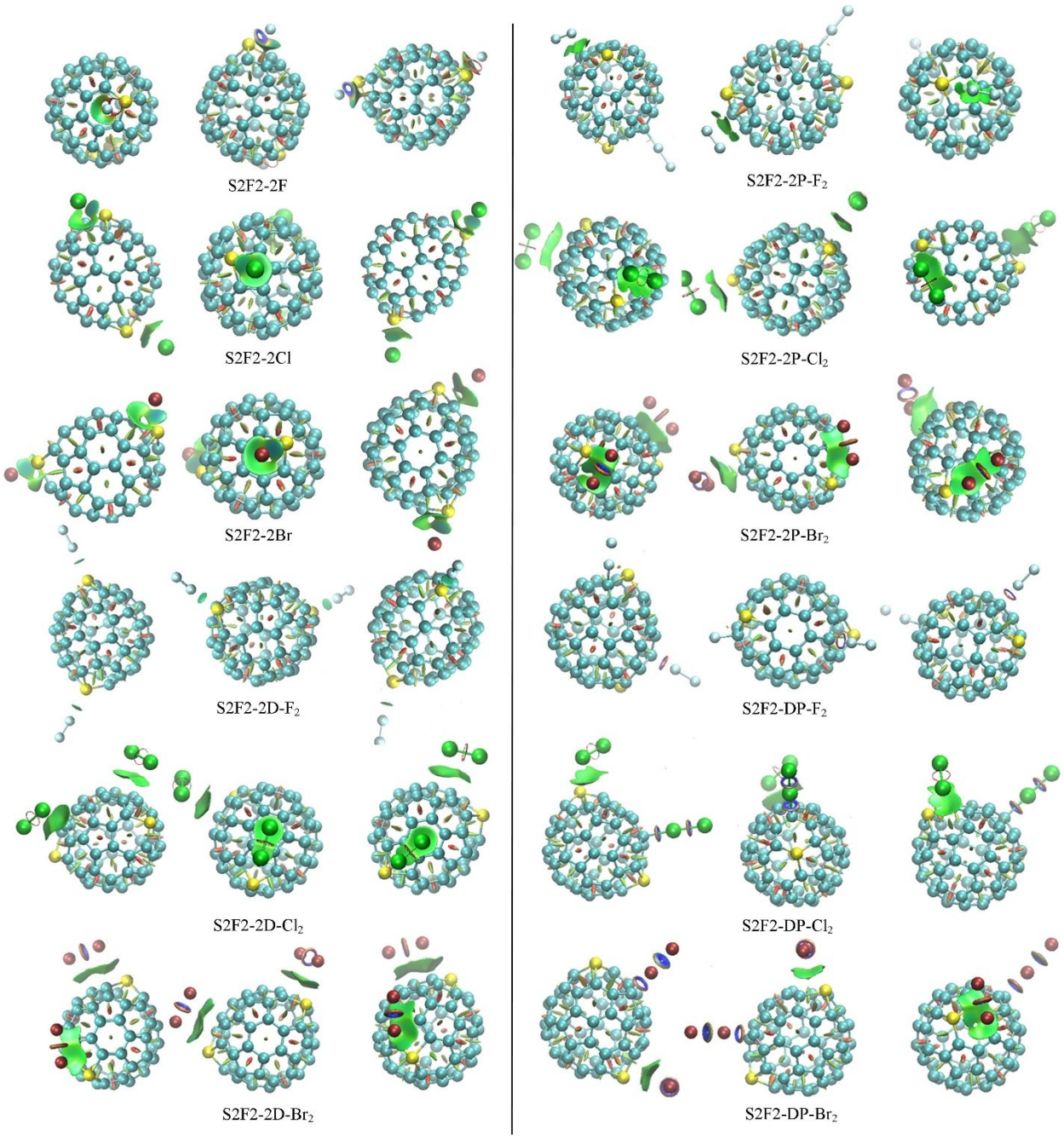

Figure S5. Noncovalent interaction isosurfaces obtained from RDG and electron density frames for interactions of S2F2 model with halogens and halides