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Supporting Information for "The Interaction of Halogen Atoms and Molecules with Borophene"

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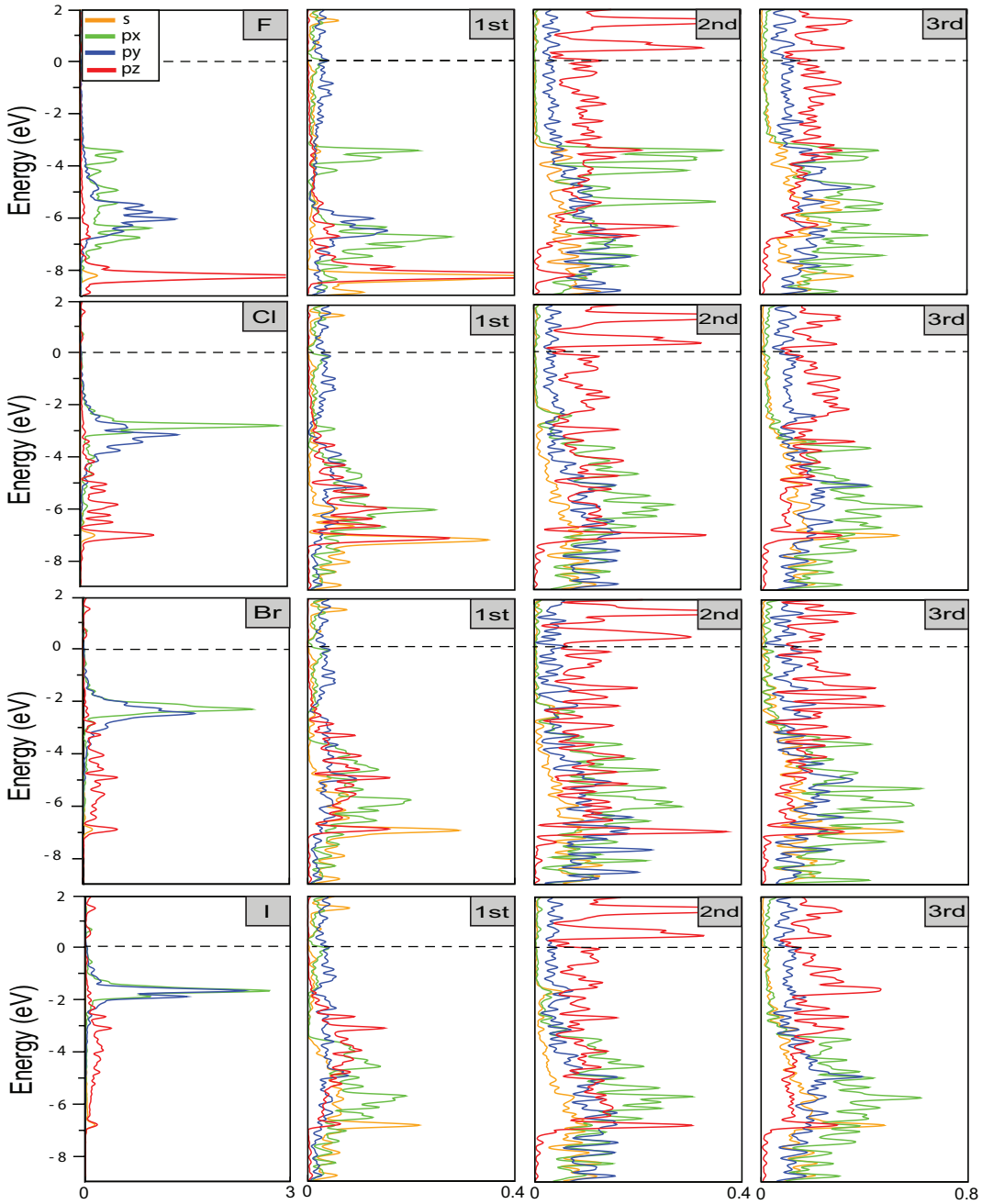

Figure 1: Orbital decomposed projected density of states (PDOS) of all halogen atoms and first, second, third nearest B atoms.

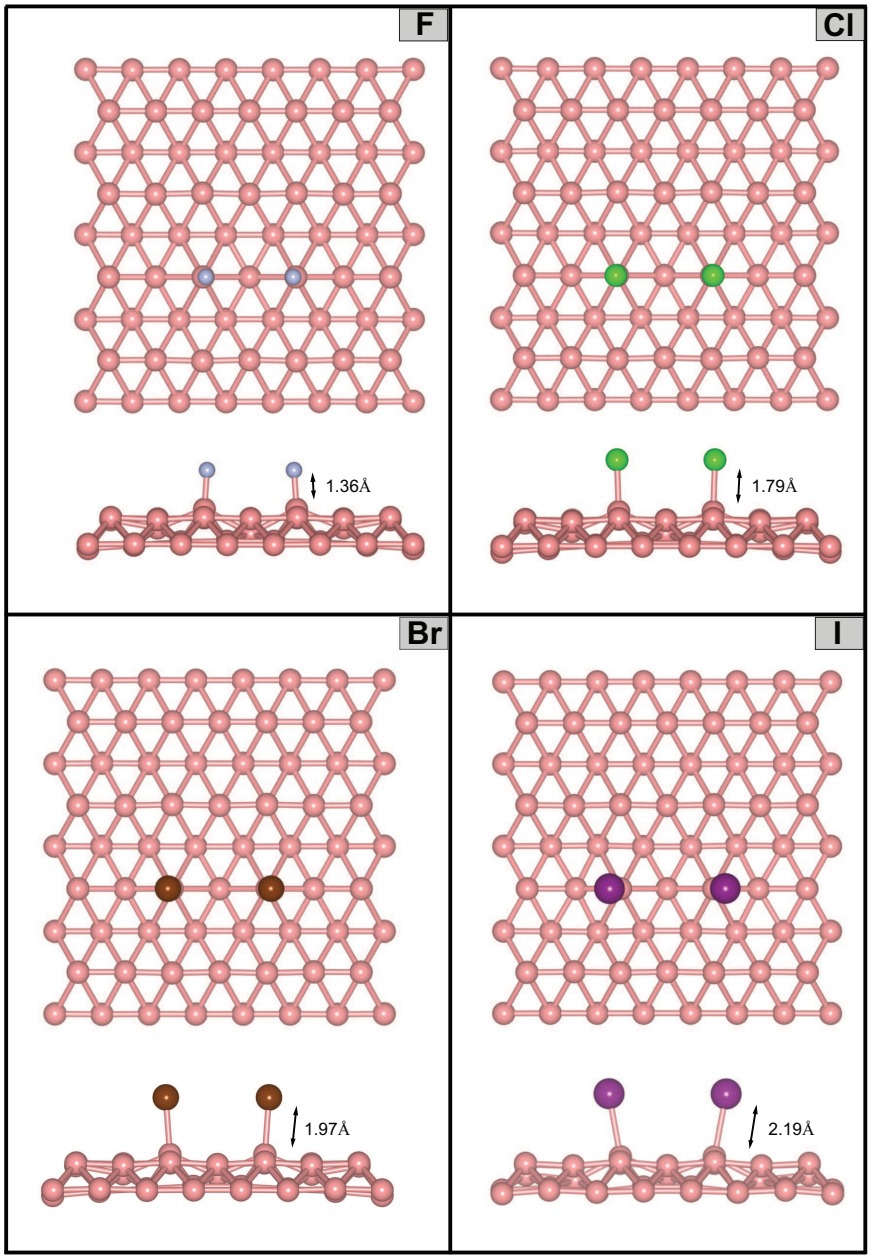

Figure 2: The final configurations of halogen molecule adsorption on borophene. All halogen molecules dissociates into separate atoms.

Lattice vectors and coordinates

Borophene + F

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0.0000000000	11.4547996521	0.0000000000
0.0000000000	0.0000000000	14.9732999802

B	F
56	1

Cartesian

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11.305632241	8.591947726	7.902937534	B4
1.614906209	11.453780293	7.845096020	B5
1.600027952	2.838877347	7.838402433	B6
1.600027952	5.752188084	7.838432778	B7
1.614906209	8.592084961	7.845111192	B8
3.224702444	11.449323923	7.883996469	B9
3.211429519	2.837663230	7.968730136	B10
3.211429519	5.753402030	7.968805105	B11
3.224702444	8.596529041	7.884026813	B12
4.847759811	11.448556501	7.860428796	B13
4.852802397	2.829312572	7.968730136	B14
4.852802397	5.761752858	7.968835449	B15
4.847759811	8.597285538	7.860473420	B16
6.457816161	11.448568108	7.860533216	B17
6.452796487	2.829335444	7.968910417	B18
6.452796487	5.761729645	7.969014837	B19
6.457816161	8.597273931	7.860577840	B20
8.080884648	11.449335530	7.884041093	B21
8.094157909	2.837674666	7.968880073	B22
8.094157909	5.753391106	7.968955041	B23
8.080884648	8.596518117	7.884056265	B24
9.690669764	11.453791899	7.845096020	B25
9.705536734	2.838888783	7.838447950	B26
9.705536734	5.752176477	7.838492574	B27
9.690669764	8.592073354	7.845111192	B28
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0.798205050	4.295526997	8.775506356	B30
0.802263783	7.169948620	8.800946448	B31
0.808074920	10.022938089	8.757762997	B32
2.406101808	1.411059510	8.795511256	B33
2.403942384	4.295526997	8.615442171	B34
2.406101808	7.180017271	8.795555880	B35
2.419238947	10.022938089	8.772512092	B36
4.038723950	1.424736544	8.742820234	B37
4.074438842	4.295526997	8.357497222	B38
4.038723950	7.166328631	8.742895202	B39
4.041855771	10.022938089	8.738088314	B40
5.652782427	1.393923106	8.854610271	B41
5.652748396	4.295481252	9.140421068	B42
5.652782427	7.197130632	8.854685239	B43
5.652782427	10.022938089	8.809256313	B44
7.266851686	1.424725108	8.742895202	B45

7.231170824	4.295526997	8.357796202	B46
7.266851686	7.166340238	8.742954998	B47
7.263731658	10.022938089	8.738058862	B48
8.899474333	1.411036552	8.795646020	B49
8.901633420	4.295526997	8.615742044	B50
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10.507404953	4.295526997	8.775567045	B54
10.503323309	7.169948620	8.800946448	B55
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5.652578917	4.295389421	10.503215686	F1

Borophene + Cl

11.3057003021	0.0000000000	0.0000000000
0.0000000000	11.4547996521	0.0000000000
0.0000000000	0.0000000000	14.9732999802

B	Cl
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Cartesian

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1.599293094	5.749828468	7.833746375	B7
1.614352286	8.592451602	7.841711743	B8
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3.223978705	8.597125090	7.885238798	B12
4.847692087	11.447285204	7.857598748	B13
4.853684159	2.829404232	7.926655143	B14
4.853695278	5.761661369	7.926789907	B15
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6.457906460	11.447308417	7.857822760	B17
6.451925844	2.829473020	7.927164748	B18
6.451925844	5.761604017	7.927299512	B19
6.457906460	8.598545229	7.857868276	B20
8.081664992	11.448751771	7.885194174	B21
8.093196968	2.839576151	7.959012833	B22
8.093196968	5.751500545	7.959087802	B23
8.081664992	8.597101876	7.885238798	B24
9.691257381	11.453436865	7.841711743	B25
9.706294166	2.841271442	7.833790998	B26
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     5.652669216         4.295458380         9.104695165  B42
     5.652782427         7.192583455         8.841763940  B43
     5.652793546        10.022938089         8.810214834  B44
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Borophene + Br
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        0.0000000000        11.4547996521         0.0000000000
        0.0000000000         0.0000000000        14.9732999802
    B   Br
   56    1
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    11.305666609         8.592943872         7.908343275  B4
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     1.599338243         2.841958639         7.832503152  B6
     1.599338243         5.749118398         7.832547776  B7
     1.614205213         8.592967086         7.840962953  B8
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     3.212978415         2.840011410         7.953292941  B10
     3.212978415         5.751065628         7.953383081  B11
     3.223775196         8.597056131         7.885463703  B12
     4.847703543        11.447056479         7.856520634  B13
     4.853718190         2.830572604         7.911233119  B14
     4.853718190         5.760492485         7.911397335  B15
     4.847703543         8.598786243         7.856580430  B16
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7.264025466	10.022938089	8.737444837	B48
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8.899394816	4.295526997	8.613166352	B50
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8.886754994	10.022938089	8.778696073	B52
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10.502418972	7.167634749	8.798520692	B55
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5.650702183	4.295228973	11.046956260	Br1

Borophene + I

11.3057003021	0.0000000000	0.0000000000
0.0000000000	11.4547996521	0.0000000000
0.0000000000	0.0000000000	14.9732999802

B	I
56	1

Cartesian

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4.848359221	8.598064566	7.852882000	B16
6.457397687	11.447834825	7.853361261	B17
6.451247255	2.834112199	7.900646542	B18
6.451235799	5.756964668	7.900736683	B19
6.457397687	8.598007215	7.853436229	B20
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8.091455682	2.841637913	7.945252604	B22
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8.081472938	8.597285538	7.886706925	B24
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4.073183755	4.295526997	8.381574499	B38
4.042986192	7.158493968	8.715628207	B39
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