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Supporting information

Transition of wide-band gap semiconductor h-BN(BN)/P heterostructure via single-atom-embedding

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Table S-1 ~ Table S-6:
The Bader charge analysis result of single-atom-embedded h-BN/P heterostructures.
The shown columns are represented as:
-Element : the element atom in the calculated model.
-X, Y, Z : the coordinates of each element.
-Charge : the charge according to Bader partitioning.

Table S- 1. The result of Bader charge analysis on Na doped h-BN/P (Structure A) with GLLB-sc functional

#	Element	X	Y	Z	CHARGE
1	N	-0.007534	18.465689	31.006129	9.305083
2	N	-0.004012	4.313565	31.662452	9.320535
3	N	-0.006007	9.039698	31.663848	9.317095
4	N	-0.008064	13.735359	31.010852	9.304195
5	N	4.237982	1.963492	31.346643	9.314776
6	N	4.244328	6.675578	31.741789	9.319898
7	N	4.23708	11.388179	31.345571	9.309171
8	N	4.232876	16.100958	30.963911	9.307235
9	B	2.802759	18.456003	31.060277	2.7007
10	B	2.816872	4.303652	31.616373	2.709531
11	B	2.813844	9.04927	31.613172	2.710697
12	B	2.803046	13.7442	31.059319	2.698764
13	B	7.049126	1.946487	31.346007	2.709061
14	B	7.054733	6.67905	31.818696	2.718441
15	B	7.046837	11.403789	31.338568	2.710931
16	B	7.042621	16.099686	30.947481	2.695801
17	P	0.90375	3.478656	22.698041	15.180794
18	P	0.903012	9.731147	22.777721	15.22195
19	P	0.93143	16.053466	22.938388	15.102935
20	P	5.14358	0.323584	18.696332	15.025616
21	P	5.175115	6.628568	18.352439	15.045832
22	P	5.14143	12.894467	18.760952	15.025913
23	P	3.770989	0.375651	22.880304	15.073784
24	P	3.711137	6.602213	22.64853	15.339234
25	P	3.756026	12.867176	22.934755	15.069253
26	P	7.986851	3.461525	18.453686	15.00916
27	P	7.995418	9.772913	18.537592	15.051565
28	P	7.971836	16.031788	18.80426	14.990926
29	Na	7.14899	6.4336	26.619657	10.140012

Table S- 2. The result of Bader charge analysis on Pt doped h-BN/P (Structure A) with GLLB-sc functional

#	Element	X	Y	Z	CHARGE
1	N	-0.001488	18.847112	30.578916	9.446354
2	N	0.000255	4.72006	30.900133	9.372806
3	N	-0.002882	9.441123	31.255525	9.448787
4	N	-0.001293	14.134968	30.725827	9.451143
5	N	4.237593	2.351642	30.864301	9.446348
6	N	4.229154	7.070852	31.276888	9.450837
7	N	4.237684	11.782212	30.939292	9.448711
8	N	4.239964	16.490984	30.559401	9.448438
9	B	2.807595	18.844607	30.640523	2.750389
10	B	2.835173	4.715224	31.018223	2.747396
11	B	2.80477	9.439522	31.19206	2.742146
12	B	2.808254	14.134813	30.721473	2.745973
13	B	7.038093	2.333628	30.736173	2.746111
14	B	7.034323	7.099303	31.122261	2.749873
15	B	7.052116	11.789404	30.971934	2.744229
16	B	7.051498	16.486461	30.582542	2.747208
17	P	2.092322	2.953354	23.49538	15.06446
18	P	2.101023	9.179153	23.657043	15.169185
19	P	2.07087	15.466901	23.527788	15.319513
20	P	6.305768	-0.264333	19.436671	15.237093
21	P	6.378123	6.083433	19.264268	15.257599
22	P	6.337718	12.346603	19.427688	15.216821
23	P	4.914105	-0.253765	23.552295	15.243697
24	P	4.885923	6.038295	23.346576	15.007062
25	P	4.951513	12.363497	23.528882	15.276659
26	P	9.134978	2.885069	19.380211	15.228046
27	P	9.198582	9.233214	19.503467	15.263547
28	P	9.179671	15.473667	19.4213	15.260517
29	Pt	7.863011	5.116885	26.181545	79.877234

Table S- 3. The result of Bader charge analysis on Pd doped h-BN/P (Structure A) with GLLB-sc functional

#	Element	X	Y	Z	CHARGE
1	N	-0.35909	18.855656	30.311861	9.37442
2	N	-0.358971	4.704905	30.938032	9.355523
3	N	-0.358169	9.436825	30.985056	9.371542
4	N	-0.35883	14.125942	30.317782	9.375309
5	N	3.88127	2.355351	30.639288	9.37767
6	N	3.878995	7.069482	31.03886	9.37469
7	N	3.883296	11.779263	30.638016	9.376065
8	N	3.88169	16.490646	30.252002	9.375783
9	B	2.452386	18.85035	30.370688	2.729638
10	B	2.461101	4.705456	30.904771	2.727289
11	B	2.455507	9.43709	30.921183	2.725471
12	B	2.452413	14.12964	30.371255	2.730011
13	B	6.692365	2.345051	30.625482	2.726548
14	B	6.688326	7.07495	31.02175	2.741123
15	B	6.695521	11.785692	30.638708	2.724931
16	B	6.694161	16.489377	30.254289	2.733026
17	P	1.263468	3.328471	23.124457	15.023378
18	P	1.272344	9.528542	23.07291	15.081413
19	P	1.25587	15.834418	23.114025	15.156179
20	P	5.474403	0.103055	18.992424	15.092816
21	P	5.553965	6.409763	18.771619	15.121296
22	P	5.499072	12.735659	18.929189	15.129222
23	P	4.100454	0.120417	23.10749	15.180879
24	P	4.052744	6.426989	22.863921	15.039328
25	P	4.112787	12.715202	23.043524	15.127708
26	P	8.324639	3.227452	18.996172	15.168388
27	P	8.335692	9.591644	18.941246	15.15373
28	P	8.356734	15.85543	18.99401	15.129625
29	Pd	7.383454	6.511472	25.636466	46.716287

Table S- 4. The result of Bader charge analysis on Na doped h-BN/P (Structure B) with GLLB-sc functional

#	Element	X	Y	Z	CHARGE
1	N	7.426368	0.785679	31.422769	9.215731
2	N	7.433729	5.496917	31.804398	9.229514
3	N	7.426859	10.208346	31.433906	9.211732
4	N	7.423547	14.921311	31.050304	9.207558
5	N	3.185226	3.132251	31.748578	9.230472
6	N	3.18545	7.862263	31.782068	9.22145
7	N	3.182552	12.55664	31.120254	9.216857
8	N	3.18231	17.28502	31.118073	9.216718
9	B	1.756107	0.770895	31.42762	2.683925
10	B	1.771677	5.496122	31.88421	2.691503
11	B	1.75704	10.22351	31.44556	2.686305
12	B	1.749304	14.92135	31.045142	2.673441
13	B	5.998368	3.121064	31.697062	2.688319
14	B	5.998501	7.873336	31.718057	2.691619
15	B	5.992818	12.566963	31.15717	2.677139
16	B	5.992403	17.275871	31.150997	2.677262
17	P	2.6517	2.375639	22.781346	15.087563
18	P	2.654361	8.634373	22.762037	15.040643
19	P	2.682743	14.927098	22.928342	14.916197
20	P	6.894503	18.075867	18.755194	14.832236
21	P	6.918113	5.498899	18.412538	14.905937
22	P	6.895567	11.7818	18.751296	14.891829
23	P	5.511778	18.101402	22.928871	14.913358
24	P	5.458706	5.503622	22.706082	15.180558
25	P	5.512128	11.753412	22.92427	14.969174
26	P	1.26011	2.35515	18.539619	14.90874
27	P	1.257574	8.648488	18.523513	14.859396
28	P	1.241581	14.928122	18.797739	14.881221
29	Na	8.894125	5.544575	26.679945	10.042462

Table S- 5. The result of Bader charge analysis on Pt doped h-BN/P (Structure B) with GLLB-sc functional

#	Element	X	Y	Z	CHARGE
1	N	7.781783	0.775154	30.895897	9.419856
2	N	7.790431	5.50024	30.941359	9.345062
3	N	7.781014	10.224241	30.896848	9.411445
4	N	7.777604	14.923913	30.520097	9.4195
5	N	3.538901	3.130076	31.196427	9.42114
6	N	3.538411	7.869164	31.192117	9.40865
7	N	3.535793	12.562192	30.578096	9.418873
8	N	3.535528	17.286385	30.578069	9.418871
9	B	2.107549	0.775691	30.896763	2.725461
10	B	2.138971	5.499369	31.134052	2.73195
11	B	2.10743	10.224263	30.895488	2.72689
12	B	2.103402	14.923885	30.519605	2.722197
13	B	6.335745	3.112783	30.989598	2.730244
14	B	6.336917	7.887568	30.989651	2.732387
15	B	6.349378	12.571131	30.638274	2.724435
16	B	6.349838	17.277327	30.636723	2.724536
17	P	1.741412	2.499455	23.734868	15.030122
18	P	1.735717	8.62845	23.7793	15.051088
19	P	1.761707	14.972908	23.63444	15.232767
20	P	6.000079	18.118109	19.529895	15.140811
21	P	6.081624	5.569595	19.289411	15.171872
22	P	6.011191	11.857301	19.502417	15.145542
23	P	4.60396	18.100332	23.635455	15.19456
24	P	4.548526	5.561528	23.357193	14.951256
25	P	4.618748	11.861218	23.606485	15.195856
26	P	0.36945	2.394275	19.590109	15.210165
27	P	0.381918	8.732641	19.621699	15.209934
28	P	0.377515	14.993458	19.528928	15.224761
29	Pt	7.629383	5.379397	26.214487	79.522703

Table S- 6. The result of Bader charge analysis on Pd doped h-BN/P (Structure B) with GLLB-sc functional

#	Element	X	Y	Z	CHARGE
1	N	7.783355	0.777524	30.891135	9.441778
2	N	7.787674	5.498454	30.912039	9.393005
3	N	7.783549	10.220992	30.890205	9.438928
4	N	7.782394	14.923138	30.558604	9.442975
5	N	3.544847	3.13581	30.940983	9.446887
6	N	3.543618	7.861204	30.943087	9.441821
7	N	3.538784	12.564588	30.607423	9.44484
8	N	3.538954	17.280739	30.607586	9.447767
9	B	2.110224	0.776917	30.826304	2.73065
10	B	2.133565	5.498318	30.934162	2.731664
11	B	2.110064	10.220469	30.822939	2.72842
12	B	2.106709	14.92306	30.567782	2.722093
13	B	6.34557	3.121241	30.908302	2.730481
14	B	6.344929	7.876554	30.910509	2.733838
15	B	6.352035	12.570402	30.658539	2.731636
16	B	6.351781	17.275735	30.660954	2.729999
17	P	1.854751	2.496198	23.460216	15.159853
18	P	1.855751	8.645204	23.462779	15.129738
19	P	1.859358	14.992881	23.467943	15.198239
20	P	6.090237	18.106766	19.322383	15.24027
21	P	6.163943	5.572865	19.092186	15.21781
22	P	6.090059	11.879346	19.322259	15.239372
23	P	4.698249	18.130561	23.434748	15.256736
24	P	4.661413	5.570563	23.169819	15.111626
25	P	4.700281	11.857079	23.434863	15.253596
26	P	0.450505	2.389966	19.333273	15.220878
27	P	0.455418	8.751516	19.332952	15.196174
28	P	0.468943	14.992826	19.353713	15.183001
29	Pd	7.895911	5.570394	26.038685	46.982487