Extra electronic outer-shell peculiarities accessible under a joint XPS and DFT study

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Supplementary material

Material contains the optimized coordinates of atoms, lattice constants, total (DOS) and partial (pDOS) Densities of States, and relevant views resulted from Density Functional Theory (DFT) calculations for the bilayer $C_{24}F_{12}$ (Table 1S; Figs. 1S and 1S+), $C_{24}F_{12}Br_2$ (Tables 2S-6S; Figs. 2S-6S) and C_{24} (Table 7S; Fig. 7S) unit cells with the Bernal and hexagonal (Hex) structure in terms of [20]. Table 8S gives a summary for $C_{24}F_{12}Br_2$ unit cells. Carbon planes were specified by the same C-triplets in each of $C_{24}F_{12}Br_2$ unit cells in computations the angles between C-skeleton and Br-Br axis. Atom numbering in Fig. 1S was used through each processing. The pictures have been constructed using the GiperChem 8.0.6 software.

Computational details

DFT runs have been performed by the Quantum Espresso package [16] and the non-local exchange-correlation functional in the Perdew-Burke-Ernzerhof parameterization [17]. The interactions between the ionic cores and electrons are described by the Projected Augmented Wave method [18] with a kinetic energy cutoff 40 Ry (320 Ry for the charge-density cutoff) for a plane-wave basis set. Marzari-Vanderbilt cold smearing [19] with a Gaussian spreading factor of 0.02 Ry for the Brillouin-zone integration was used.

The graphite was modeled with a bilayer C_{24} unit cell with the optimized lattice parameters (a = 2.46 Å × 3, b = 2.46 Å × 2); van der Waals interaction has been examined as in Ref. [S1]. Half-fluorinated graphite, pristine and imbedded with the Br_2 molecule was modeled with a bilayer $C_{24}F_{12}$ and $C_{24}F_{12}Br_2$ unit cell, respectively, with the optimized lattice parameters a = 2.51 Å × 3 and b = 2.46 Å × 2; there were F attached to C atoms on both sides of the slab and 40 Bohr space between slabs to prevent the interactions. The Brillouin zone integration was performed on a 20 × 20 × 1 grid of Monkhorst-Pack k-points [22]. The accuracy was verified by testing the energy convergence. The excess number of bands NB = 384 and 288 accepted for C_{24} and $C_{24}F_{12}$ unit cell has resulted in the same occupied DOS structure, but the extended vacant DOS energy range as compared to the default NB = 58 and 108, respectively.

References (under the same numbering as in the text of a paper)

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Table 1S Optimized bilayer Bernal and hexagonal $C_{24}F_{12}$ unit cells

(a) Cartesian coordinates of atoms numbered as in Fig. 1S (Å)

Top $C_{12}F_6$ Layer				Lower $C_{12}F_6$ Layer			
			Bernal				
No.	X	Y	Z	No.	X	Y	Z
C #1	0.01775	1.57486	3.2118	C #1	-1.21447	3.39593	-0.02946
C #2	1.26611	0.89618	3.21327	C #2	-1.23293	2.04545	-0.7502
C #3	2.52768	1.57494	3.21168	C #3	0.0156	1.16594	-0.74977
C #4	2.54616	2.92557	3.93217	C #4	-0.00283	-0.18622	-0.031
C #5	1.29766	3.80507	3.93142	C #5	1.27713	2.04534	-0.75007
C #6	0.03628	2.92543	3.93234	C #6	2.52562	1.1658	-0.74936
C #7	3.80765	3.80502	3.93163	C #7	2.50718	-0.18634	-0.03057
C #8	5.05616	2.92545	3.93245	C #8	3.78704	2.04537	-0.75009
C #9	5.03773	1.57504	3.21153	C #9	5.0356	1.16594	-0.74977
C #10	3.77609	0.89639	3.21261	C #10	5.01718	-0.18623	-0.03098
C #11	-1.2123	3.80486	3.93212	C #11	1.29558	3.3959	-0.02946
C #12	6.2861	0.89633	3.21283	C #12	3.80555	3.396	-0.02968
F #13	-1.21477	4.34486	5.22432	F #13	0.01814	0.62598	-2.04198
F #14	0.03926	2.38681	5.22536	F #14	2.52822	0.62548	-2.04143
F #15	1.29505	4.34561	5.22341	F #15	5.03814	0.62598	-2.04197
F #16	2.54862	2.38717	5.22525	F #16	-1.2355	2.58431	-2.04309
F #17	3.805	4.34545	5.22369	F #17	1.27481	2.58401	-2.04303
F #18	5.05845	2.38681	5.22542	F #18	3.78425	2.58403	-2.04307
			Hexagonal				
C #1	-1.21401	3.56695	3.71168	C #1	-1.21401	3.56693	-0.36682
C #2	-1.2309	2.21551	4.43349	C #2	-1.23091	2.21552	-1.08862
C #3	0.01748	1.33521	4.43362	C #3	0.01748	1.3352	-1.08877
C #4	6.29305E-4	-0.01619	3.71171	C #4	6.27169E-4	-0.01617	-0.36685
C #5	1.2791	2.21549	4.43373	C #5	1.2791	2.2155	-1.08888
C #6	2.52751	1.3352	4.43373	C #6	2.52751	1.33518	-1.08888
C #7	2.51064	-0.01619	3.71183	C #7	2.51064	-0.01617	-0.36698
C #8	3.78913	2.21548	4.43362	C #8	3.78913	2.21549	-1.08877
C #9	5.03752	1.33518	4.43349	C #9	5.03752	1.33517	-1.08862
C #10	5.02063	-0.01626	3.71168	C #10	5.02063	-0.01624	-0.36682
C #11	1.29598	3.56688	3.71183	C #11	1.29597	3.56686	-0.36698
C #12	3.80599	3.56688	3.71171	C #12	3.80599	3.56686	-0.36685
F #13	0.01617	0.79537	5.72565	F #13	0.01615	0.79537	-2.38079
F #14	2.52633	0.79535	5.72576	F #14	2.52632	0.79535	-2.38091
F #15	5.0364	0.79526	5.72549	F #15	5.03639	0.79525	-2.38062
F #16	-1.22978	2.75543	5.72549	F #16	-1.22977	2.75544	-2.38062
F #17	1.28029	2.75534	5.72576	F #17	1.28029	2.75534	-2.38091
F #18	3.79045	2.75532	5.72565	F #18	3.79047	2.75532	-2.38079

(b) Structural properties: lattice parameters (a, b), interlayer distances (d_{layer}), C−C bond lengths (d_{C-C}), C−F bond length (d_{C-F}) (Å)

			Bernal	
a	*b*	d_{layer}	d_{C-C}	d_{C-F}
7.53	4.92	3.75; 3.98	1.42; 1.43; 1.53; 1.53; 1.53; 1.54	1.40
			Hexagonal	
7.53	4.92	4.08, 5.52	1.42, 1.42, 1.53, 1.53, 1.54, 1.54	1.40

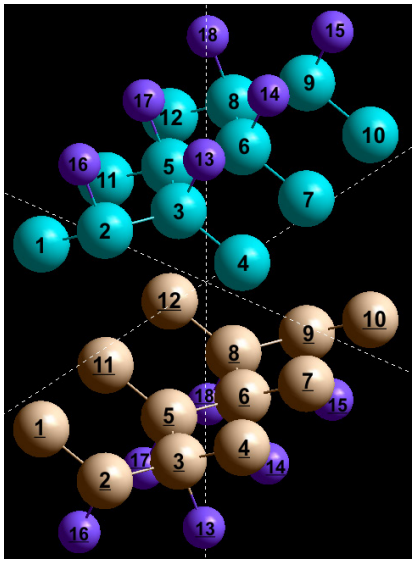
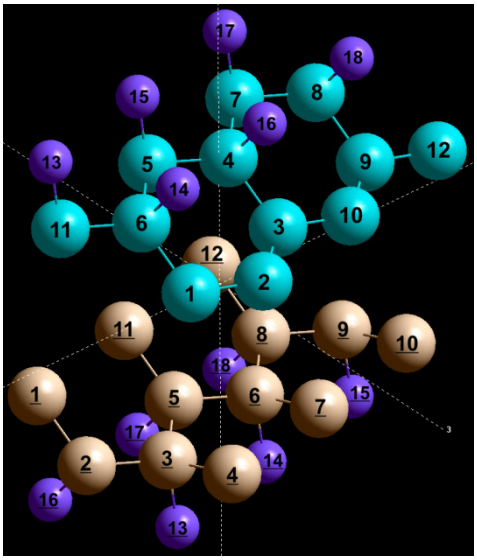
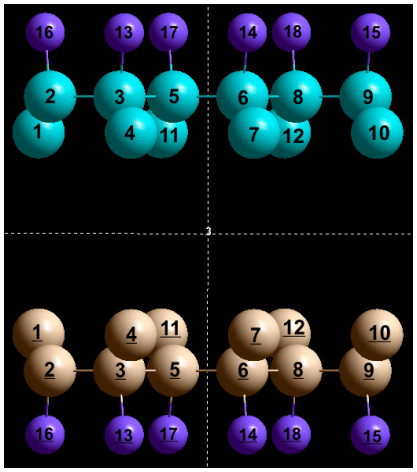
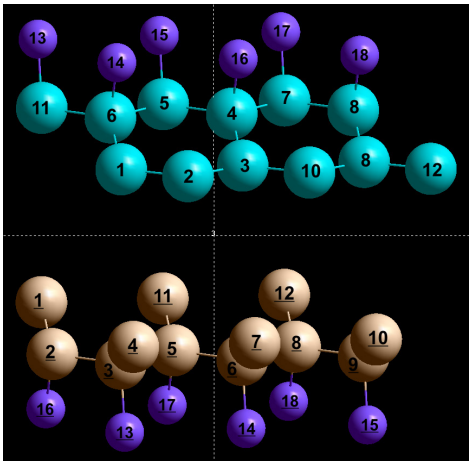
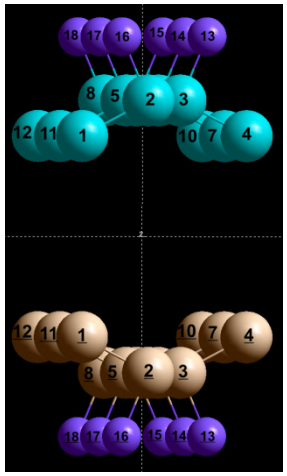
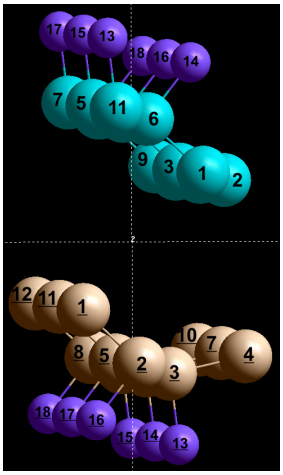
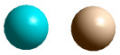
View	Hex Total formation energy -1138.80072 Ry	Bernal Total formation energy -1138.80650 Ry
Optional		
X-Z		
Y-Z		
	Carbon 	Fluorine 

FIG. 1S Atom numbering in relevant views of the Hex and Bernal $C_{24}F_{12}$ unit cell

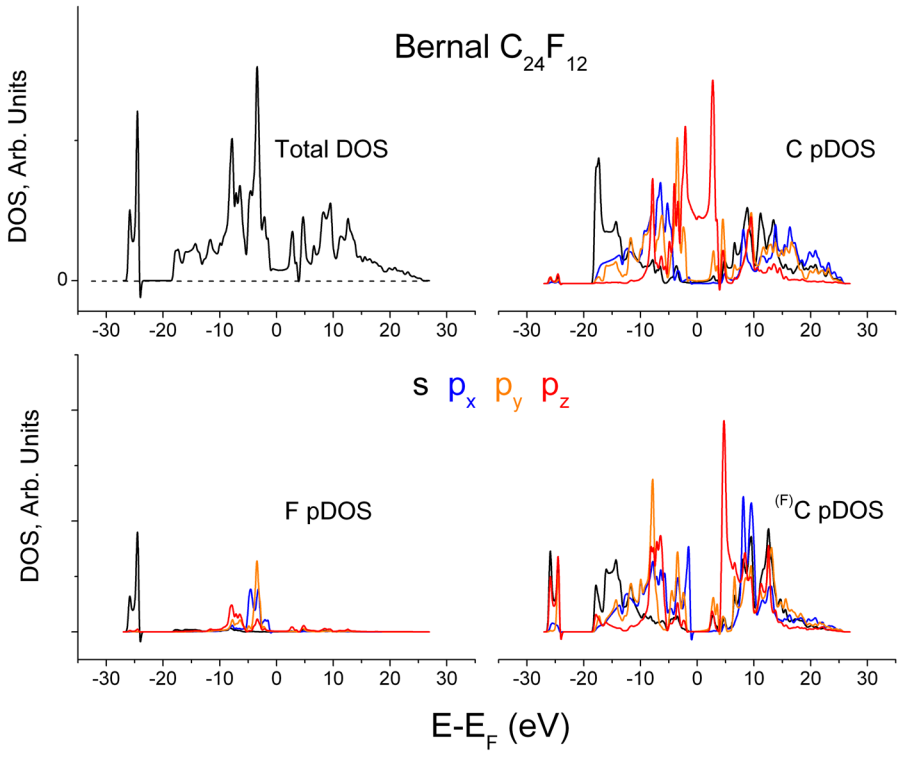


FIG. 1S+ Total and partial DOS of the Bernal $C_{24}F_{12}$ unit cell, close to those of Hex structure; there is a preference 0.08 eV in the formation energy as compared to Hex $C_{24}F_{12}$

Table 2S Optimized bilayer hexagonal $C_{24}F_{12}Br_2$ unit cell #1; $\alpha_0 = 0^\circ$

(a) Optimized Cartesian coordinates of atoms numbered as in Fig. 1S (Å)

Top C_{12} Layer				Lower C_{12} Layer			
No.	X	Y	Z	No.	X	Y	Z
C #1	5.01567	0.00684	4.12294	C #1	5.01614	0.00586	-0.77668
C #2	5.03752	1.36	4.82889	C #2	5.03816	1.35938	-1.48197
C #3	3.7898	2.23866	4.83553	C #3	3.79031	2.23776	-1.48916
C #4	3.80421	3.58067	4.1129	C #4	3.80477	3.57974	-0.76642
C #5	2.52874	1.36115	4.84741	C #5	2.52945	1.3599	-1.50069
C #6	1.2786	2.23563	4.84808	C #6	1.27928	2.23452	-1.50147
C #7	1.29924	3.58149	4.13861	C #7	1.29998	3.58036	-0.79158
C #8	0.01674	1.35899	4.8357	C #8	0.01722	1.35821	-1.48827
C #9	-1.23091	2.23806	4.82792	C #9	-1.23031	2.23752	-1.48004
C #10	-1.20982	3.5919	4.12173	C #10	-1.20926	3.59117	-0.77327
C #11	2.5072	0.01683	4.13714	C #11	2.50798	0.01598	-0.78934
C #12	0.00177	0.01761	4.11248	C #12	0.00234	0.01679	-0.76487
F #13	3.79263	2.78297	6.12957	F #13	3.79317	2.78174	-2.78332
F #14	1.27286	2.7743	6.14508	F #14	1.27345	2.77286	-2.79854
F #15	-1.23718	2.7793	6.12386	F #15	-1.23662	2.77952	-2.77567
F #16	5.04447	0.82108	6.12604	F #16	5.04559	0.82087	-2.7793
F #17	2.53738	0.82078	6.1442	F #17	2.5383	0.81848	-2.79701
F #18	0.01347	0.81389	6.1298	F #18	0.01334	0.81291	-2.78225
Br #1	3.5122	1.66995	1.6731	Br #2	0.28869	1.9726	1.67354

(b) Angles between the Br-Br axis and Carbon triplets representing the planes

Top C_{12} Layer			Lower C_{12} Layer		
C #4, 6, 10	C #3, 5, 9	C #1, 5, 12	C #4, 6, 10	C #3, 5, 9	C #1, 5, 12
2.4°	0.2°	2.4°	2.4°	0.2°	2.4°

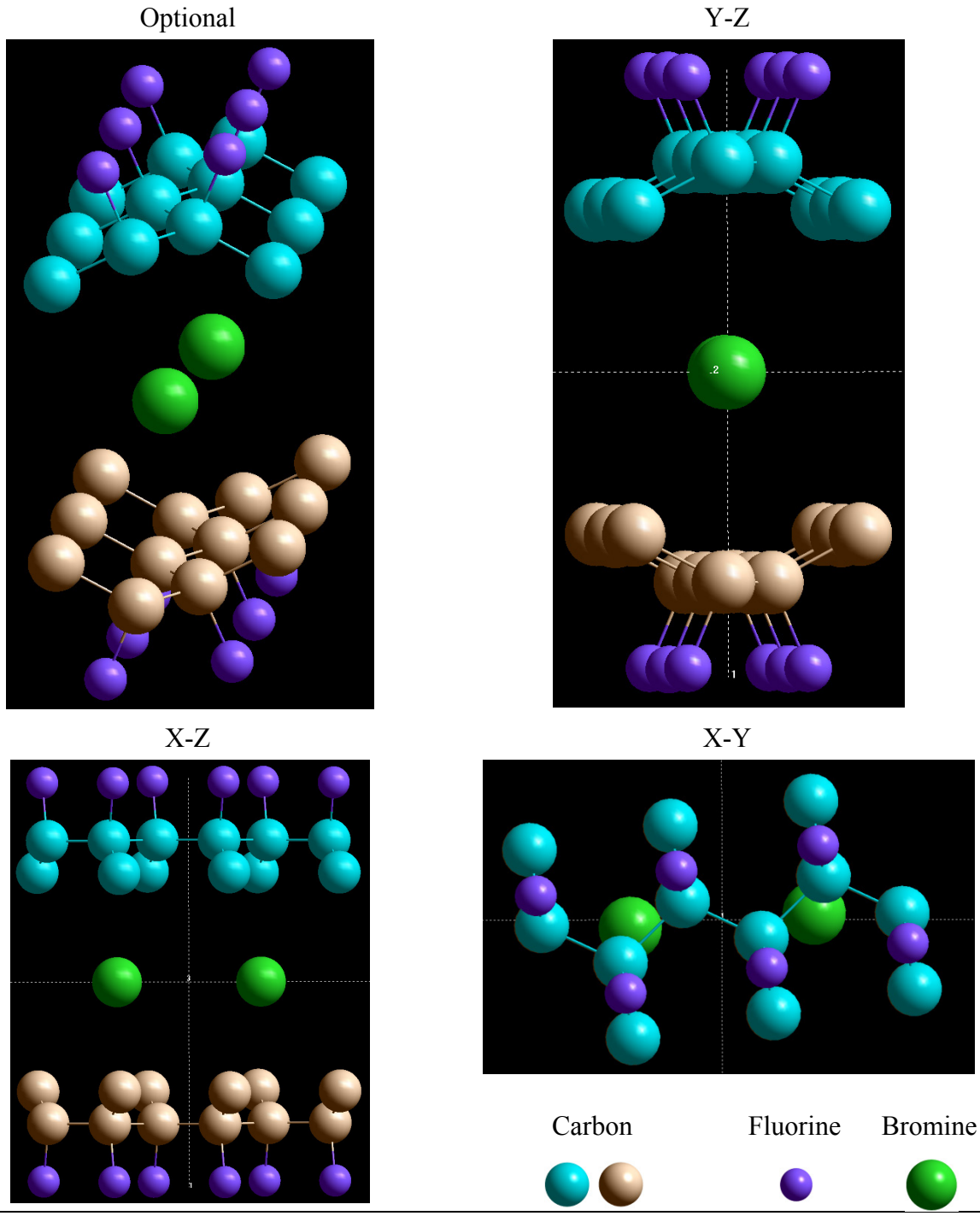


FIG. 2S Relevant views of the hexagonal $C_{24}F_{12}Br_2$ unit cell #1

Table 3S Optimized bilayer hexagonal $C_{24}F_{12}Br_2$ unit cell #2; $\alpha_0 = 90^\circ$

(a) Optimized Cartesian coordinates of atoms numbered as in Fig. 1S (Å)

Top $C_{12}F_6$ Layer				Lower $C_{12}F_6$ Layer			
No.	X	Y	Z	No.	X	Y	Z
C #1	5.02893	-0.01045	5.04187	C #1	5.00753	-0.0328	-1.69633
C #2	5.04379	1.34488	5.75767	C #2	5.01628	1.31693	-2.42001
C #3	3.7954	2.22631	5.75548	C #3	3.76804	2.19853	-2.42163
C #4	3.80421	3.57595	5.03147	C #4	3.78345	3.55385	-1.70663
C #5	2.53721	1.34292	5.76871	C #5	2.50583	1.32226	-2.4274
C #6	1.28591	2.21804	5.77348	C #6	1.25705	2.20616	-2.44064
C #7	1.30101	3.56976	5.06322	C #7	1.27085	3.53297	-1.67299
C #8	0.02478	1.3372	5.77626	C #8	-0.00365	1.32494	-2.43716
C #9	-1.22399	2.22114	5.76356	C #9	-1.2548	2.19956	-2.43351
C #10	-1.19839	3.57359	5.05274	C #10	-1.24078	3.55419	-1.72273
C #11	2.5233	-0.01142	5.05702	C #11	2.47995	-0.0305	-1.71691
C #12	0.01116	0.0103	5.00899	C #12	-0.01909	-0.02708	-1.72836
F #13	3.80172	2.77525	7.04544	F #13	3.77122	2.73567	-3.71613
F #14	1.28557	2.75967	7.06732	F #14	1.26204	2.74486	-3.72844
F #15	-1.23079	2.76906	7.05498	F #15	-1.26079	2.73008	-3.73123
F #16	5.03943	0.80738	7.0518	F #16	5.00896	0.76806	-3.70988
F #17	2.54471	0.80992	7.0654	F #17	2.5145	0.77388	-3.71861
F #18	0.01855	0.7987	7.06412	F #18	-0.00312	0.78274	-3.73096
Br #1	0.84147	2.51396	0.7117	Br #2	0.46565	1.03463	2.6313

(b) Angles between the Br-Br axis and Carbon triplets representing the planes

Top C_{12} Layer			Lower C_{12} Layer		
C #4, 6, 10	C #3, 5, 9	C #1, 5, 12	C #4, 6, 10	C #3, 5, 9	C #1, 5, 12
23.7°	50.8°	78.0°	77.3°	51.7°	24.2°

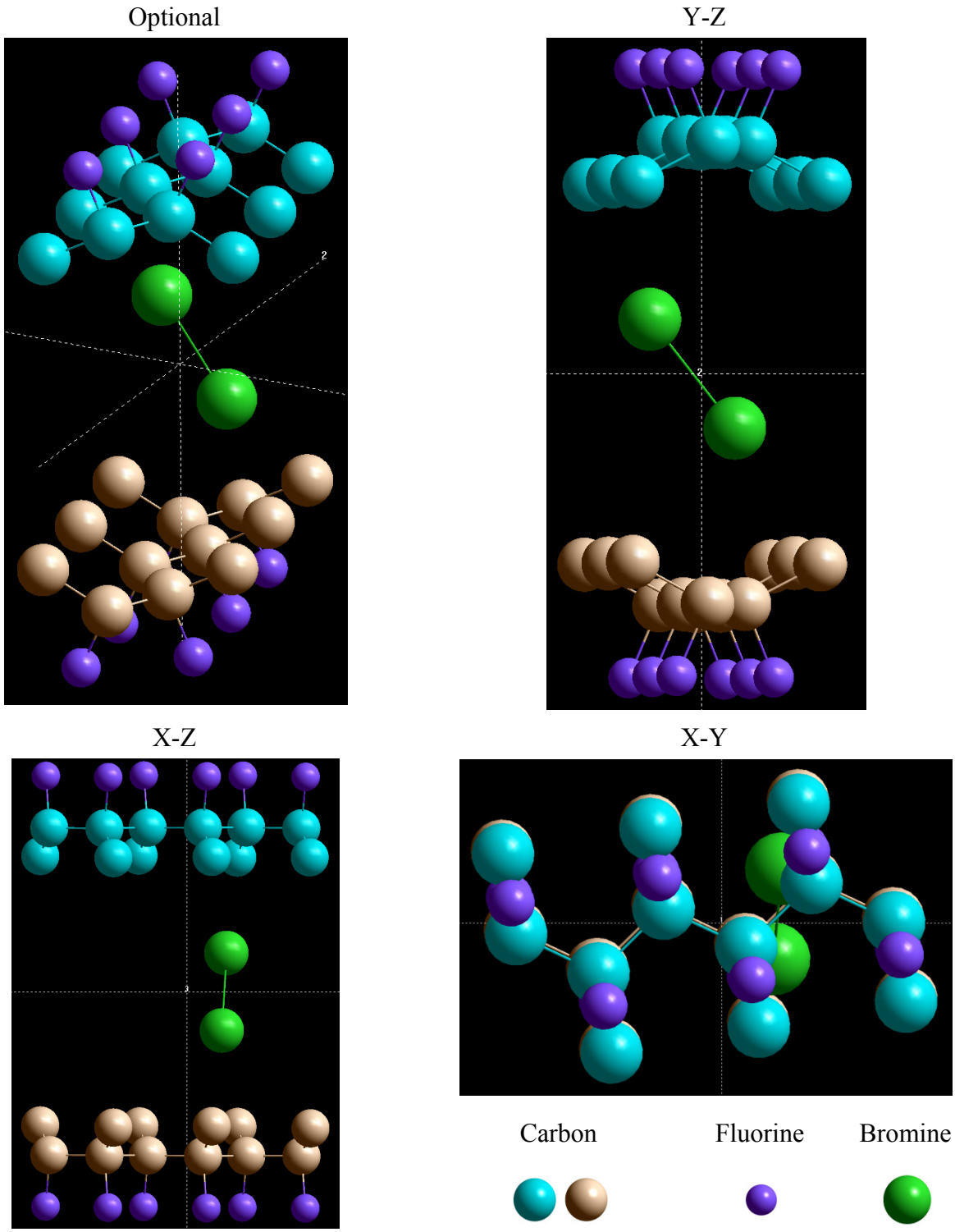


FIG. 3S Relevant views of the hexagonal $C_{24}F_{12}Br_2$ unit cell #2

Table 4S Optimized bilayer Bernal $C_{24}F_{12}Br_2$ unit cell #3; $\alpha_0 = 0^\circ$

(a) Optimized Cartesian coordinates of atoms numbered as in Fig. 1S (Å)

Top $C_{12}F_6$ Layer				Lower $C_{12}F_6$ Layer			
No.	X	Y	Z	No.	X	Y	Z
C #1	0.0827	1.39277	4.9707	C #1	-1.30555	3.32322	-1.69635
C #2	1.32988	0.71346	4.97347	C #2	-1.32225	1.9722	-2.41741
C #3	2.59193	1.39131	4.96803	C #3	-0.07359	1.09179	-2.41616
C #4	2.61015	2.74472	5.68395	C #4	-0.09063	-0.26053	-1.69777
C #5	1.36212	3.62419	5.68661	C #5	1.18794	1.97005	-2.416
C #6	0.10104	2.74477	5.68867	C #6	2.43682	1.0905	-2.4158
C #7	3.87107	3.62361	5.68478	C #7	2.4198	-0.26026	-1.69725
C #8	5.11987	2.74479	5.68791	C #8	3.69692	1.97044	-2.41646
C #9	5.1012	1.39414	4.97097	C #9	4.94686	1.09285	-2.41958
C #10	3.83994	0.715	4.96869	C #10	4.92978	-0.25931	-1.70427
C #11	-1.14819	3.6232	5.69033	C #11	1.20497	3.32379	-1.70022
C #12	6.34841	0.71581	4.97132	C #12	3.71394	3.32373	-1.70157
F #13	-1.1496	4.16165	6.98408	F #13	-0.07243	0.55183	-3.70878
F #14	0.10515	2.20459	6.98147	F #14	2.43931	0.54914	-3.70855
F #15	1.36133	4.16491	6.97974	F #15	4.94836	0.55563	-3.71383
F #16	2.61302	2.20491	6.97722	F #16	-1.32235	2.51518	-3.70883
F #17	3.86781	4.16579	6.97696	F #17	1.18685	2.50886	-3.70912
F #18	5.12096	2.20738	6.98239	F #18	3.6941	2.51232	-3.70873
Br #1	1.80501	2.37914	1.70353	Br #2	3.79739	3.64548	1.95866

(b) Angles between the Br-Br axis and Carbon triplets representing the planes

Top C_{12} Layer			Lower C_{12} Layer		
C #2, 3, 12	C #1, 4, 9	C #5, 6, 8	C #4, 6, 10	C #3, 5, 9	#1, 5, 12
6.4°	8.9°	6.2°	20.2°	6.2°	8.9°

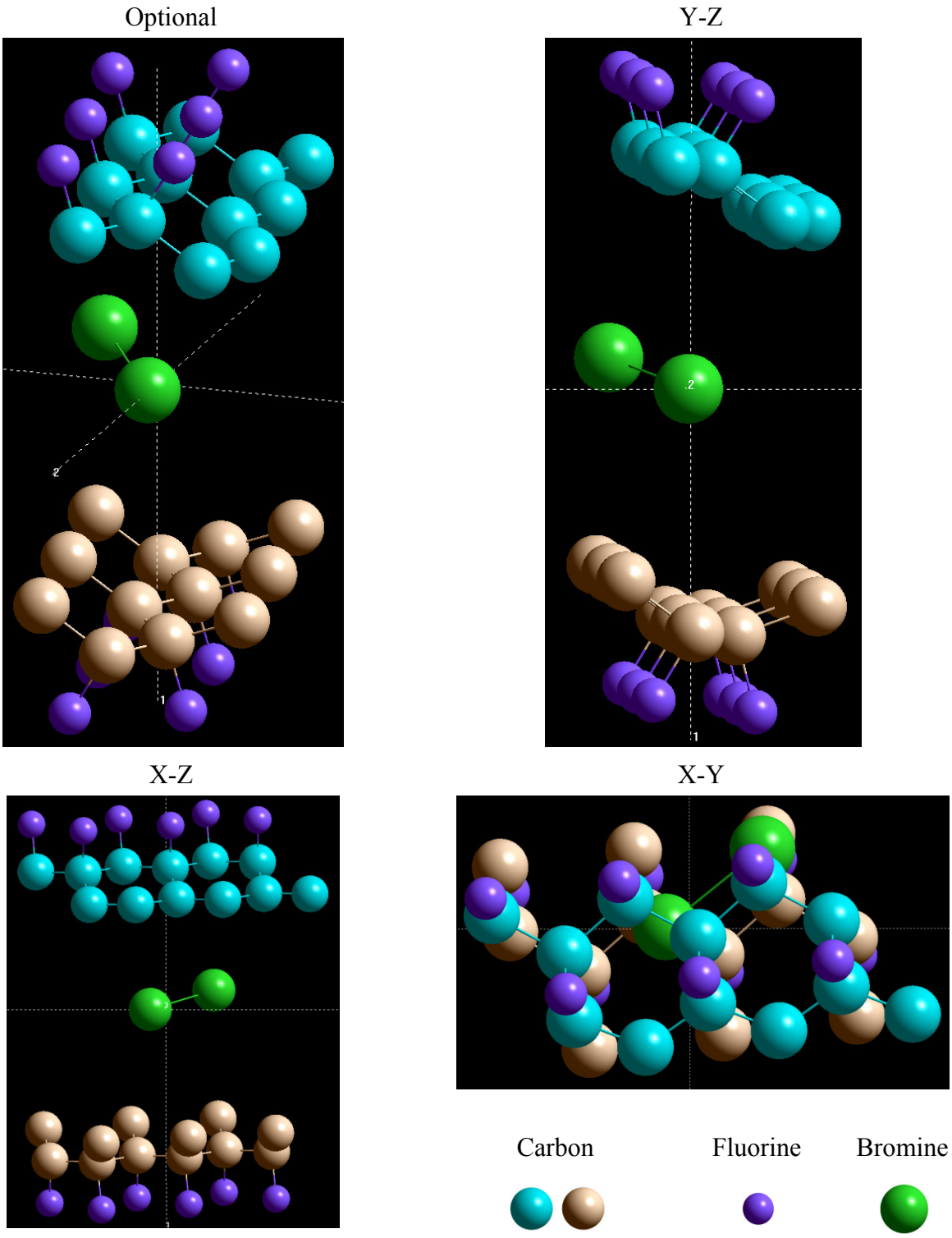


FIG. 4S Relevant views of the Bernal $C_{24}F_{12}Br_2$ unit cell #3

Table 5S Optimized bilayer Bernal $C_{24}F_{12}Br_2$ unit cell #4; $\alpha_0 = 90^\circ$

(a) Optimized Cartesian coordinates of atoms numbered as in Fig. 1S (Å)

Top Layer Nos. 1-12				Lower Layer Nos. 1-12			
No.	X	Y	Z	No.	X	Y	Z
C #1	0.17566	1.83587	3.9331	C #1	-1.23931	3.27862	-1.04744
C #2	1.45365	1.05036	4.14863	C #2	-1.25455	1.92679	-1.76644
C #3	2.64758	1.7314	4.2524	C #3	-0.00508	1.04713	-1.76623
C #4	2.68217	3.09304	4.9438	C #4	-0.01995	-0.30483	-1.04701
C #5	1.42569	3.94489	4.94354	C #5	1.2552	1.92731	-1.76621
C #6	0.15943	3.04701	4.90897	C #6	2.5048	1.04791	-1.76658
C #7	3.94873	3.99166	4.9148	C #7	2.48849	-0.30312	-1.04636
C #8	5.18579	3.07351	4.8992	C #8	3.7656	1.92689	-1.76623
C #9	5.11509	1.7283	4.15349	C #9	5.01507	1.04706	-1.76504
C #10	3.9214	1.04671	4.25447	C #10	4.99932	-0.3047	-1.04409
C #11	-1.07712	3.96554	4.89537	C #11	1.27125	3.2784	-1.04387
C #12	6.39289	0.9421	3.93718	C #12	3.78133	3.27667	-1.04436
F #13	-1.09218	4.48801	6.19411	F #13	-0.00505	0.50633	-3.05896
F #14	0.151	2.45085	6.14766	F #14	2.50565	0.50735	-3.05884
F #15	1.38105	4.46068	6.24464	F #15	5.01424	0.50479	-3.05653
F #16	2.72436	2.57472	6.24385	F #16	-1.25531	2.46515	-3.06002
F #17	3.95471	4.58258	6.15546	F #17	1.25525	2.46802	-3.0583
F #18	5.20373	2.55307	6.1989	F #18	3.76617	2.46781	-3.05838
Br #1	-1.24157	-0.00181	2.16056	Br #2	0.28781	2.78119	2.15228

(b) Angles between the Br-Br axis and Carbon triplets representing the planes

Top C_{12} Layer			Lower C_{12} Layer		
C #2, 3, 12	C #1, 4, 9	C #5, 6, 8	C #4, 6, 10	C #3, 5, 9	#1, 5, 12
9.9°	31.4°	2.2°	24.2°	0.1°	24.5°

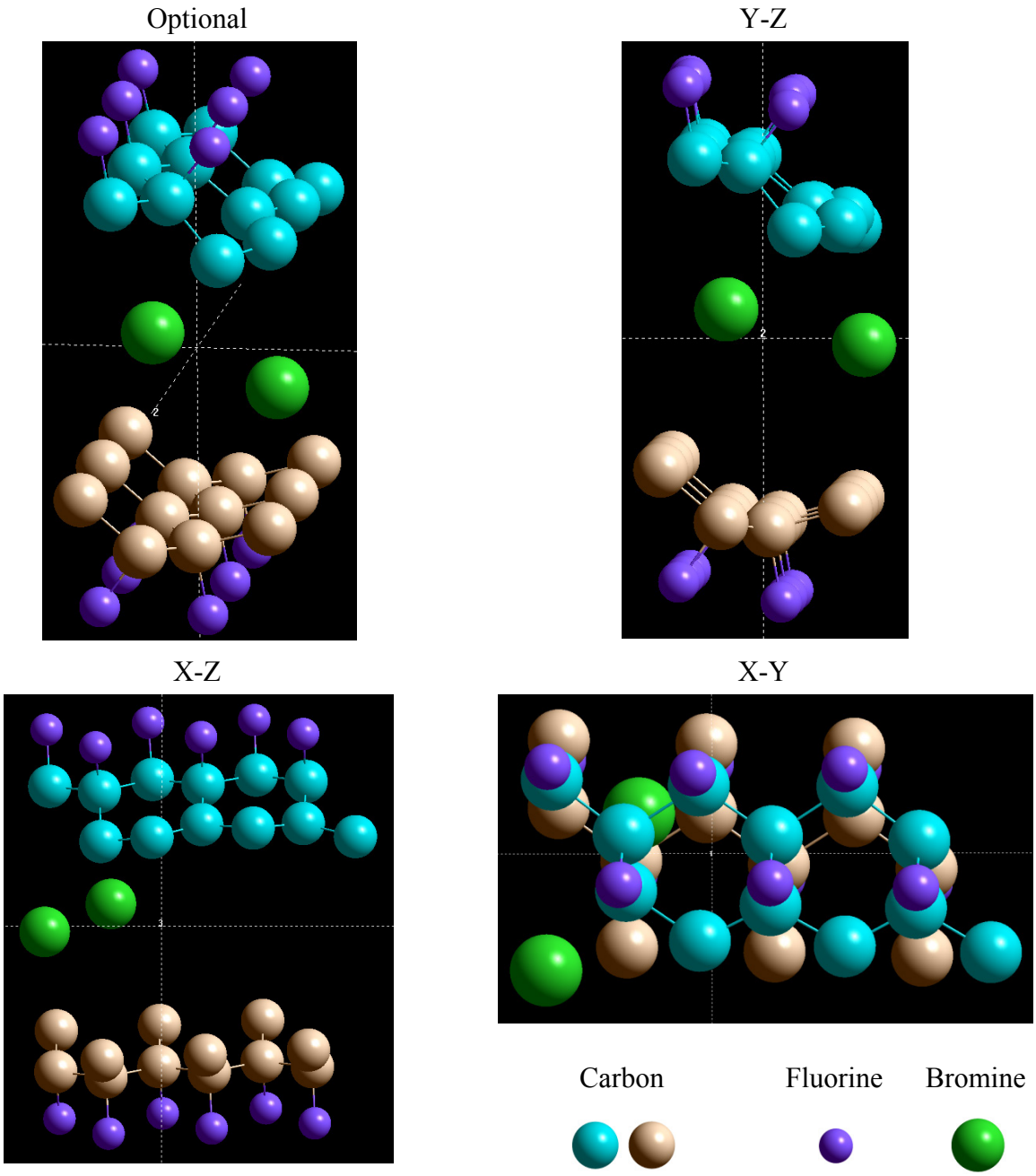


FIG. 5S Relevant views of the Bernal $C_{24}F_{12}Br_2$ unit cell #4

Table 6S Optimized bilayer Bernal $C_{24}F_{12}Br_2$ unit cell #5; $\alpha_0 = 52^\circ$

(a) Optimized Cartesian coordinates of atoms numbered as in Fig. 1S (Å)

Top $C_{12}F_6$ Layer				Lower $C_{12}F_6$ Layer			
No.	X	Y	Z	No.	X	Y	Z
C #1	0.07857	1.35946	4.24895	C #1	-1.23307	3.59509	-1.04998
C #2	1.32901	0.68114	4.25326	C #2	-1.28426	2.2493	-1.76944
C #3	2.58793	1.35914	4.25178	C #3	-0.03833	1.36315	-1.7338
C #4	2.60743	2.7101	4.97423	C #4	-0.0639	0.0811	-0.86513
C #5	1.35856	3.59003	4.97594	C #5	1.2213	2.24282	-1.71441
C #6	0.097	2.71008	4.97291	C #6	2.46633	1.36011	-1.76111
C #7	3.86824	3.59097	4.97404	C #7	2.41499	0.01125	-1.04736
C #8	5.11689	2.71106	4.97569	C #8	3.73081	2.24706	-1.76698
C #9	5.09758	1.35933	4.25626	C #9	4.98289	1.36049	-1.76941
C #10	3.83757	0.68027	4.2524	C #10	4.99995	0.0157	-1.05734
C #11	-1.151	3.59035	4.97394	C #11	1.24676	3.53665	-0.85015
C #12	6.34534	0.6812	4.25176	C #12	3.71578	3.59121	-1.05545
F #13	-1.15268	4.13131	6.26617	F #13	-0.01531	0.77698	-2.98786
F #14	0.09949	2.16686	6.26382	F #14	2.46435	0.85407	-3.06699
F #15	1.35447	4.12808	6.26859	F #15	4.96536	0.82435	-3.06716
F #16	2.61266	2.17009	6.26668	F #16	-1.28975	2.76003	-3.07344
F #17	3.8661	4.13427	6.26511	F #17	1.20505	2.85163	-2.96026
F #18	5.12104	2.17475	6.27024	F #18	3.74688	2.77922	-3.0667
Br #1	-0.11852	0.40013	1.14058	Br #2	1.31456	3.4143	1.18964

(b) Angles between the Br-Br axis and Carbon triplets representing the planes

Top C_{12} Layer			Lower C_{12} Layer		
C #2, 3, 12	C #1, 4, 9	C #5, 6, 8	C #4, 6, 10	C #3, 5, 9	#1, 5, 12
0.9°	24.4°	0.7°	29.9°	0.7°	22.6°

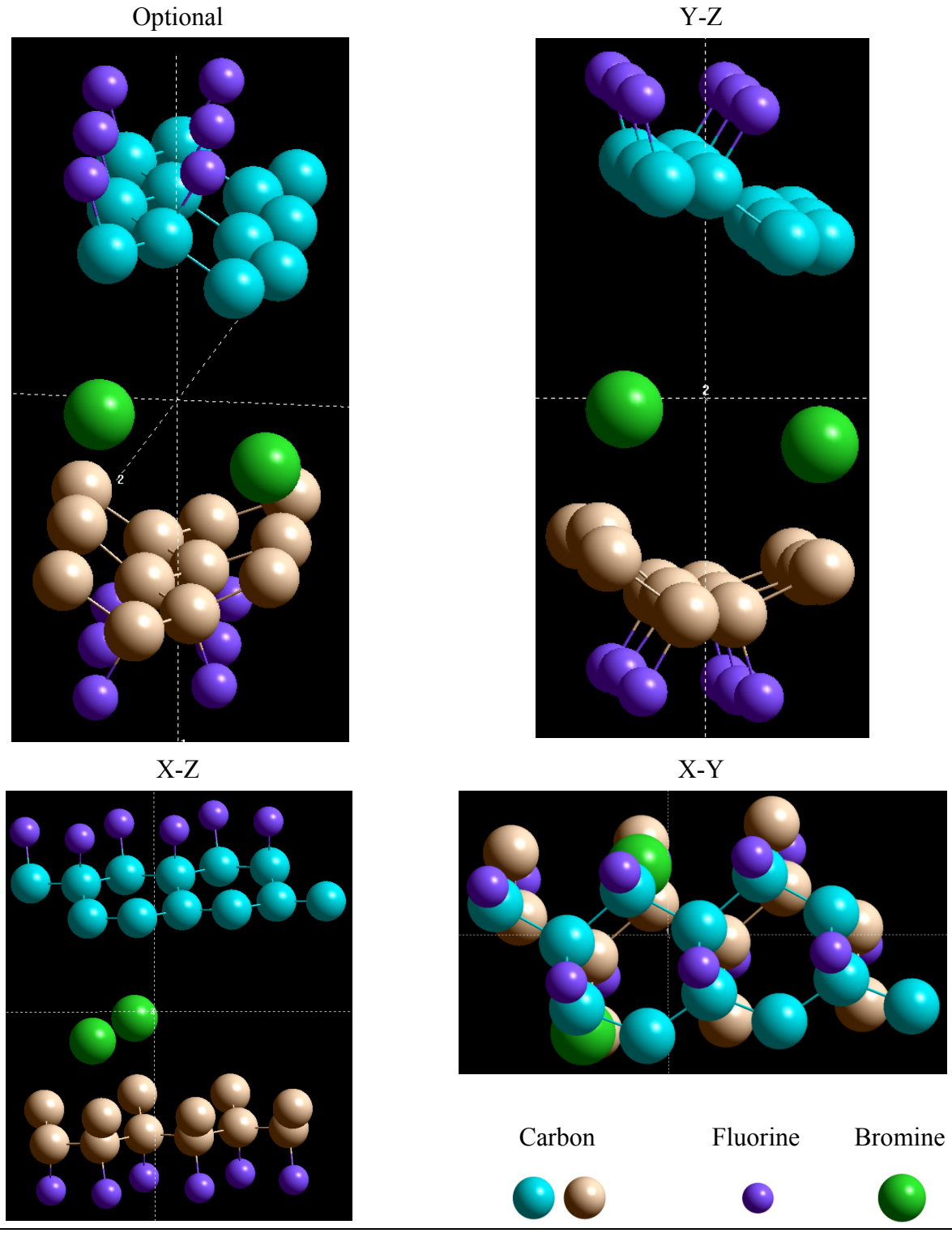


FIG. 6S Relevant views of the Bernal $C_{24}F_{12}Br_2$ unit cell #5

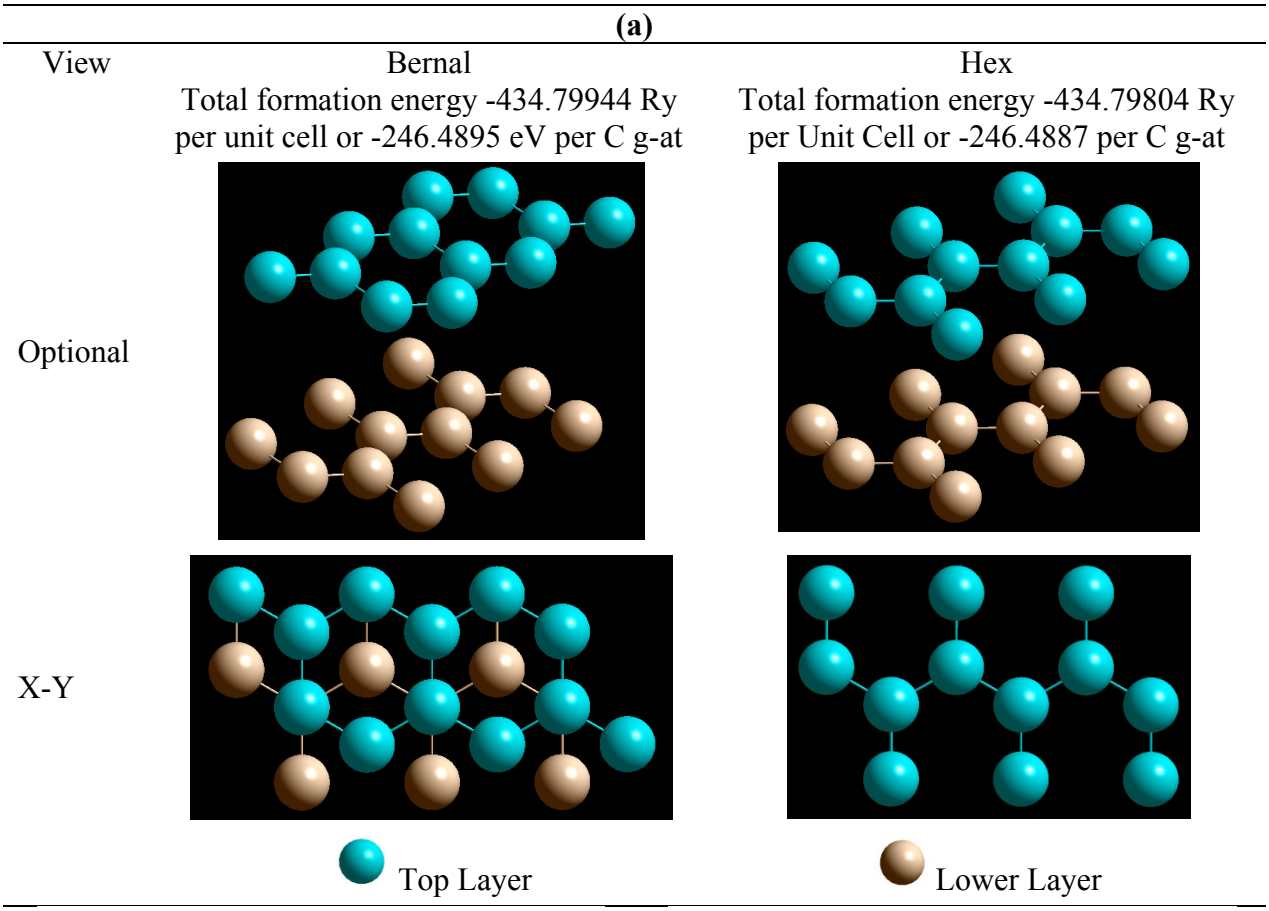
Table 7S Optimized bilayer Bernal and hexagonal C_{24} unit cells

(a) Lattice parameters (*a, b*), interlayer space (d_{layer}) and C-C (d_{C-C}) bond length (Å)

a	*b*	d_{layer}	d_{C-C}
7.38	4.92	3.96	1.42

(b) Optimized Cartesian coordinates of atoms (Å) numbered as in Fig. 1S

Top C_{12} Layer				Lower C_{12} Layer			
			Bernal				
No.	X	Y	Z	No.	X	Y	Z
C #1	9.65796E-5	1.59046	3.57131	C #1	-1.23016	3.38041	-0.38863
C #2	1.22977	0.88037	3.5708	C #2	-1.23	1.9601	-0.38858
C #3	2.4601	1.59045	3.57114	C #3	2.706E-5	1.24994	-0.38803
C #4	2.45995	3.01075	3.57092	C #4	1.74901E-4	-0.17035	-0.3882
C #5	1.22992	3.72091	3.57045	C #5	1.22999	1.96011	-0.38842
C #6	-5.89441E-5	3.01076	3.57114	C #6	2.46002	1.24995	-0.3879
C #7	3.68992	3.72091	3.5705	C #7	2.46017	-0.17034	-0.38802
C #8	4.91995	3.01076	3.57112	C #8	3.69	1.9601	-0.3885
C #9	4.9201	1.59045	3.57111	C #9	4.92003	1.24994	-0.38807
C #10	3.68978	0.88036	3.57053	C #10	4.92018	-0.17035	-0.38817
C #11	-1.23009	3.72092	3.57071	C #11	1.22984	3.38041	-0.38856
C #12	6.14977	0.88037	3.57068	C #12	3.68985	3.3804	-0.38872
			Hexagonal				
C #1	-1.23016	3.38041	3.5708	C #1	-1.23016	3.38041	-0.38863
C #2	-1.23	1.9601	3.5708	C #2	-1.23	1.9601	-0.38858
C #3	2.706E-5	1.24994	3.5708	C #3	2.706E-5	1.24994	-0.38803
C #4	1.74901E-4	-0.17035	3.5708	C #4	1.74901E-4	-0.17035	-0.3882
C #5	1.22999	1.96011	3.5708	C #5	1.22999	1.96011	-0.38842
C #6	2.46002	1.24995	3.5708	C #6	2.46002	1.24995	-0.3879
C #7	2.46017	-0.17034	3.5708	C #7	2.46017	-0.17034	-0.38802
C #8	3.69	1.9601	3.5708	C #8	3.69	1.9601	-0.3885
C #9	4.92003	1.24994	3.5708	C #9	4.92003	1.24994	-0.38807
C #10	4.92018	-0.17035	3.5708	C #10	4.92018	-0.17035	-0.38817
C #11	1.22984	3.38041	3.5708	C #11	1.22984	3.38041	-0.38856
C #12	3.68985	3.3804	3.5708	C #12	3.68985	3.3804	-0.38872



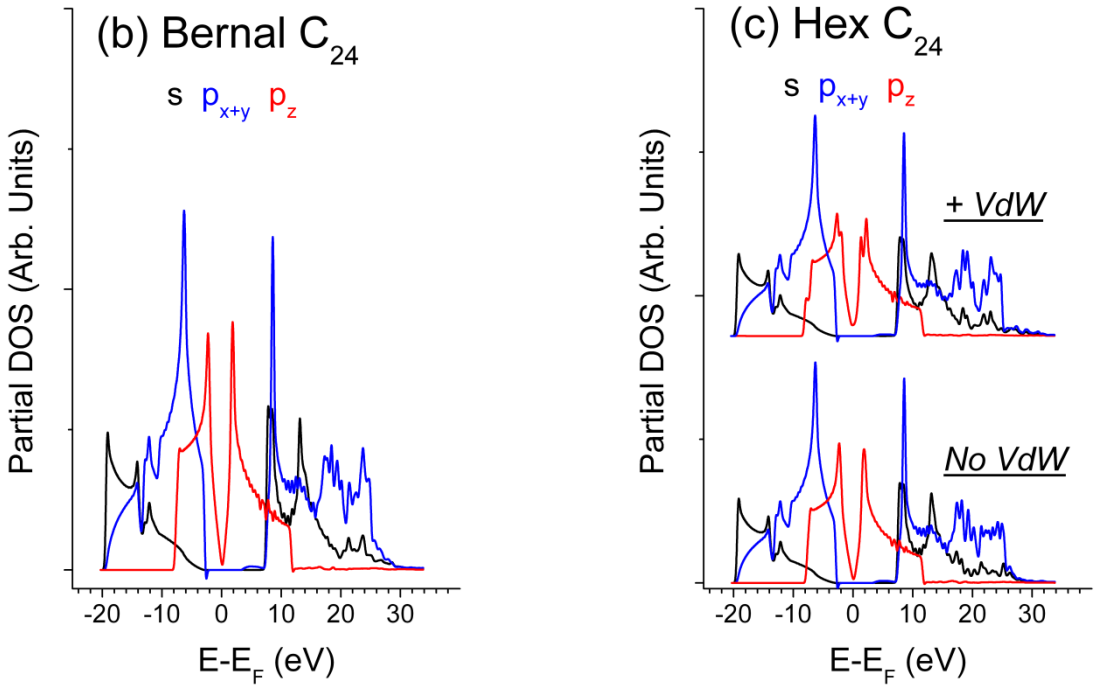


FIG. 7S (a) Relevant views of the bilayer Bernal and Hex C_{24} Unit Cell; **(b)** Partial DOS of the Bernal C_{24} unit cell, close to those of hexagonal structure ($p_x = p_y$); **(c)** Partial DOS affected by the van der Waals (VdW) interaction in Hex C_{24} unit cell ($p_x = p_y$).

Table 8S Optimized bilayer $C_{24}F_{12}Br_2$ unit cells: Summary

Total E and relative ΔE formation energy; enthalpy ΔH of reaction $C_{24}F_{12} + Br_2 \rightarrow C_{24}F_{12}Br_2$; interlayer distance ($d_{layer}$); C-C ($d_{C-C}$), C-F ($d_{C-F}$), and Br-Br ($d_{Br-Br}$) bond length/distance at lattice parameters a = 2.51 Å × 3, b = 2.46 Å × 2 and angles between Br-Br axis and skeleton C planes before (α_0) and after (α) optimization

E per Unit Cell (Ry)	ΔE per C_2F (eV)	ΔH per Unit Cell (eV)	d_{layer} (Å)	d_{C-C} (Å)	d_{C-F} (Å)	d_{Br-Br} (Å)
Hexagonal $C_{24}F_{12}Br_2$ unit cell #1; $\alpha_0 = 0^\circ$; α = 0.2-2.4°						
-1540.50463	0	+0.25456	4.88, 6.32	1.43, 1.43, 1.52, 1.53, 1.53, 1.54	1.40	3.24, 4.92*
Hexagonal $C_{24}F_{12}Br_2$ unit cell #2; $\alpha_0 = 90^\circ$; α = 23.7-78.0°						
-1540.56292	0.0661	-0.53851	6.74, 8.21	1.43, 1.45, 1.53, 1.53, 1.53, 1.54	1.40	2.45, 4.92*
Bernal $C_{24}F_{12}Br_2$ unit cell #3; $\alpha_0 = 0^\circ$; α = 6.2-20.2°						
-1540. 52977	0.0285	-0.00884	7.38, 7.39	1.42, 1.43, 1.53, 1.53, 1.53, 1.54	1.40	2.37, 4.92*
Bernal $C_{24}F_{12}Br_2$ unit cell #4; $\alpha_0 = 90^\circ$; α = 0.1-31.4°						
-1540. 59827	0.1061	-0.94083	5.70, 5.98, 6.02	1.33, 1.42, 1.44, 1.53, 1.54, 1.55	1.37 1.40	3.18, 4.25*, 4.92*
Bernal $C_{24}F_{12}Br_2$ unit cell #5; $\alpha_0 = 52^\circ$; α = 0.7-29.9°						
-1540.55885	0.0615	-0.40450	5.11, 5.82, 6.74	1.36, 1.42, 1.43, 1.45, 1.50, 1.52, 1.53, 1.54	1.38 1.39 1.40	3.34, 4.09*, 4.92*

*For Br atoms in X-Y adjacent cells