

First-principles Analysis of Seven Novel Phases of Phosphorene with Chirality

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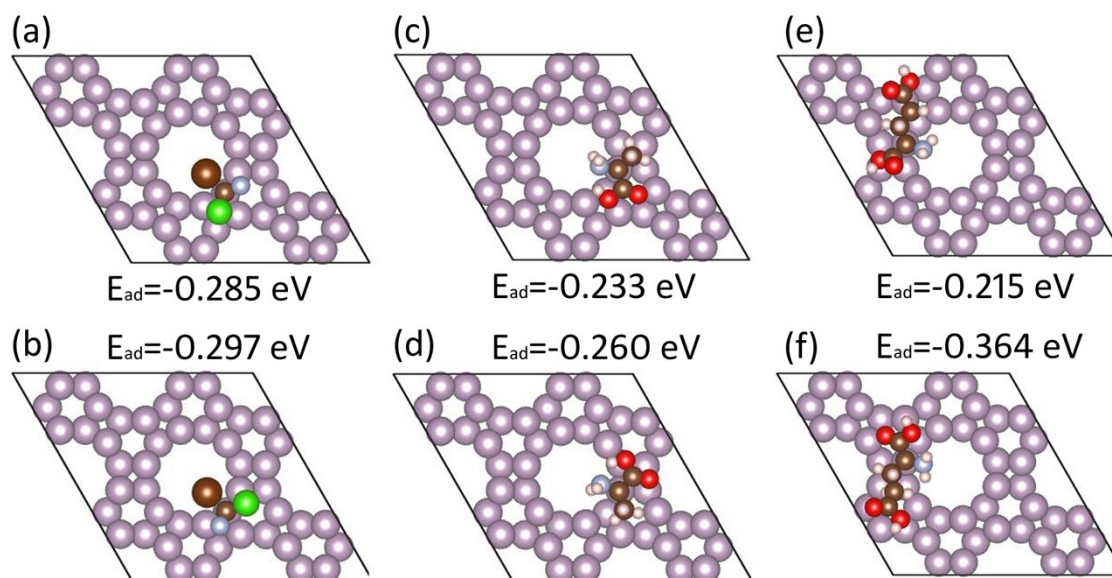


Figure S1. Adsorption structures of enantiomers of CHFClBr (a)(b), alanine (c)(d) and glutamic acid (e)(f). The adsorption energy was denoted and the differences of adsorption energy between enantiomers of CHFClBr, alanine and glutamic acid are 0.012, 0.028 and 0.149 eV, respectively.

Structures of porous phosphorene, IGP-S, DHPP-S and DHPP-2-S (in POSCAR formation):

porous phosphorene

```
1.0000000000000000
  9.8310003281000000    0.0000000000000000    0.0000000000000000
 -4.9155001640000000    8.5138960286999996    0.0000000000000000
  0.0000000000000000    0.0000000000000000    20.0000000000000000
H    P
  6    12
```

Direct

```
0.1555913162346911  0.3074276987611526  0.5132179273602020
0.3075167133905836  0.1539091960439620  0.4868100554797365
0.8480470250410050  0.1544956767659116  0.4870691811226777
0.1544420361109573  0.8471466079712400  0.5132262343232341
0.6948602663109682  0.8474201954605860  0.5130509237697396
0.8473552432369402  0.6942446394938386  0.4869757317633017
0.4459288994968418  0.2231937285515855  0.5278228172968937
0.5551169178629110  0.1090533735788455  0.4673795777853513
0.7783685891401078  0.2235967313054061  0.5278522011455991
0.1093298275083256  0.5544336386873070  0.5326379778567514
0.2239246533770256  0.4457123328404293  0.4721505547536609
0.4472504887365361  0.5552382145324586  0.5325259735309658
0.5550274567311533  0.4463128229706399  0.4672915561646818
0.7781967637686904  0.5555658595045827  0.5278255983933349
0.8926064776744411  0.4467507209960218  0.4673781286848850
0.2235765836331396  0.7778147398265247  0.4722240607192632
0.4470028811138178  0.8921373044290775  0.5325422093949541
0.5565078456318702  0.7783864762804384  0.4720293334547918
```

IGP-P-S

1.0000000000000000		
8.9092840767069461	0.0000000000000000	0.0000000000000000
-4.4546420383534731	7.7156663399942271	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.9630213569575226

P

12

Direct

0.4559558325213615	0.3330815938542955	0.5297020695073726
0.4557740200770866	0.1228922807305324	0.4702759419226297
0.6693150359913602	0.1232930980062150	0.5299430529095375
0.1235638930724363	0.4551475368739162	0.5297377626375379
0.3333454022452997	0.4552518186057881	0.4700269993783195
0.5466199839989585	0.6682653185201275	0.5298707192538998
0.6689254397361424	0.5463034608201554	0.4698473675007904
0.8783764041152580	0.5459192332161535	0.5296174963526568
0.8787474698474469	0.3327249500007738	0.4700346846445598
0.1238729338284728	0.6688504456976005	0.4702914693204008
0.3332498400953483	0.8784156951873001	0.5301514107220910
0.5463537734708410	0.8782045984871445	0.4703809838501911

DHPP-S

1.0000000000000000

9.4454588212821644	0.0000000000000000	0.0000000000000000
-4.7227294105915636	8.1800072896338776	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.2155685892749410

P

12

Direct

0.5265568298622867	0.4176234855164012	0.5271520601980413
0.5184994000592624	0.2219526354798305	0.4577454074055396
0.6156158679285184	0.1291859990407787	0.5410384787713127
0.2098879581871671	0.5328323476715084	0.5428237598116041
0.4044422791349405	0.5395109134888898	0.4731674455472259
0.6072635927263477	0.7370229658100413	0.5345200721694781
0.7235688964952729	0.6196477781742971	0.4651548037604556
0.8909794816470367	0.5519839323497919	0.5257061912598076
0.7869592400432239	0.3125443422110692	0.4636876616787546
0.1164557515643594	0.6280286818860006	0.4589552193115765
0.2998922449707067	0.8009103327468239	0.5359124657858700
0.5392884543808663	0.9041863156245853	0.4739464433003278

DHPP-2-S

1.0000000000000000		
10.4126714580131772	0.0000000000000000	0.0000000000000000
-3.9047517967549417	6.7632285029254211	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.5159056176365944

P

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Direct

0.5483640113789150	0.1581244143538996	0.4661014271631174
0.7771307059931232	0.2503926015197422	0.5035626766325549
0.1258663674263545	0.4924085370087852	0.4392687326530549
0.1773997610172984	0.4401595531887281	0.5407819862469481
0.3782155462024051	0.4358612809978766	0.4985863338905290
0.4938105443531029	0.2938812295201032	0.5522686022214387
0.6623205410562321	0.5620939888289982	0.4984224817437450
0.8631480065965107	0.5580583841074613	0.5408197487586577
0.2633141823317189	0.7475700285947298	0.5032585757576769
0.4921903303852417	0.8400806742753204	0.4656579786840354
0.5470547413265407	0.7049890151342808	0.5519081752333364
0.9145352239325533	0.5050003634700531	0.4393632810149128