Electronic Supplementary Information (ESI)

High throughput screening of Ohmic contact in 2D Metal-Semiconductor van der Waals heterojunctions

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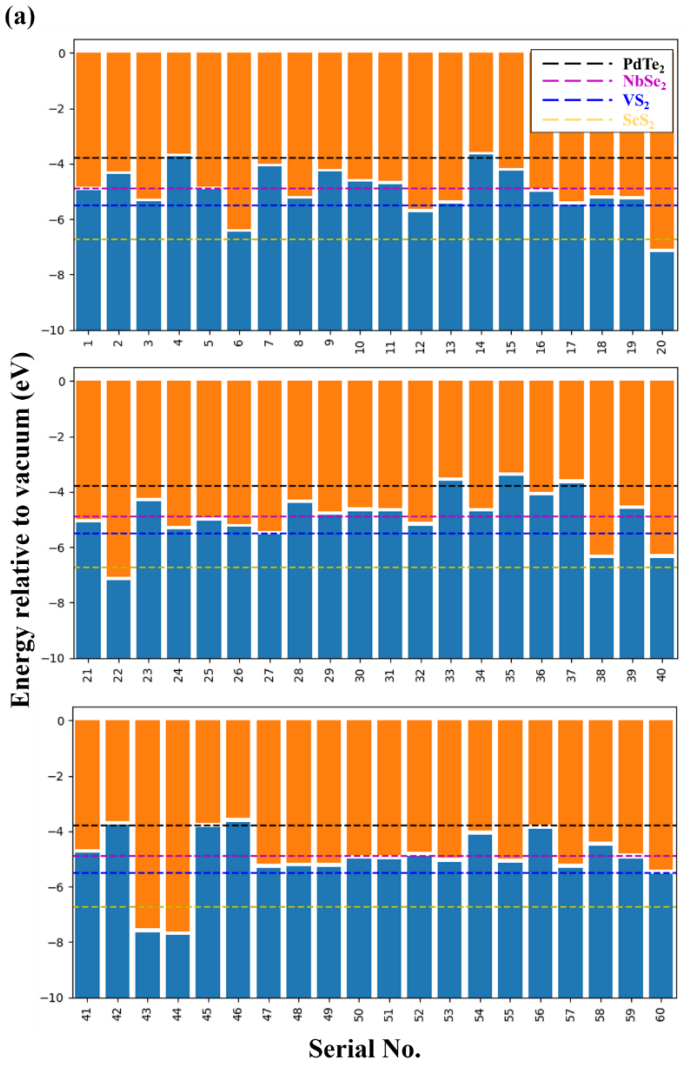

FIG S1 (a) Band alignment (PBE) of monolayers with serial numbers 1 – 60

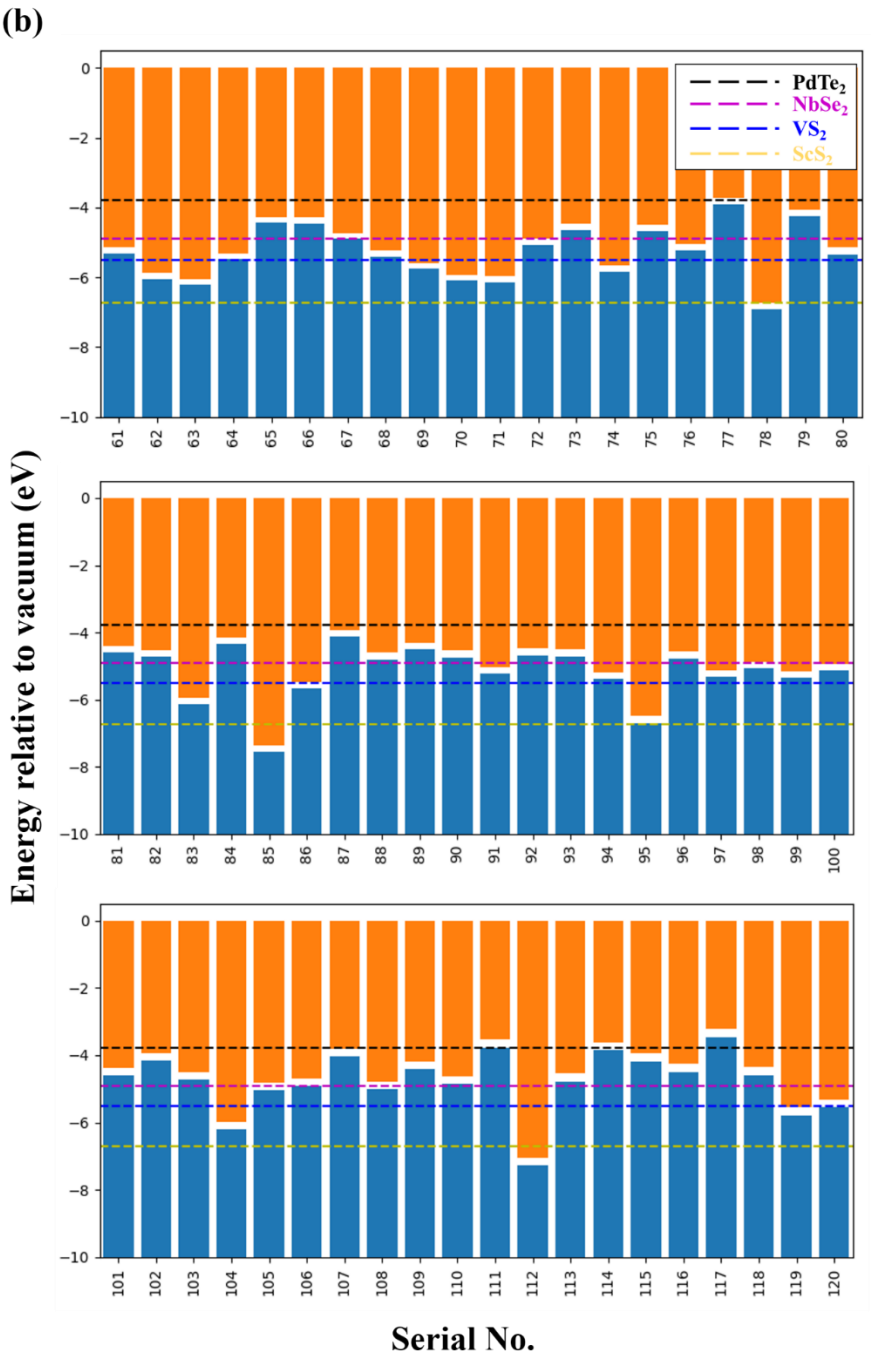

FIG S1 (b) Band alignment (PBE) of monolayers with serial numbers 61 – 120

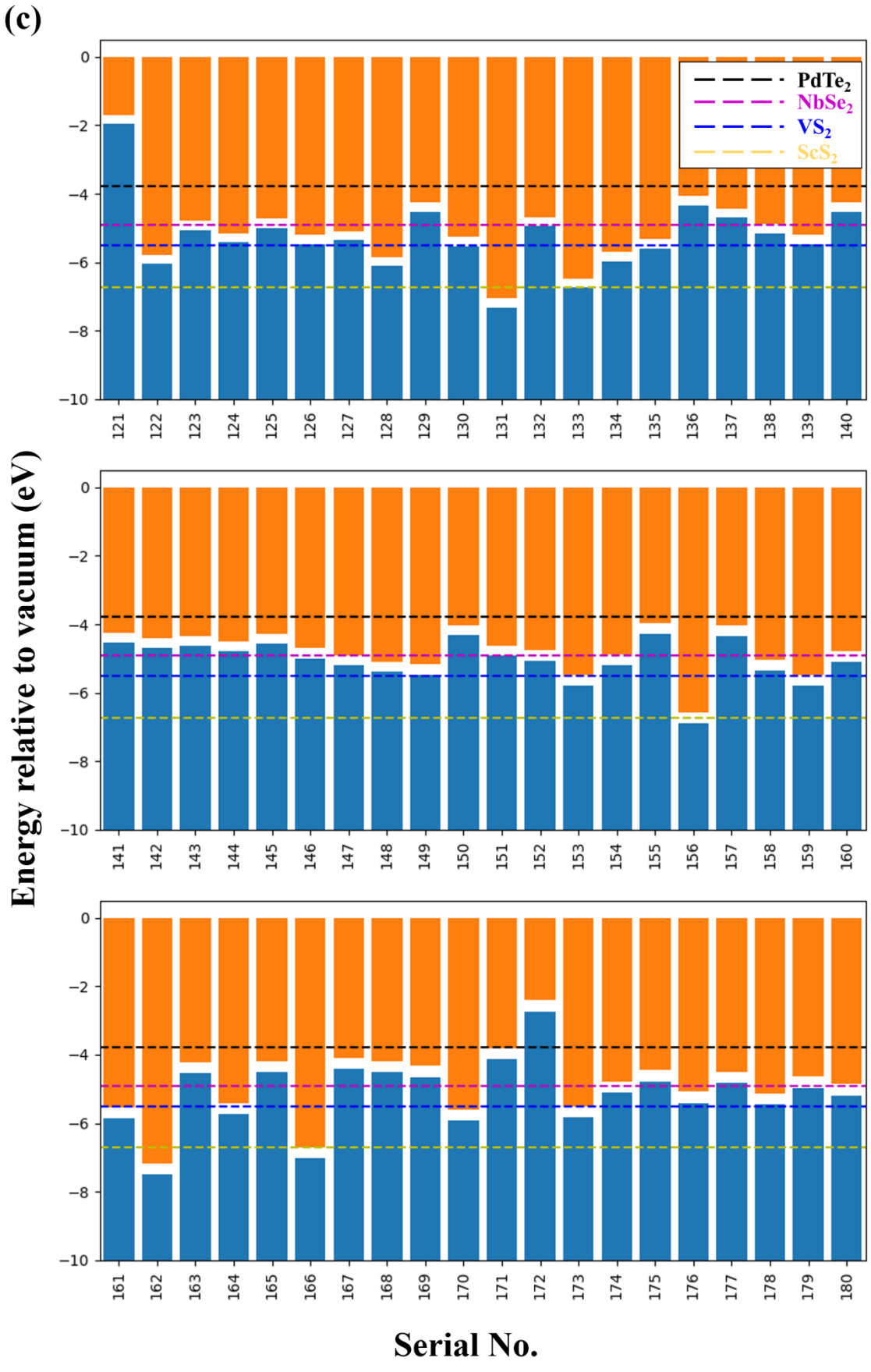

FIG S1 (c) Band alignment (PBE) of monolayers with serial numbers 121 – 180

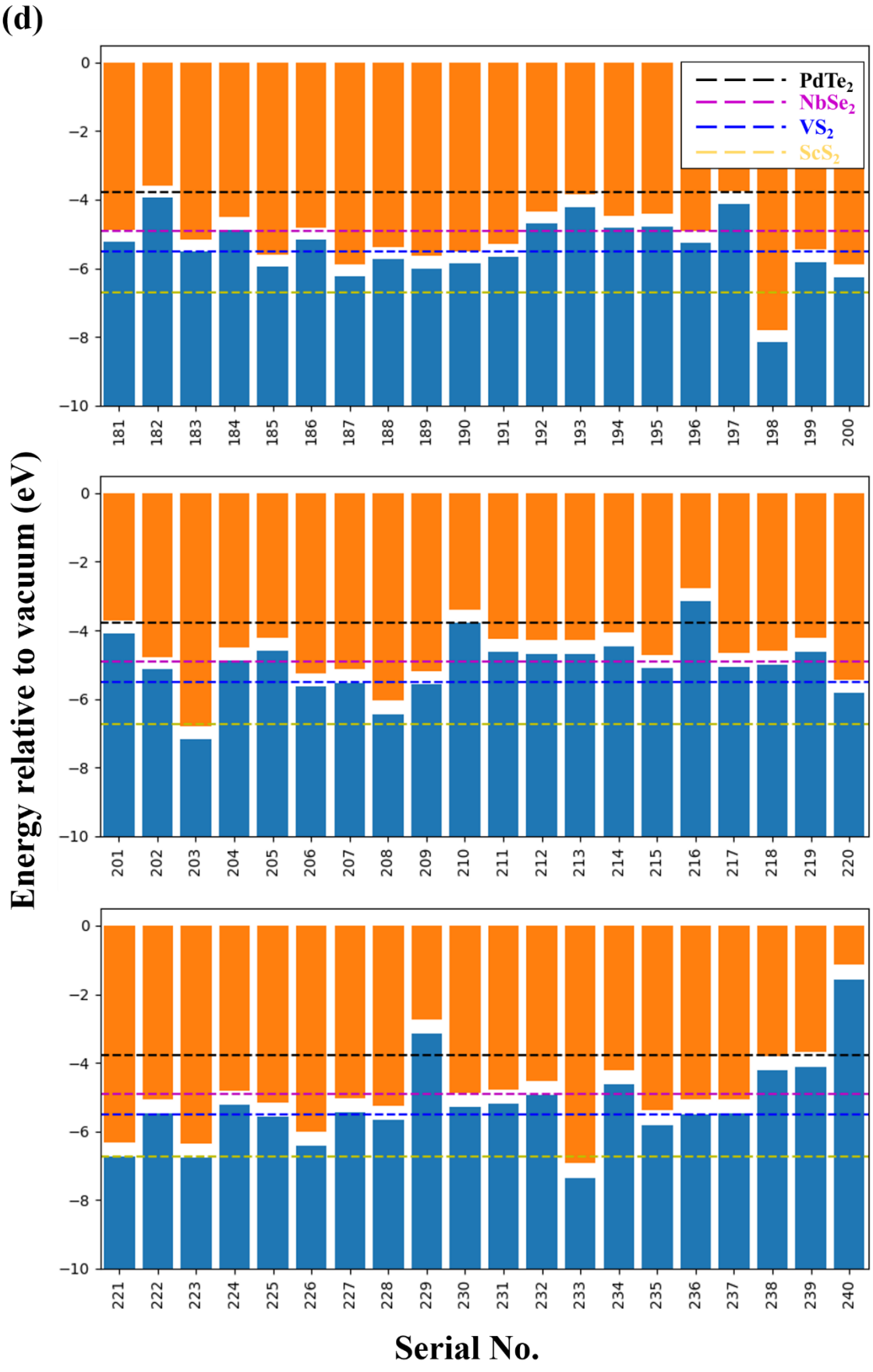

FIG S1 (d) Band alignment (PBE) of monolayers with serial numbers 181 – 240

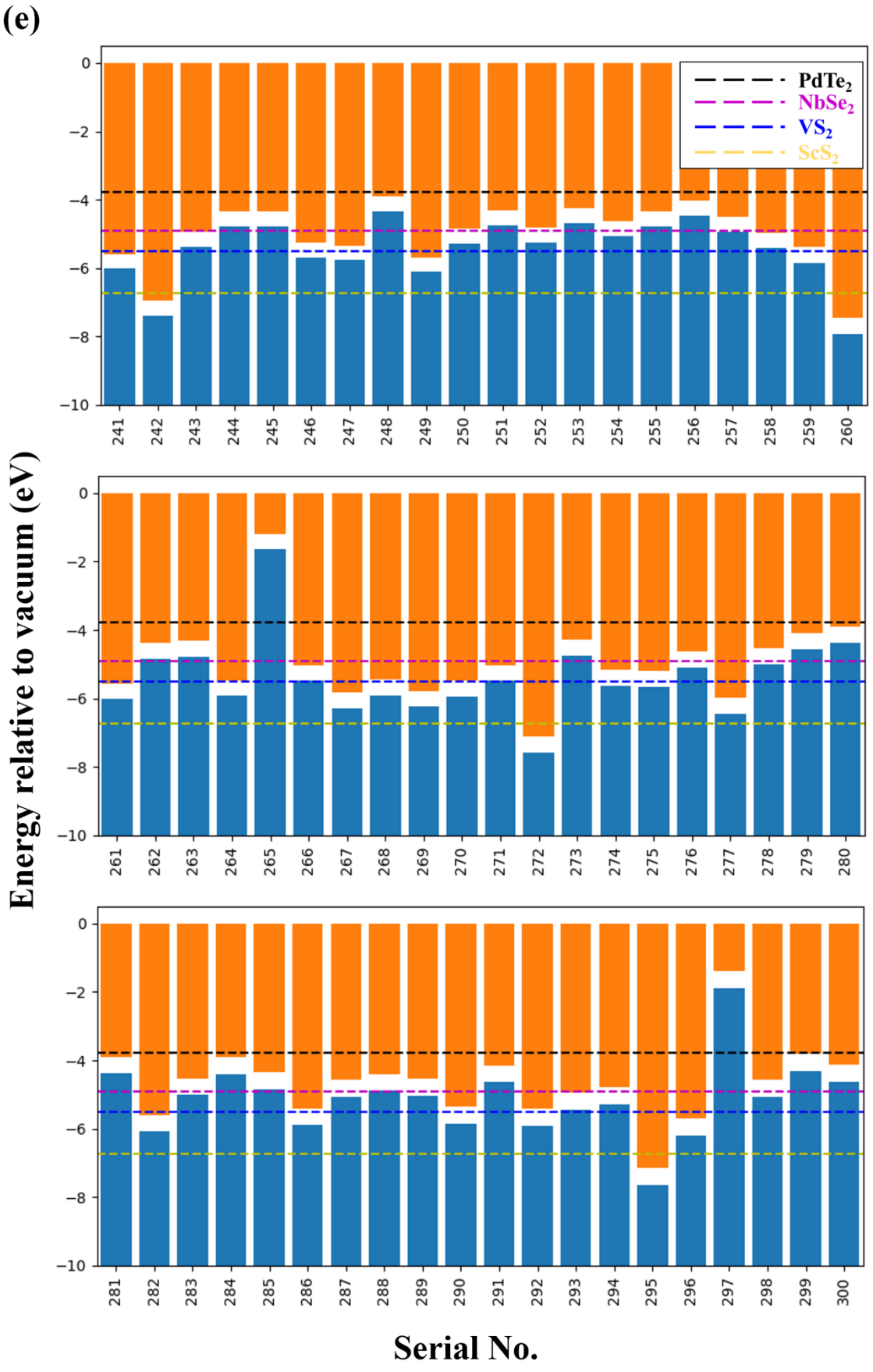

FIG S1 (e) Band alignment (PBE) of monolayers with serial numbers 241 – 300

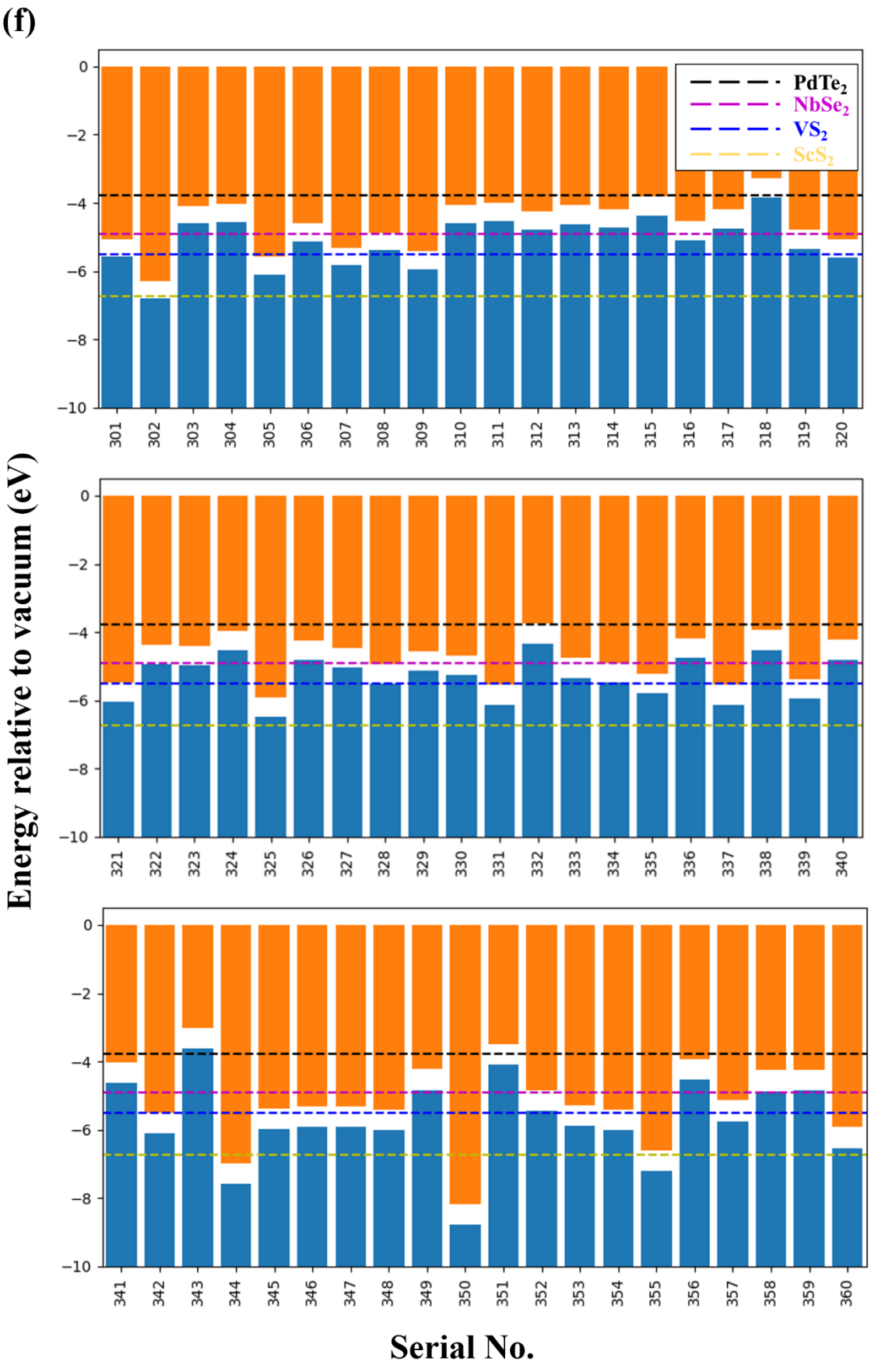

FIG S1 (f) Band alignment (PBE) of monolayers with serial numbers 301 – 360

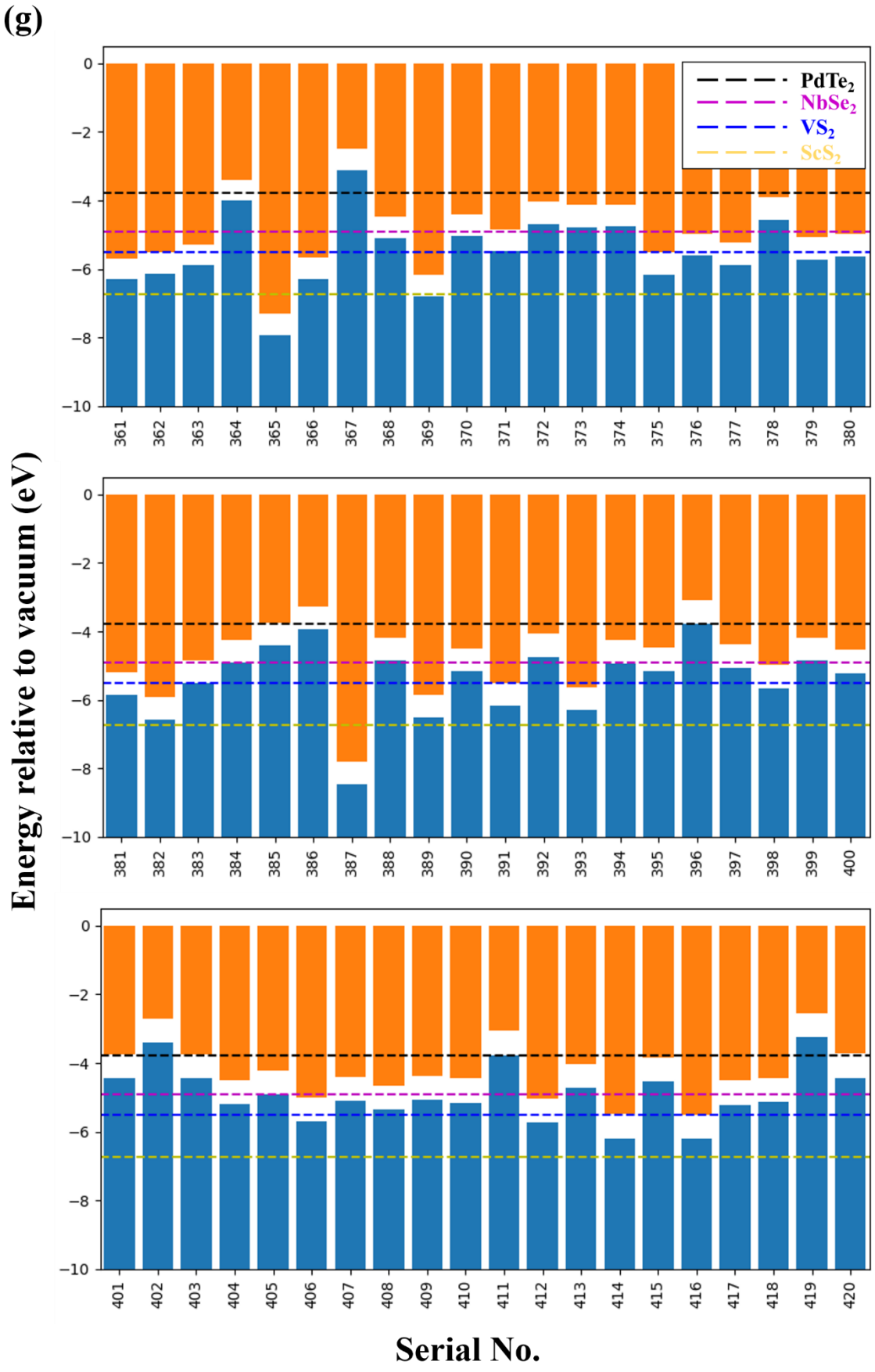

FIG S1 (g) Band alignment (PBE) of monolayers with serial numbers 361 – 420

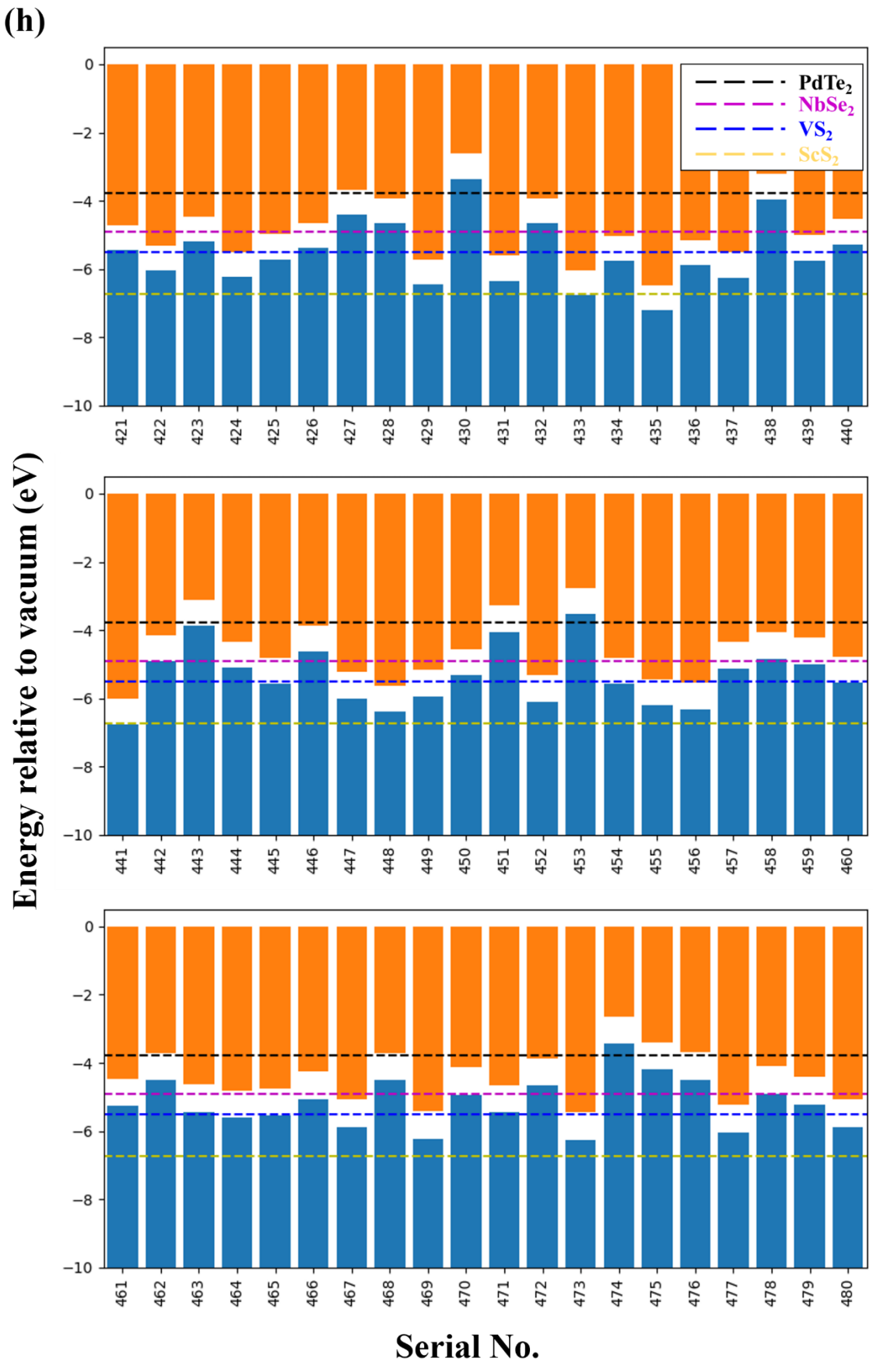

FIG S1 (h) Band alignment (PBE) of monolayers with serial numbers 421 – 480

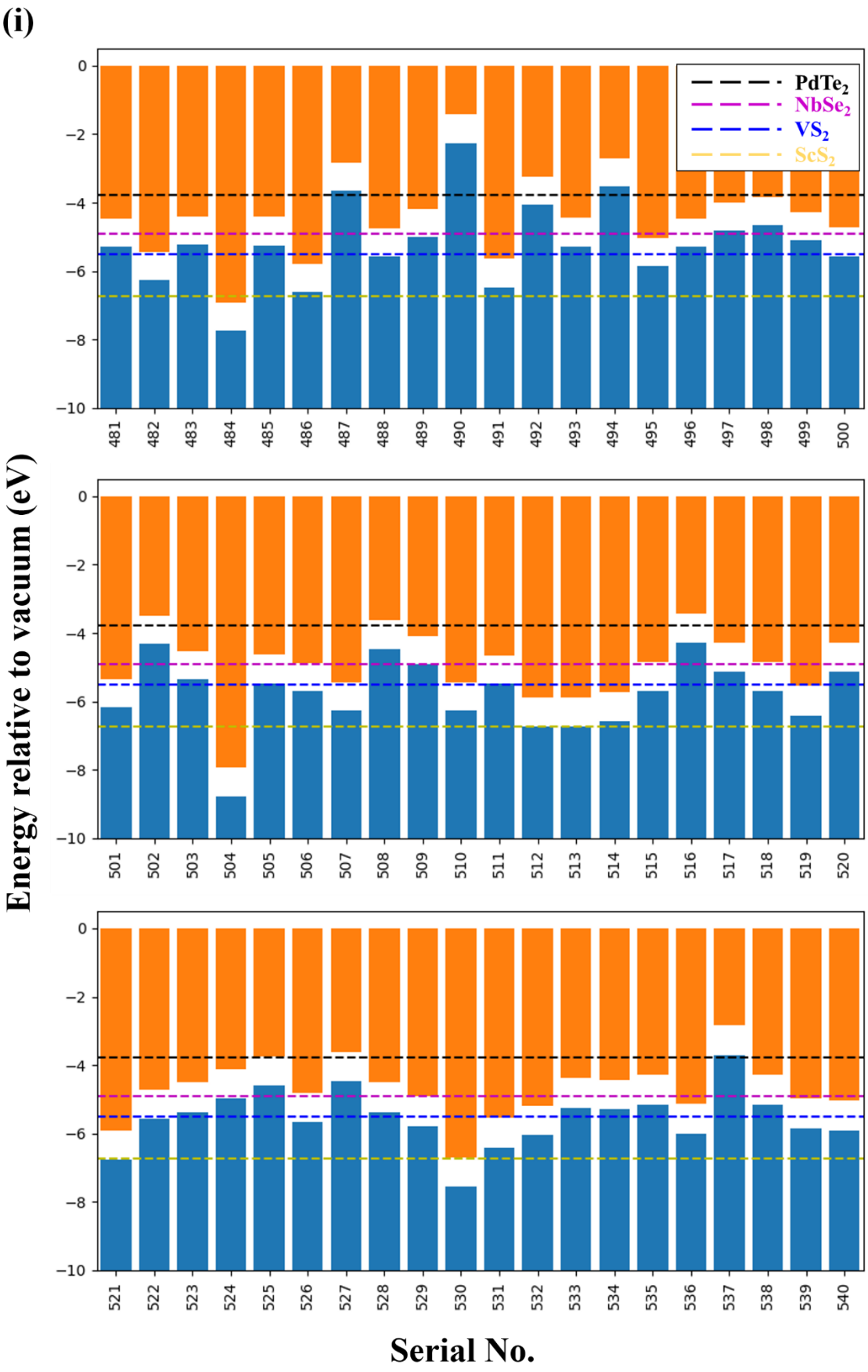

FIG S1 (i) Band alignment (PBE) of monolayers with serial numbers 481 – 540

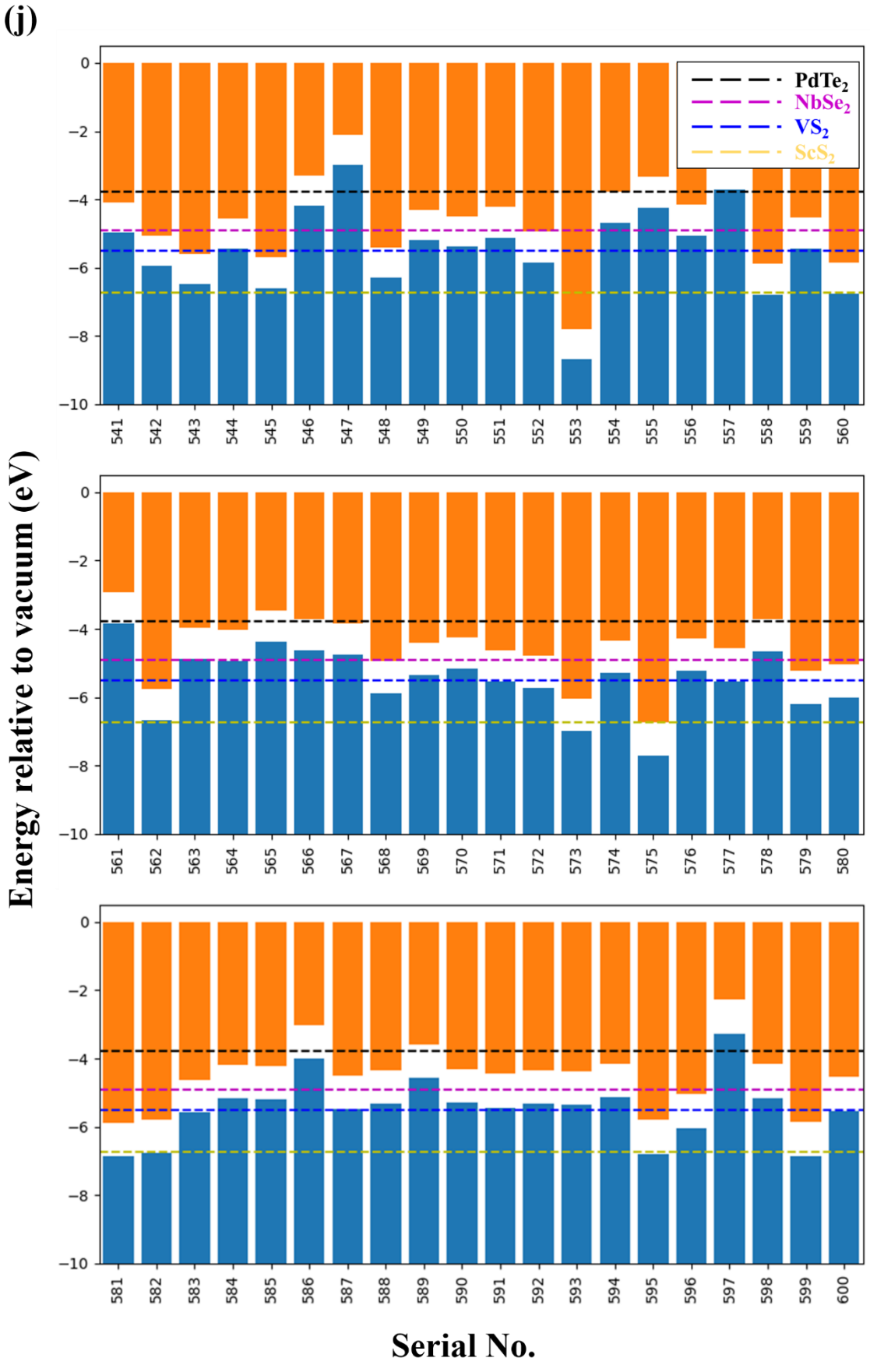

FIG S1 (j) Band alignment (PBE) of monolayers with serial numbers 541 – 600

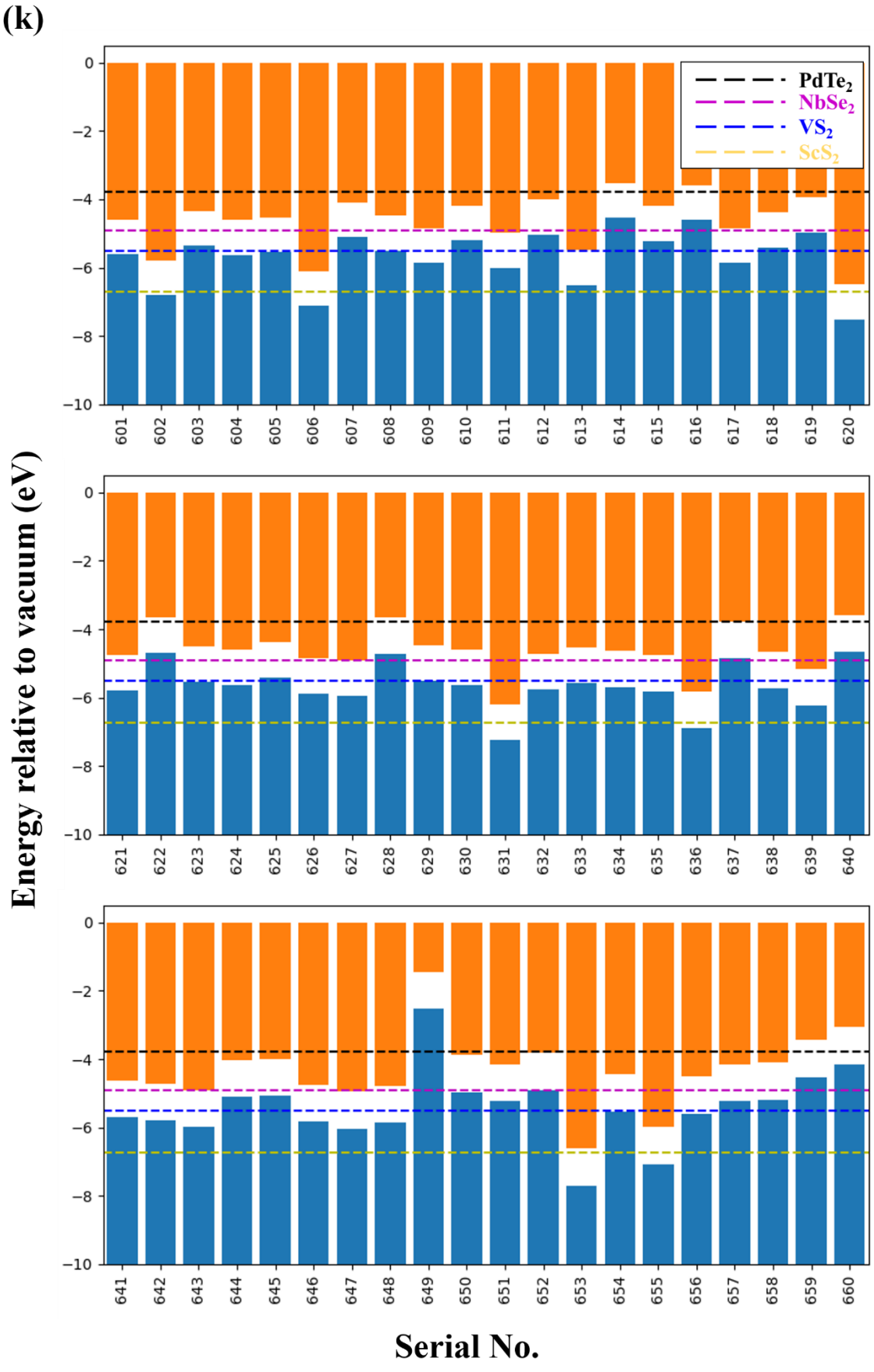

FIG S1 (k) Band alignment (PBE) of monolayers with serial numbers 601 – 660

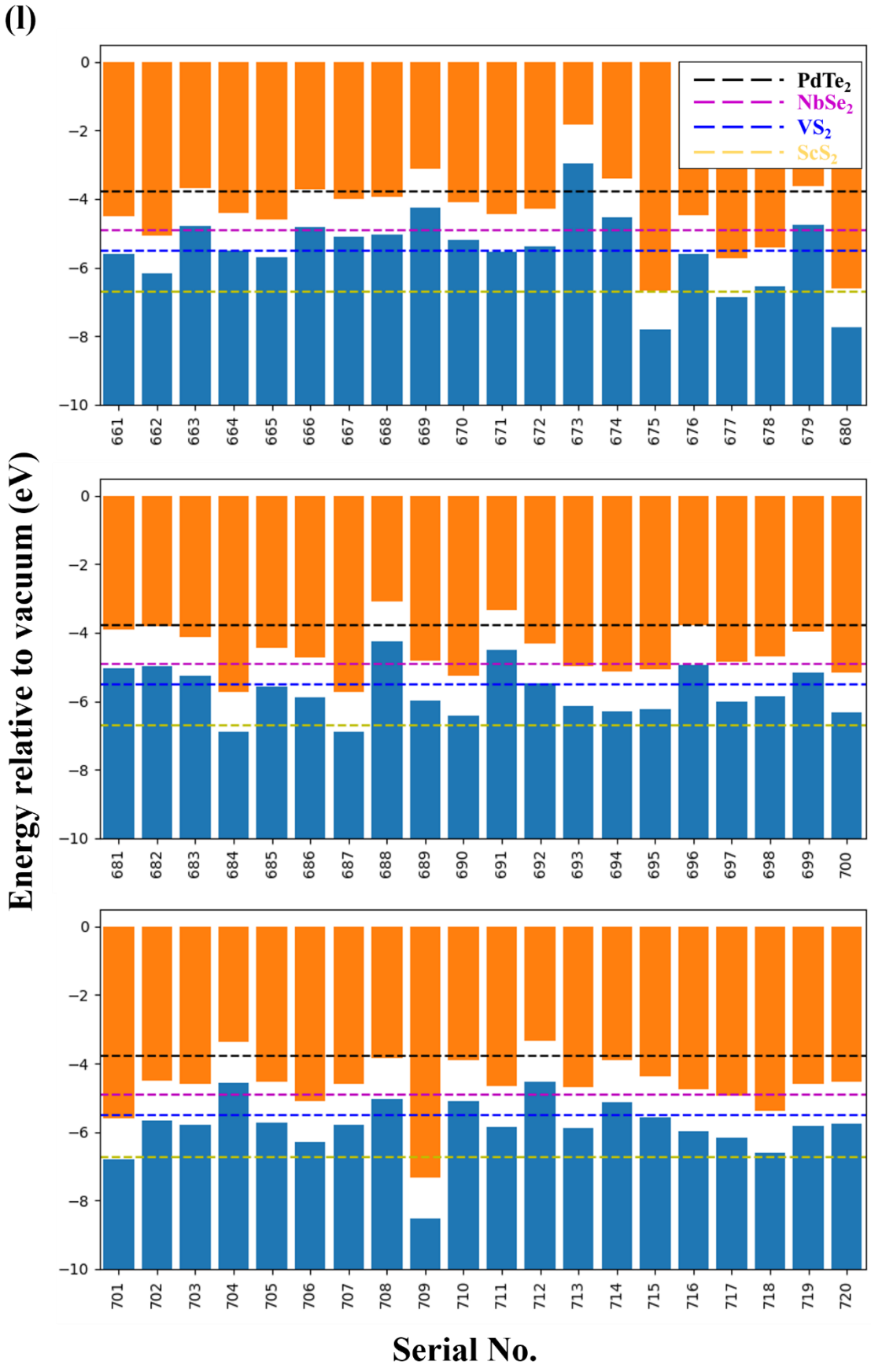

FIG S1 (l) Band alignment (PBE) of monolayers with serial numbers 661 – 720

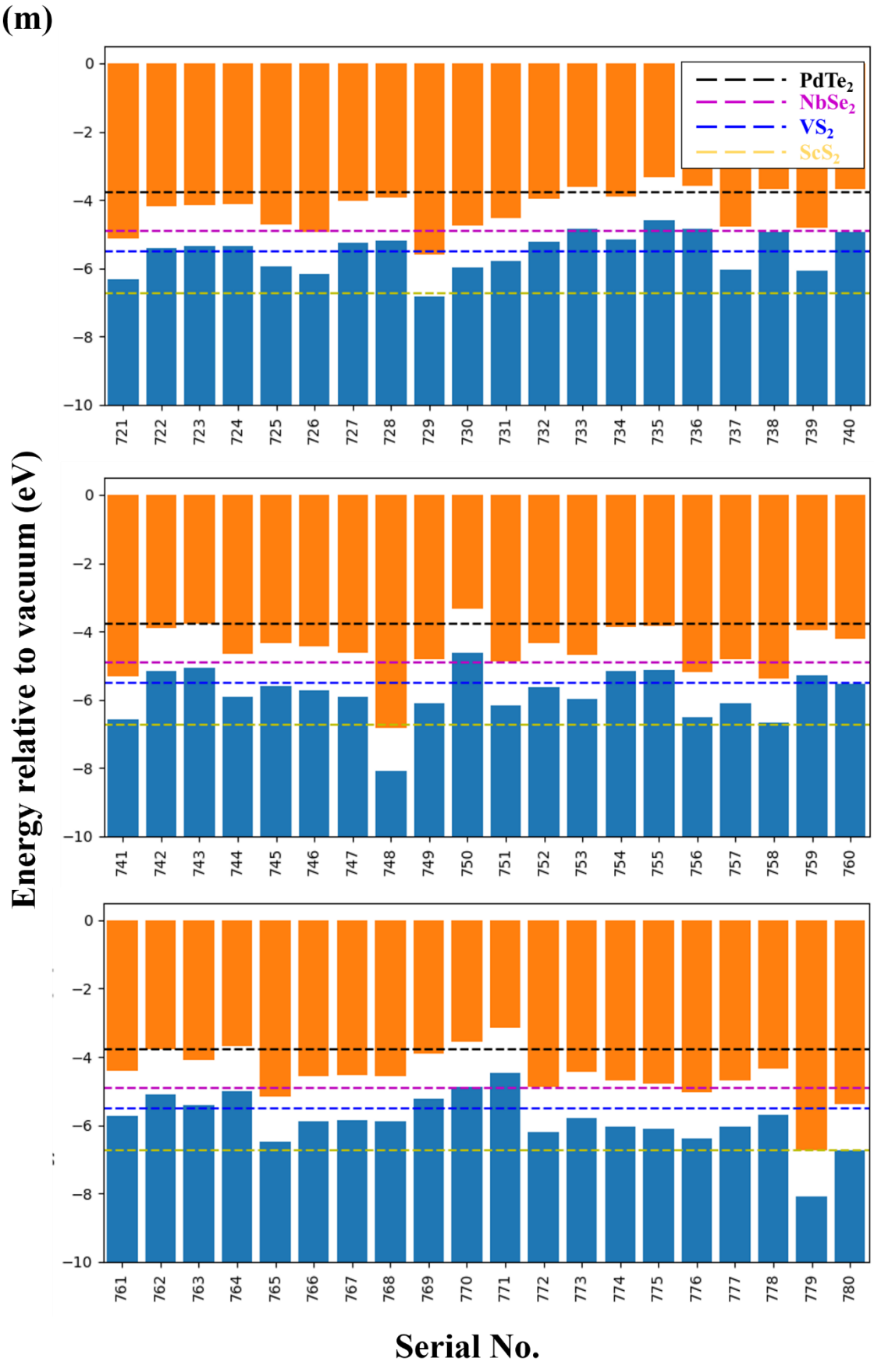

FIG S1 (m) Band alignment (PBE) of monolayers with serial numbers 721 – 780

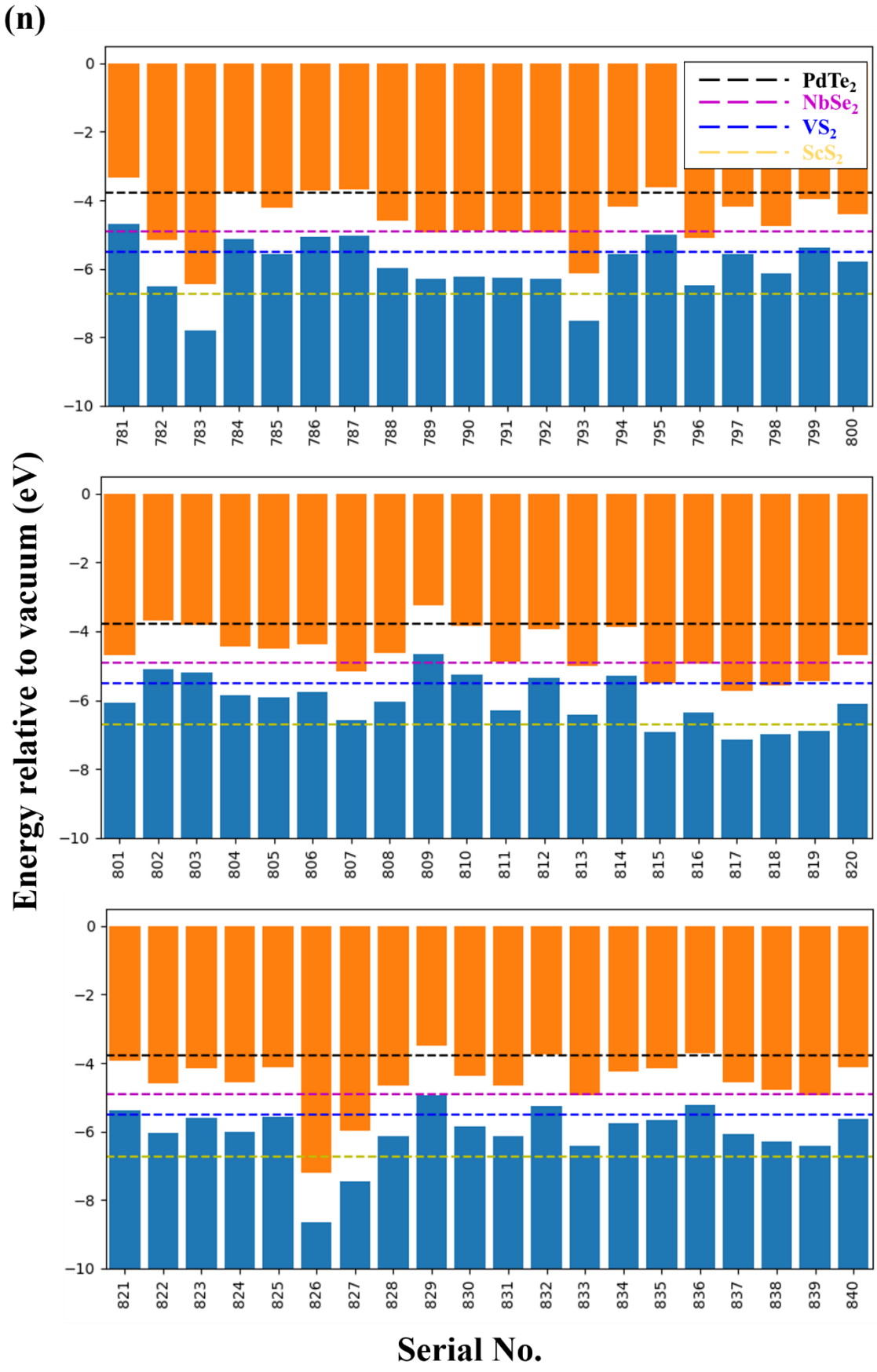

FIG S1 (n) Band alignment (PBE) of monolayers with serial numbers 781 – 840

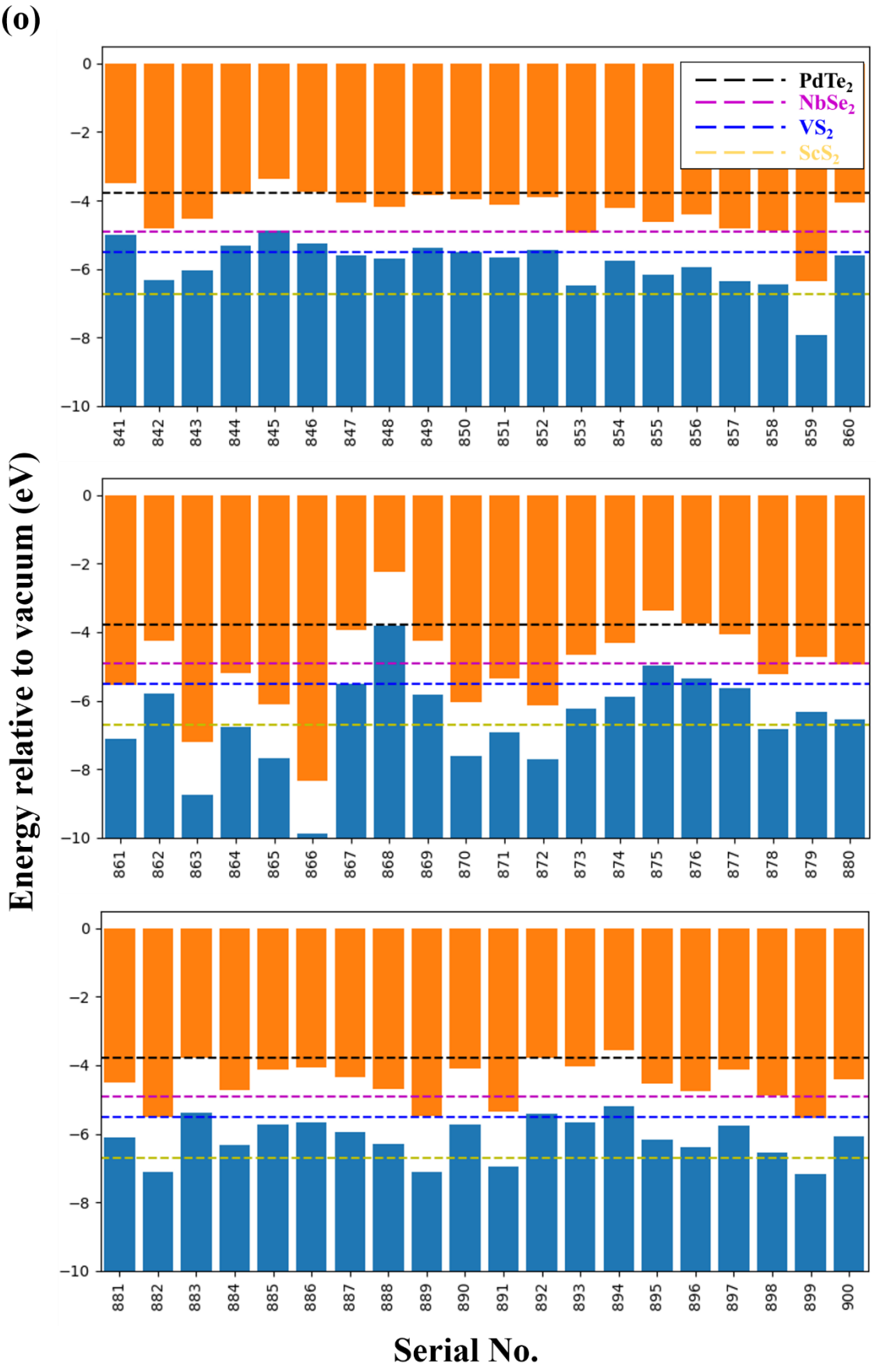

FIG S1 (o) Band alignment (PBE) of monolayers with serial numbers 841 – 900

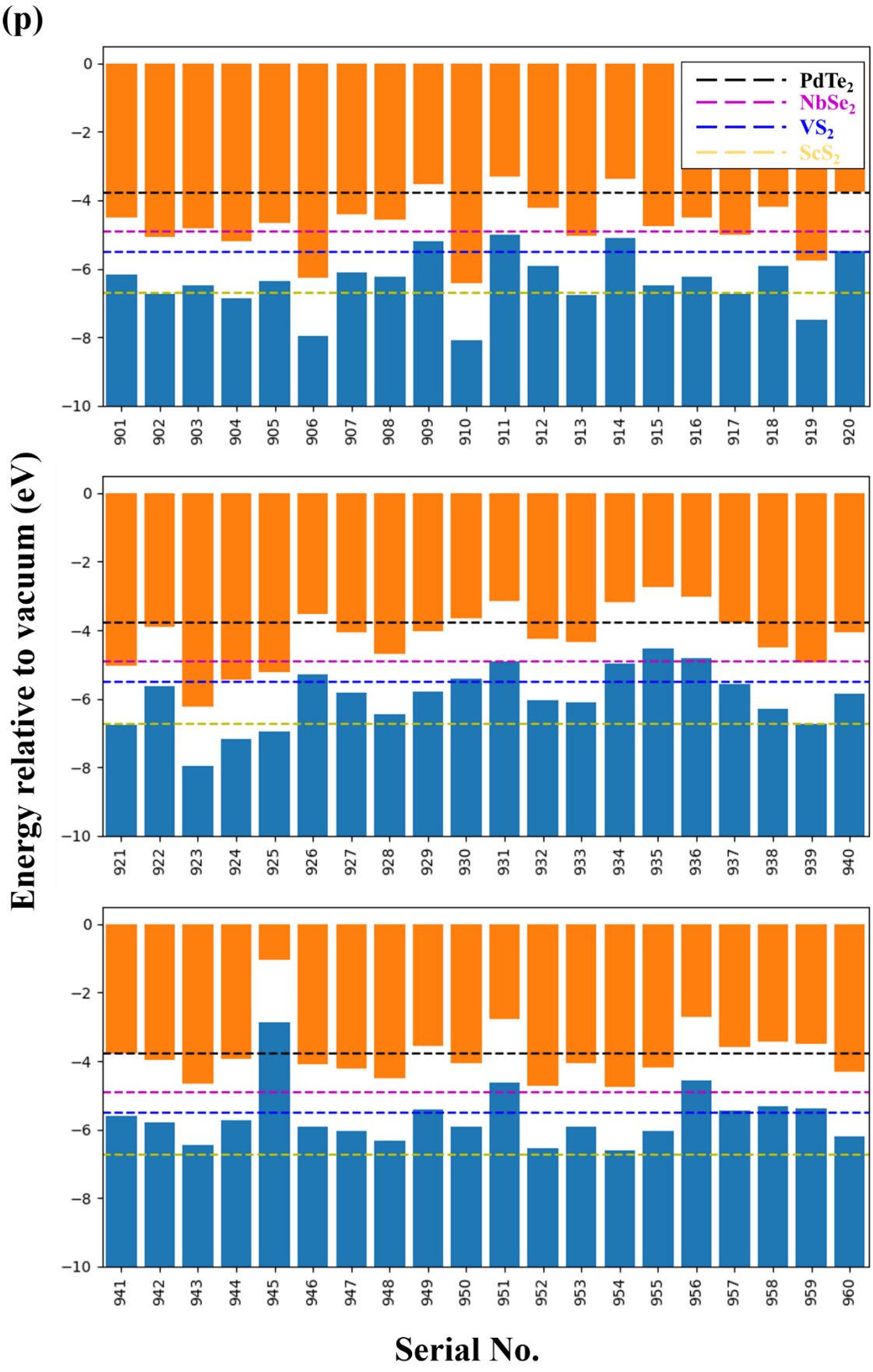

FIG S1 (p) Band alignment (PBE) of monolayers with serial numbers 901 – 960

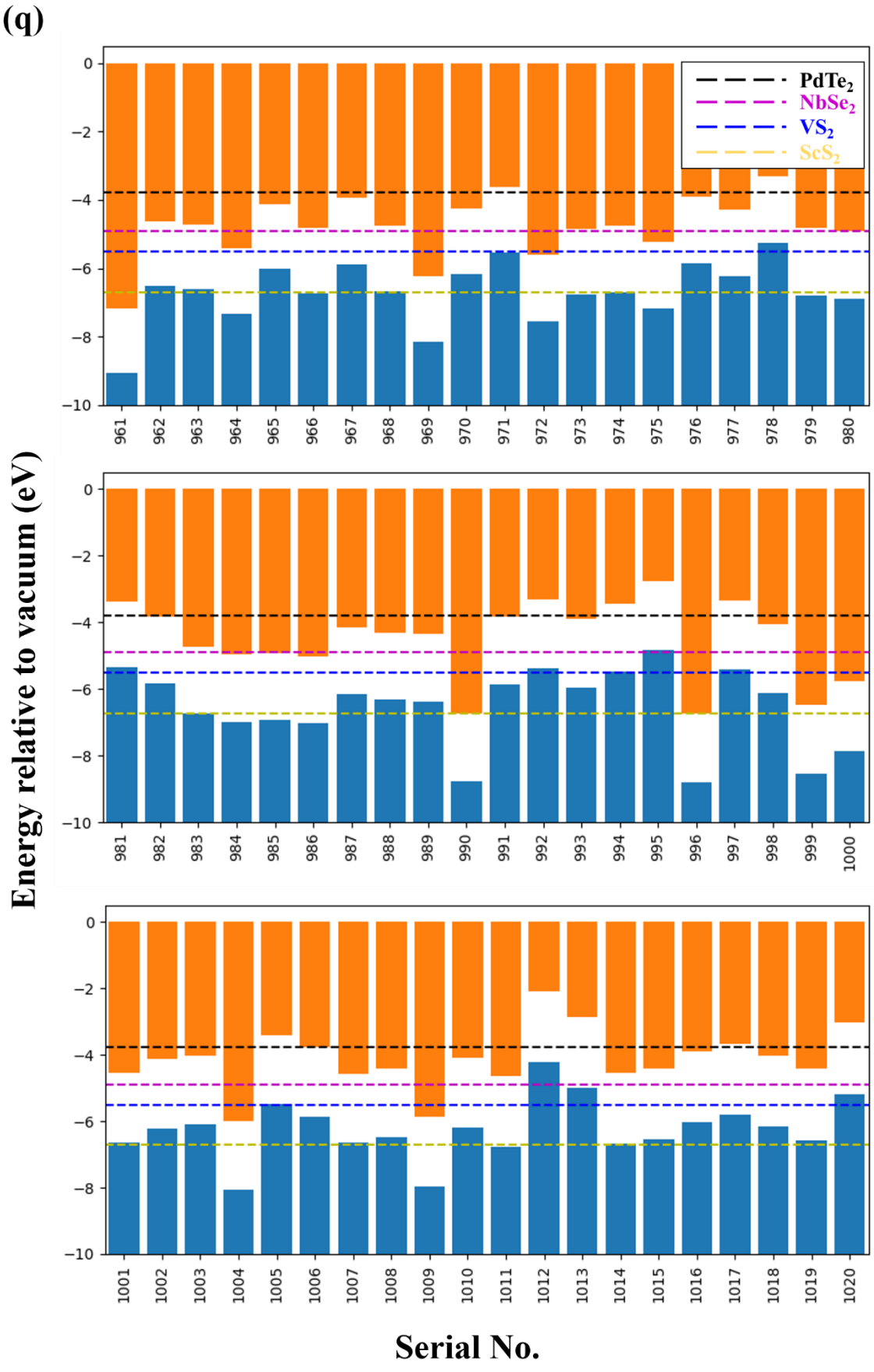

FIG S1 (q) Band alignment (PBE) of monolayers with serial numbers 961 – 1020

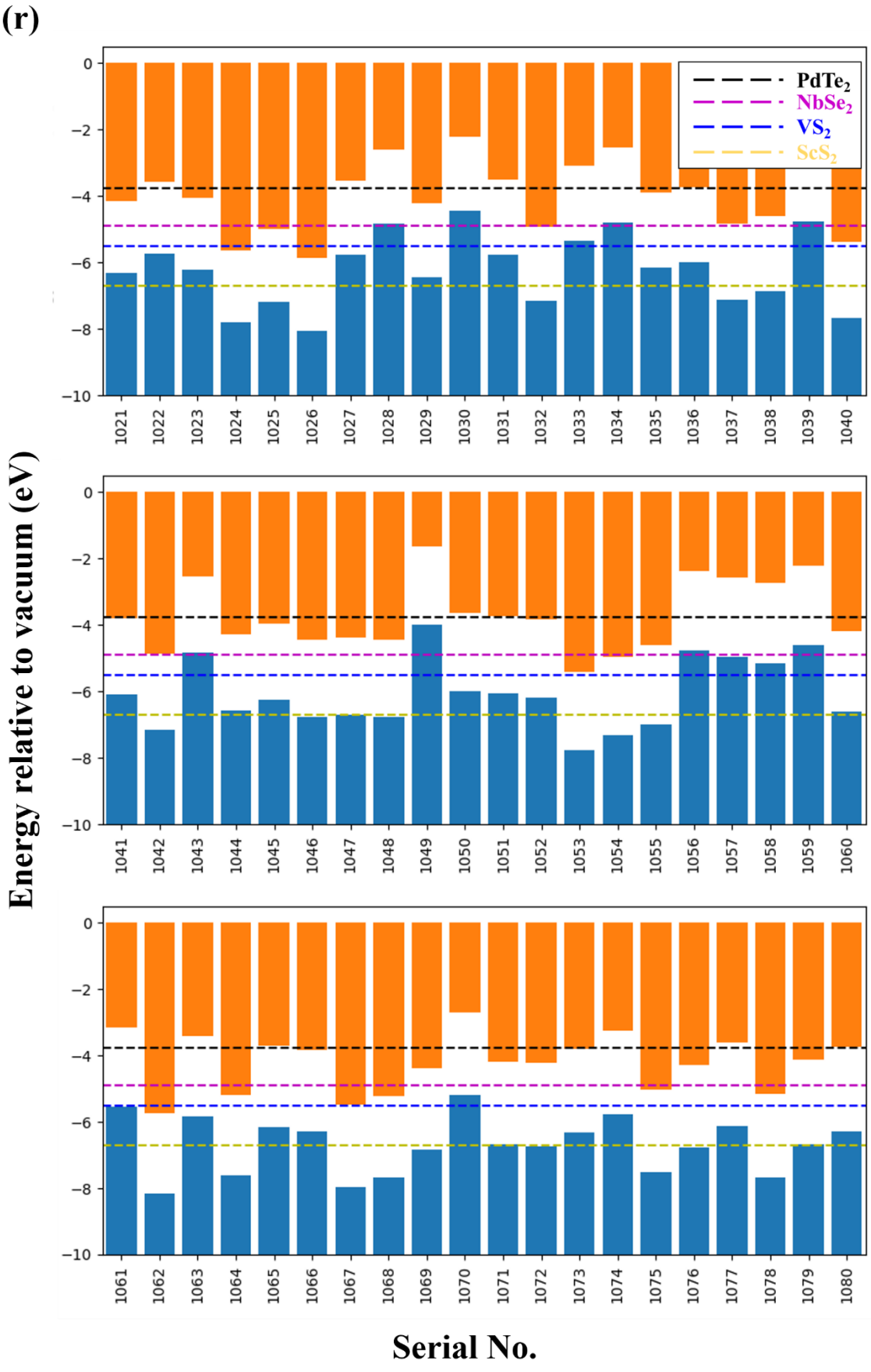

FIG S1 (r) Band alignment (PBE) of monolayers with serial numbers 1021 – 1080

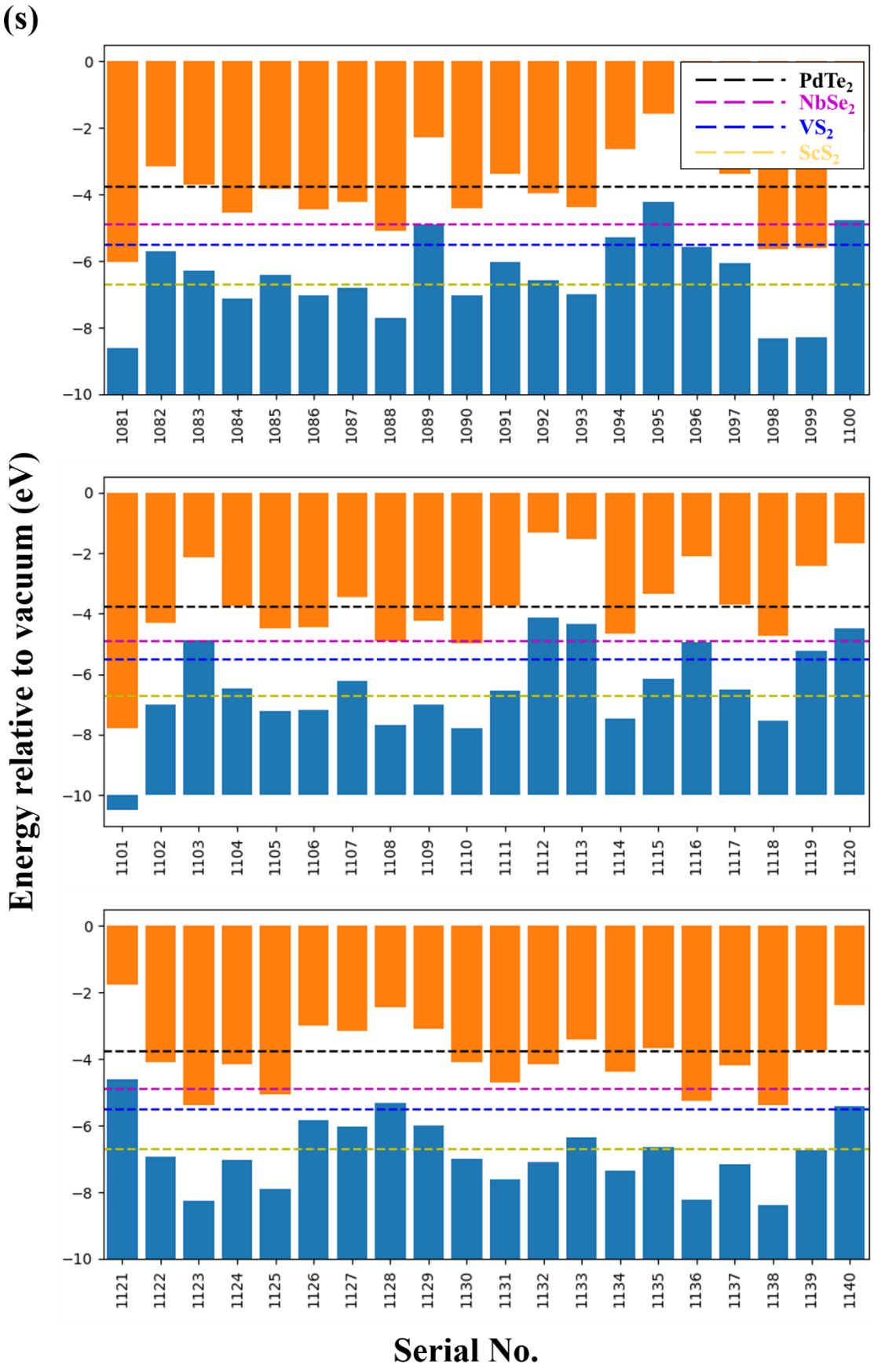

FIG S1 (s) Band alignment (PBE) of monolayers with serial numbers 1081 – 1140

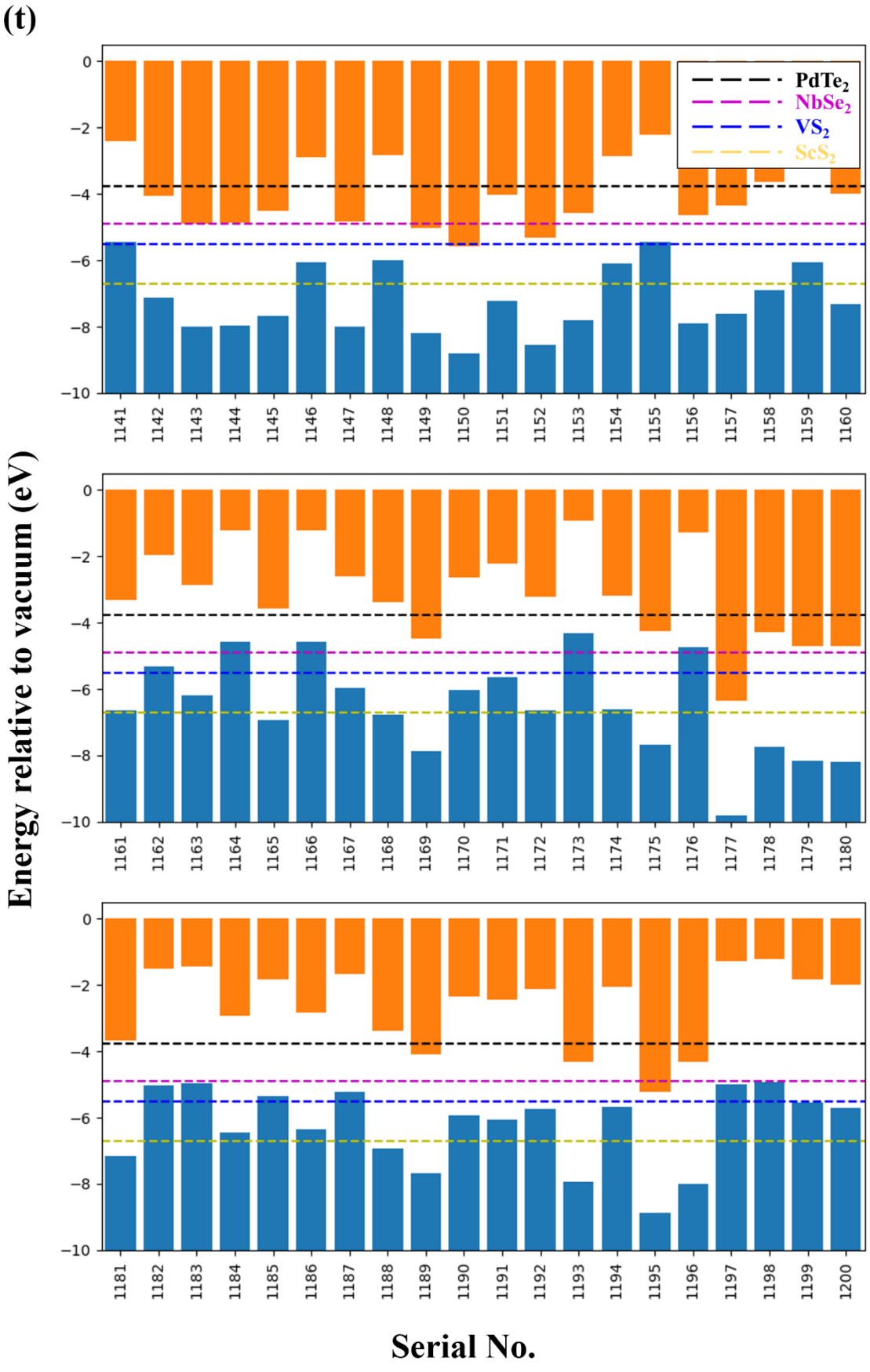

FIG S1 (t) Band alignment (PBE) of monolayers with serial numbers 1141 – 1200

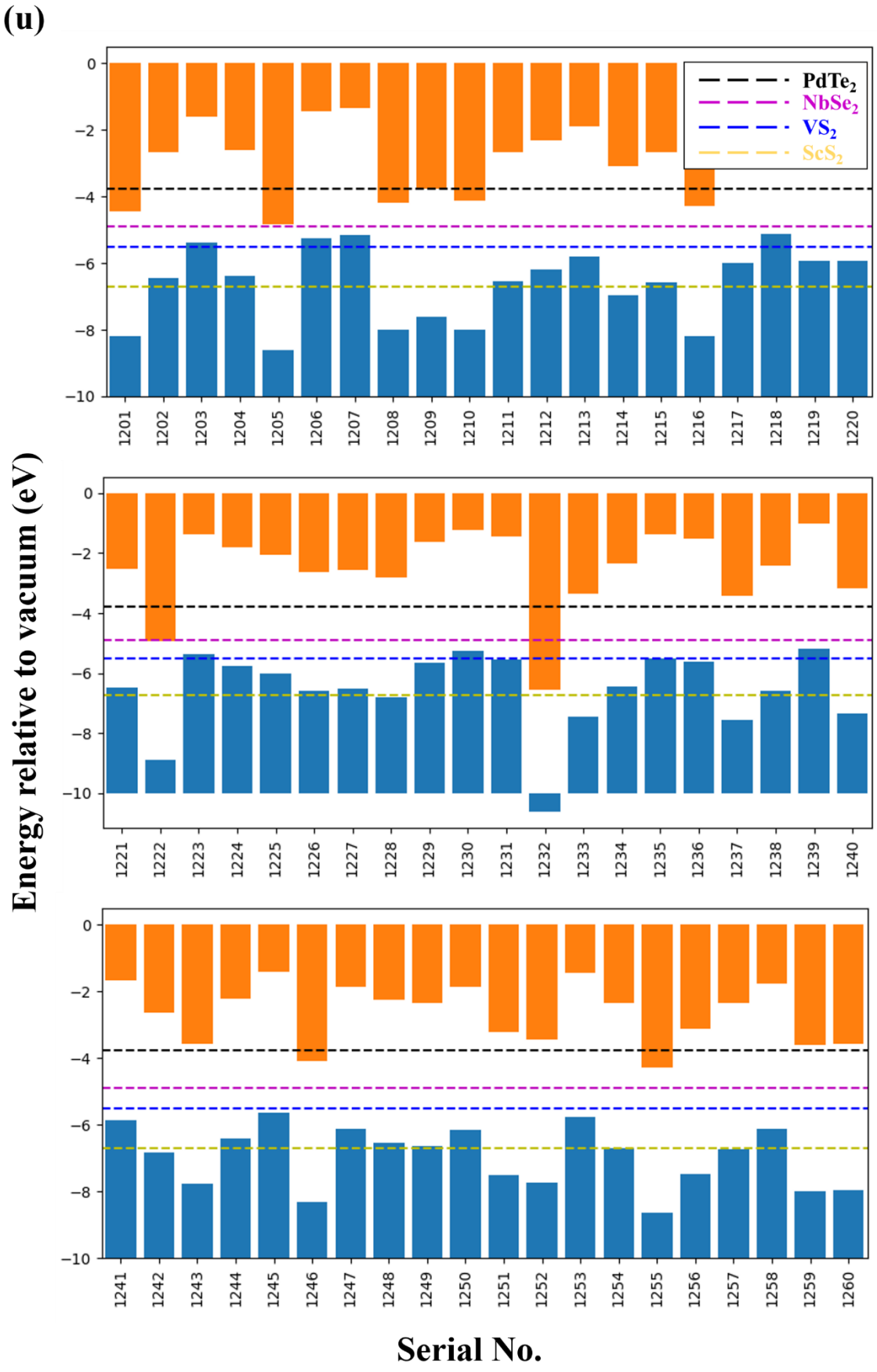

FIG S1 (u) Band alignment (PBE) of monolayers with serial numbers 1201 – 1260

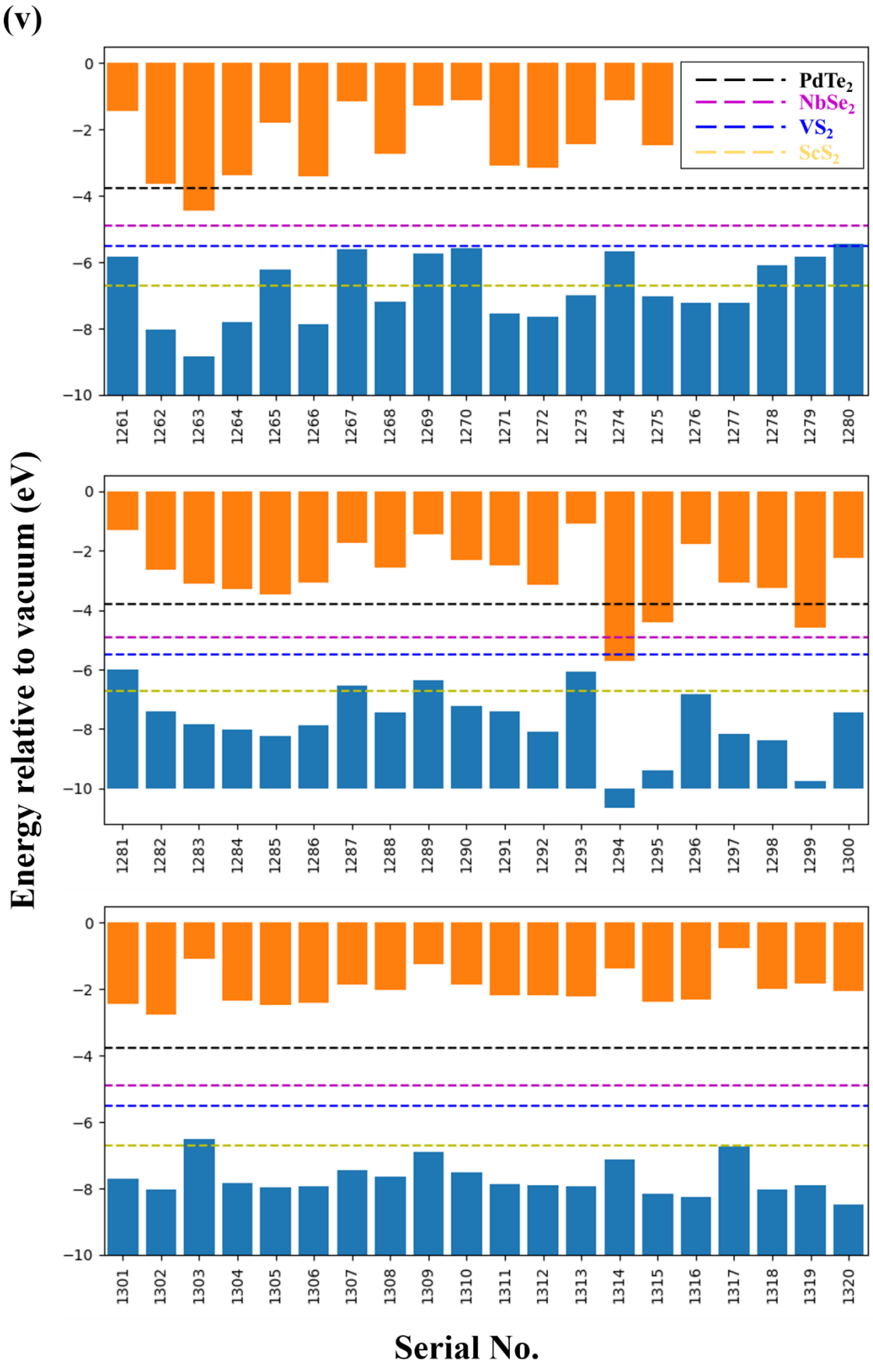

FIG S1 (u) Band alignment (PBE) of monolayers with serial numbers 1261 – 1320

Table – S1 List of analyzed monolayers along with their corresponding serial numbers

Serial No.	Material
1	$Mn_2P_2Se_6$
2	Rh_2Se_2
3	Ru_2Se_4
4	ScI_2
5	NiI_2
6	Cu_2Br_6
7	$ScCl_2$
8	$Mn_2P_2S_6$
9	$Rh_2P_2Te_6$
10	Ti_2Te_2
11	Bi_2MnTe_4
12	Bi_2Se_2Te
13	Os_2S_4
14	Re_2I_4
15	Pb_2Te_4
16	Os_2Te_4
17	HgSe
18	$Ti_2Zr_2Te_8$
19	$Pt_2Br_2N_2$
20	F_2Ge_2
21	VSeTe
22	$Cr_2Cu_2O_8$
23	Bi_2O_2
24	Bi_2SeTe_2
25	Ti_2Cl_6
26	Pb_2F_2
27	Ir_2O_2
28	$Mn_2Br_2S_4Sb_2$
29	$PbTe_2$
30	$Cr_2Ge_2Te_6$
31	$Fe_2P_2Te_6$
32	$HfTe_2$
33	Zr_2S_2
34	Mo_2S_4
35	Hf_2S_2
36	Ir_2Se_2
37	Ca_2I_2
38	Hg_2Cl_2
39	Re_2I_6
40	FeF_2
41	Re_2Br_6
42	$Bi_2Cu_2S_4$
43	$Zn_4Cl_4O_4$
44	CdO_2
45	Re_2I_6
46	YI_2
47	HfSeTe
48	Hf_3ZrTe_8
49	Os_2Se_4
50	FeI_2
51	$PtBr_2$
52	$Hg_2Pt_4Se_6$
53	HgTe
54	Ti_2I_4
55	Ru_2Te_4
56	$ScBr_2$
57	Bi_2STe_2
58	Hf_2Te_{10}
59	Bi_2Se_2
60	Ag_2O_2
61	$Hf_2Zr_2Te_8$
62	$CoCl_2$
63	Os_2O_4
64	Ag_2ReI_6
65	Ga_2NiS_4
66	Pb_2S_2
67	Ti_2Br_6
68	Au_2O_2
69	$CoBr_2$
70	$Mn_2Cl_2N_2$
71	$Cr_2Cl_2Se_2$
72	$Co_4Br_4O_4$
73	MoOTe
74	$Cr_2Br_2Se_2$
75	$Ta_2P_2Te_6$
76	Cu_2ReI_6
77	Sb_4
78	Au_2ReF_6
79	$Cu_2Sb_2Se_4$
80	$TiZr_3Te_8$
81	Zr_2Te_{10}
82	Pb_2O_2
83	Hg_2Br_2
84	Nb_3I_8
85	CuV_2O_6
86	$PdBr_2$
87	W_2Br_6
88	$Ru_2P_2Te_6$
89	WSTe
90	MoSTe
91	$Cr_2Ta_4O_{12}$
92	Nb_3Cl_8
93	Zr_2Te_2
94	ZrSTe
95	Au_2Cl_6
96	Ti_2I_6
97	$Cu_2C_4H_4O_8$
98	VTe_2
99	$HfZr_3Te_8$
100	V_2S_2
101	$Ir_2I_2S_2$
102	Au_2MoTe_4
103	Ti_2Te_2
104	Rh_2Cl_6
105	AsIS
106	Bi_2OTe_2
107	W_2I_6
108	V_2Te_2
109	$Ir_2P_2Te_6$
110	V_2Te_2
111	$PdSe_2$
112	Hg_2O_4
113	Sn_2H_2
114	Re_2S_2
115	$OsCl_2$
116	Sb_2Se_2
117	Pb_2O_2
118	Ru_2Se_6
119	$Y_3N_2O_2$
120	VSe_2
121	MnH_2O_2
122	$Tl_2I_2S_2$
123	V_2Se_2
124	$ZrTe_2$
125	CrSTe
126	ZrSeTe
127	FeO_2
128	OsO_2
129	$Mn_2Br_2Sb_2Se_4$
130	Ir_2Cl_6
131	Ag_2Cl_6
132	Pb_2Te_6
133	$K_2Pt_2Cl_6N_2$
134	Bi_2Se_3
135	Rh_2Br_6
136	Pb_2Te_2
137	$Cr_2Si_2Te_6$
138	Hf_2Se_6
139	$RuBr_2$
140	Fe_2Te_4
141	Ge_2S_4
142	$Zr_2I_2N_2$
143	$Ga_2P_2Te_6$
144	Sc_2Te_2
145	Nb_3Br_8
146	$Ta_2P_2Se_6$
147	Tl_2Te_2
148	Ti_2S_6
149	$PbSe_2$
150	$Ir_2Br_2O_2$
151	Ir_2S_2
152	$PbSb_2Te_4$

153	CoF_2
154	HgO
155	$PtTe_2$
156	V_4O_8
157	Ir_2Se_2
158	Bi_2S_2
159	$Li_2V_4O_{10}$
160	$MnZrCl_6$
161	$Tl_2I_2O_2$
162	$Cu_4Cl_4O_4$
163	Ag_2MoTe_4
164	$CrMoF_6$
165	BSb
166	Sn_2F_2
167	$CoC_4Cl_2H_4N_2$
168	$Hf_3N_2O_2$
169	Ti_2Cl_4
170	Co_4S_8
171	Au_2WTe_4
172	$CuLi_2O_2$
173	Ti_2CO_2
174	$Ru_2P_2S_6$
175	$AsITe$
176	$Cr_2I_2S_2$
177	Bi_2Te_2
178	$ZrSe_2$
179	Sb_2Te_3
180	Tl_2Te_2
181	$Ir_2Br_2S_2$
182	YBr_2
183	$BiITe$
184	Bi_2Se_2
185	$CoBr_2$
186	$AgVP_2Se_6$
187	$CoCl_2$
188	$FeCl_2$
189	Bi_2SSe_2
190	$Pt_2Cl_2N_2$
191	$Ir_2Cl_2S_2$
192	$Mn_2Cl_2S_4Sb_2$
193	$Cu_2S_4Sb_2$
194	S_2Sb_2
195	$Hg_2P_2Te_6$
196	$Co_2H_2S_4$
197	ScH_2
198	$Y_2Cl_2O_4$
199	Au_2Br_2
200	K_2C_4
201	YCl_2
202	$TiTe_2$
203	Fe_2Cl_6
204	Nb_4S_{12}
205	Cu_2MoTe_4
206	$Zr_3C_2O_2$
207	$Cu_4F_4H_4O_4$
208	In_2O_2
209	$CoZrBr_6$
210	Si_2Te_2
211	$SnTe_2$
212	$Co_2H_2O_4$
213	$Bi_2P_2Te_6$
214	$CoC_4H_8N_2O_4$
215	$Zr_2P_2Se_6$
216	C_6N_2
217	Sc_2Se_2
218	Sb_2SeTe_2
219	$Zr_3N_2O_2$
220	$BiIS$
221	$Cu_4Cl_4H_4O_4$
222	$PtCl_2$
223	$NiZrF_6$
224	Zr_2Se_6
225	In_2S_4
226	Bi_2S_2Se
227	$CdGaInS_4$
228	$BiITe$
229	HfH_2O_2
230	Rh_2Cl_4
231	Sc_2S_2
232	$Pt_2P_2Se_6$
233	CrO_2
234	$Nb_4Ge_2Te_8$
235	$Hf_3C_2O_2$
236	Pb_2Cl_2
237	Sb_2Se_3
238	Pb_2S_2
239	Zr_2I_4
240	$Sc_2CH_2O_2$
241	$Cu_2O_6Si_2$
242	Cu_2Cl_6
243	$HfSe_2$
244	$Cr_2P_2Se_6$
245	$Sn_2P_2Te_6$
246	Pt_2O_2
247	$BiISe$
248	Pb_2Te_2
249	In_2Se_3
250	Cl_2Sb_2
251	Sb_2Se_2
252	Pb_2Br_2
253	Cr_3WTe_8
254	Br_2Sb_2
255	$Ir_2Cl_2O_2$
256	Pb_2Te_2
257	$AsISe$
258	Cu_2Se_2
259	Tl_2Se_2
260	$Cu_4O_{12}Te_2$
261	$Ni_2As_2O_7$
262	Zr_2Te_2
263	$CrTe_2$
264	$Cr_2Br_2S_2$
265	$Y_2CH_2O_2$
266	Nb_4O_8
267	$Cr_2Cl_2S_2$
268	Bi_2OSe_2
269	$PdCl_2$
270	$RuCl_2$
271	SSb_2Se_2
272	$Co_2F_2O_4$
273	Cr_3MoTe_8
274	Se_2Si
275	Cu_2ReCl_6
276	$Hf_2P_2Se_6$
277	Bi_2S_3
278	SSb_2Te_2
279	$InSb$
280	Sn_2Se_4
281	$Co_2H_4O_8Se_2$
282	Rb_2C_4
283	Ag_2Te_2
284	Pb_2Se_2
285	OSb_2Te_2
286	Au_2Br_2
287	In_2Te_4
288	W_2Cl_6
289	$CuInP_2Se_6$
290	Tl_2Se_2
291	$Cr_2W_2Te_8$
292	Ag_2F_2
293	$Cr_2Br_2O_2$
294	VI_2O
295	HgO_2
296	$TiSSe$
297	RuH_2O_2
298	Mo_2Cl_6
299	$Nb_2P_2S_6$
300	$P_2Sb_2Te_6$
301	OSb_2Se_2
302	$CoRe_2O_8$
303	$Nb_4Si_2Te_8$
304	$Zr_2Ge_2Te_8$
305	$TiSe_2$
306	Co_2I_6
307	$BiBrTe$
308	Os_2S_4
309	$BiClTe$
310	$WOTe$
311	CrW_3Te_8

312	Zn_2Te_2
313	$Hf_2I_2N_2$
314	Ir_4Te_8
315	TaO_2
316	Ag_2F_2
317	$Cr_2Mo_2Te_8$
318	Bi_2
319	$PdSe_2$
320	$ScSe_2$
321	Ag_2ReBr_6
322	$GeSe_2$
323	Nb_3I_7Te
324	$Hf_2Ge_2Te_8$
325	Bi_2OS_2
326	Os_2Se_4
327	CrSeTe
328	Sb_2Se_2Te
329	Fe_2Se_4
330	Pb_2Se_6
331	Ti_3ZrSe_8
332	Zr_2Br_4
333	Ta_4O_8
334	Rh_4Se_8
335	NiS_2
336	I_2Sb_2
337	$HfTi_3Se_8$
338	Ag_2WTe_4
339	BiBrTe
340	$Zn_2P_2Te_6$
341	Au_2MoSe_4
342	OS_2Sb_2
343	TiI_2
344	V_2F_8
345	Rh_4S_8
346	S_2Sb_2Se
347	S_3Sb_2
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367	HfI_2
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375	$Hf_2Ti_2Se_8$
376	$NiC_2N_2S_2$
377	$Cr_2Cl_2O_2$
378	Cu_2WTe_4
379	Fe_2S_4
380	$Bi_2P_2S_6$
381	In_2I_6
382	$Bi_2Br_2Se_2$
383	$MnZrF_6$
384	$FeZrI_6$
385	$Pt_4Tl_2Te_6$
386	Al_2FeS_4
387	SnO_2
388	Ta_3I_7Se
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409	Ga_2Se_2
410	$Sn_2O_6P_2$
411	Sc_2O_2
412	HgI_2
413	W_2I_6
414	$Bi_2I_2Se_2$
415	W_2Cl_6
416	$TiZr_3Se_8$
417	Cr_3MoSe_8

418	$Au_2I_2Te_4$
419	HfBrI
420	Os_2Te_4
421	$Au_2I_2Se_4$
422	ScS_2
423	$Sn_2P_2Se_6$
424	Hf_3TiSe_8
425	Ru_2S_4
426	$W_2H_4O_8$
427	WTe_2
428	Pb_2Se_4
429	GeS_2
430	$HfBr_2$
431	BiBrSe
432	$FeBr_2$
433	TiS_2
434	$Cu_2I_4O_{12}$
435	$CoCl_2O_8$
436	$Ga_2Br_2Se_2$
437	$ZrSe_2$
438	TiClI
439	Ag_2Se_2
440	MoOSe
441	PbS_2
442	AsB
443	$TiBr_2$
444	$Cr_2W_2Se_8$
445	$Zr_2P_2S_6$
446	Au_2WSe_4
447	$SnSe_2$
448	SnS_2
449	VBr_2O
450	Nb_3Cl_7Te
451	HgH_2O_2
452	Tl_2I_6
453	ZrBrI
454	Bi_2I_2
455	BiIS
456	Ag_2ReCl_6
457	Ru_2Se_4
458	$FeHfI_6$
459	Au_2I_2
460	CrSSe
461	$ZrTe_2$
462	Pb_2Se_2
463	$Cu_2I_2Se_4$
464	ISSb
465	Al_2I_6
466	Au_2MoS_4
467	S_2Sb_2Te
468	MoW_3Te_8
469	VCl_2O
470	$Cd_2P_2Te_6$

471	Nb_3Br_7S
472	$B_3C_{10}N_3$
473	$HfSe_2$
474	HfClI
475	Ge_2Te_2
476	Re_4Te_8
477	$CuC_6H_4N_6O_2$
478	$Ge_2P_2Te_6$
479	$Cr_2Mo_2Se_8$
480	$Ga_2I_2Se_2$
481	Ni_2S_4
482	$HfZr_3Se_8$
483	Ir_4Se_8
484	Cu_2F_4
485	$Sc_2P_2S_6$
486	$CoHfF_6$
487	$ZrBr_2$
488	$Cu_2Cl_2Se_4$
489	Au_2I_2
490	OsH_2O_2
491	ZrSSe
492	TiBrCl
493	$Co_2Br_4O_6Sb_4$
494	HfBrCl
495	$Ga_2I_2S_2$
496	$Cu_2Hg_2Cl_2Se_2$
497	$Pd_4Tl_2Se_6$
498	As_4
499	$Cu_2I_2Te_4$
500	$Cu_2Br_2Se_4$
501	$Bi_2I_2S_2$
502	$Cu_2C_6H_8I_2N_2$
503	ISbTe
504	$Ca_2C_2F_2O6$
505	$In_2P_2S_6$
506	$Au_2Br_2Se_4$
507	$Hf_2Zr_2Se_8$
508	Hf_2Cl_4
509	$FeCl_2$
510	Hf_3ZrSe_8
511	Cd_2Te_2
512	$Ti_2Zr_2S_8$
513	Ti_3ZrS_8
514	BiClSe
515	$NiZrI_6$
516	Hf_2Br_4
517	$Cu_2Cl_2Te_4$
518	$Cu_2I_2S_4$
519	$K_2Os_2F_{10}N_2O_2$
520	$NiC_6Cl_2H_4N_2$
521	$HfTi_3S_8$
522	$Hf_2P_2S_6$
523	$SnSe_2$
524	$Ta_2I_4O_2$
525	$Mo_2W_2Te_8$
526	$HfNiI_6$
527	$FeGa_2S_4$
528	$AgInP_2Se_6$
529	Cr_3WS_8
530	Pd_2F_2
531	Pd_2Cl_4
532	Bi_2Br_2
533	$FeZrBr_6$
534	Cu_2ReF_6
535	$Cu_2Br_2Te_4$
536	$NiBr_2$
537	ZrClI
538	MnI_2
539	CrS_2
540	$TiSe_2$
541	CrW_3Se_8
542	Sc_2CCl_2
543	HfSSe
544	Cr_2I_6
545	BiBrS
546	$V_2H_4O_{10}Se_2$
547	SnH_2O_2
548	Bi_2Cl_2
549	Cu_2MoSe_4
550	ZnI_2
551	BP
552	Cr_3MoS_8
553	$Zr_3F_2N_2O_2$
554	Mo_3WTe_8
555	$TiCl_2$
556	P_4
557	$HfCl_2$
558	$Ag_2Au_2Cl_8$
559	$AgGaP_2Se_6$
560	$Hf_2Ti_2S_8$
561	ZrBrCl
562	MoO_2
563	Ge_2H_2
564	Ni_2Te_4
565	Sn_2Se_2
566	PbTe
567	$MoTe_2$
568	$Cu_2Br_2S_4$
569	Hf_2CO_2
570	$FeHfBr_6$
571	Ag_2MoS_4
572	$Cr_2W_2S_8$
573	$Bi_2Cl_2S_2$
574	Zr_2CO_2
575	$Fe_2Mo_2Cl_2O_8$
576	$CrMo_3Se_8$
577	Au_2Se_2
578	Zn_2Te_4
579	Ag_2S_2
580	Co_2Br_6
581	ZrS_2
582	$Bi_2Br_2S_2$
583	Pb_2P2Se_6
584	$P_2Sb_2Se_6$
585	Mo_2I_6
586	$ZrCl_2$
587	$Au_2Cl_2Te_4$
588	AsITe
589	Sb_2
590	$Ge_2P_2Se_6$
591	In_2I_2
592	$HfTe_2$
593	Rh_2I_6
594	MoSTe
595	$TiZr_3S_8$
596	$Ag_2Cr_2P_4S_{12}$
597	Ca_4As_4
598	$Ga_2I_2O_2$
599	BiClS
600	ISbSe
601	$BiCuP_2Se_6$
602	Hf_3TiS_8
603	ISbTe
604	ISbSe
605	GeI_2
606	$Tl_2Br_2O_2$
607	$V_2F_2O_7Te_2$
608	$Au_2Br_2Te_4$
609	$Cr_2Mo_2S_8$
610	Ni_2Se_4
611	$Hg_2P_2S_6$
612	Sc_2CF_2
613	BiBrSe
614	RuI_2
615	$Nb_2I_4O_2$
616	CuBr
617	Ag_2ReF_6
618	$Ag_2I_2Te_4$
619	$PbSe_2$
620	$Tl_2Cl_2O_2$
621	$Pd_2I_4O_{12}$
622	WSeTe
623	$Sn_2P_2S_6$
624	$Nb_2Br_4O_2$
625	$Rh_2Cl_2Te_2$
626	$Mo_2O_{10}P_2$
627	$Nb_2Cl_4O_2$
628	$RuBr_2$
629	MnI_2

630	$FeZrCl_6$
631	$K_2C_2O_6$
632	BrSbTe
633	$MnZrI_6$
634	$Ag_2I_2Se_4$
635	MoOS
636	HfS_2
637	Al_2MgSe_4
638	AsBrTe
639	$In_2Cl_2Se_2$
640	Cd_2Te_4
641	$Sn_2I_2N_2$
642	Pd_4I_8
643	BrSbSe
644	Ag_2WSe_4
645	Au_2WS_4
646	$Au_4I_4Te_4$
647	$Bi_2I_2O_2$
648	$Cr_2Cu_2P_4S_{12}$
649	NiH_2O_2
650	In_2Te_5
651	$Nb_2Cl_4Se_4$
652	Pb_2S_4
653	$Fe_2W_2Cl_2O_8$
654	$FeHfCl_6$
655	Tl_2Br_6
656	SnI_2
657	$Nb_2Br_4Se_4$
658	InP
659	VClI
660	OsI_2
661	$AgBiP_2Se_6$
662	Bi_2I_6
663	$Cd_2Mn_3O_8$
664	$Pd_4P_4Se_4$
665	$Zr_2I_2N_2$
666	$Al_2Mg_2Se_5$
667	$Al_2Si_2Te_6$
668	Re_4Se_8
669	Y_2CF_2
670	GaAs
671	Pd_2S_4
672	$Pd_2O_6Se_2$
673	GeH_2O_2
674	Ge_2Se_2
675	PbO_2
676	CrW_3S_8
677	$Hf_2Zr_2S_8$
678	Co_2Cl_6
679	$Pt_4Tl_2Se_6$
680	MnO_2
681	MoSeTe
682	WSTe
683	In_2Te_2
684	Hf_3ZrS_8
685	AsISe
686	Ga_2I_6
687	$HfZr_3S_8$
688	$OsBr_2$
689	Hf_2S_6
690	ZrS_2
691	Pb_2S_2
692	$PtSe_2$
693	$Ag_2Br_2S_4$
694	PdS_2
695	ClSbSe
696	$RuCl_2$
697	Zr_2S_6
698	$CrMo_3S_8$
699	As_8Ge_4
700	$Ag_2Cl_2S_4$
701	BiBrS
702	$Nb_2I_2O_4$
703	$Ag_2I_2S_4$
704	VBrI
705	$In_2I_2O_2$
706	$Re_6Cl_2Se_8$
707	$Pd_4P_4S_4$
708	Se_2Si_2
709	TiO_2
710	$Cu_2As_4Cl_2S_3$
711	HgI_2
712	VI_2
713	$FeZrF_6$
714	Pd_2Te_4
715	$Ag_2Br_2Te_4$
716	Au_2S_2
717	BrSSb
718	$NiCl_2$
719	ISSb
720	$FeHfF_6$
721	HfS_2
722	MnI_2
723	Pt_4I_8
724	Cu_2Cl_2
725	AsBrSe
726	$In_2Br_2Se_2$
727	In_2Te_2
728	Cu_2WSe_4
729	BiClSe
730	$Ag_2Br_2Se_4$
731	AsBrTe
732	AlAs
733	WSe_2
734	WOSe
735	VBr_2
736	$Pt_4Tl_2S_6$
737	ClSbTe
738	MoW_3Se_8
739	$In_2I_2Se_2$
740	C_6N_8
741	TiS_2
742	Ga_2Te_2
743	$Mo_2W_2Se_8$
744	$SnBr_2$
745	$Cd_2P_2Se_6$
746	Re_4S_8
747	Hg_2I_2
748	NiO_2
749	AsClTe
750	VBrCl
751	Cu_3O_4P
752	$Ag_2Cl_2Te_4$
753	PbI_2
754	Ga_2Te_2
755	Mo_3WSe_8
756	$NiZrBr_6$
757	Br_2Ge
758	Re_4O_8
759	$Al_2P_2S_6$
760	$Zn_2P_2Se_6$
761	Pt_2Cl_2
762	Pt_2Te_4
763	Pd_2Se_4
764	Al_2O_2
765	ClSSb
766	$AgInP_2S_6$
767	BrSbTe
768	In_2Se_2
769	$MoSe_2$
770	$NiC_4H_8N_2O_4$
771	$OsCl_2$
772	In_2F_2
773	AsIS
774	In_2Br_2
775	$Ag_2Cl_2Se_4$
776	WO_2
777	Rh_2Br_6
778	GeS_2
779	PbO_2
780	Ga_2Br_6
781	VCl_2
782	$HfNiBr_6$
783	V_2O_5
784	Ir_2I_6
785	$HfMnI_6$
786	CdS_2
787	Cd_2Se_4
788	$Pb_2P_2S_6$

789	$Sn_2Br_2N_2$
790	Cl2Ge
791	AsClSe
792	Bi_2I_6
793	PdO_2
794	Ag_2WS_4
795	Zn_2Se_4
796	S_2Si
797	$Ba_4F_4Sb_4Se_8$
798	AsBrS
799	PbS_2
800	$Sc_2I_2Se_2$
801	ClSbTe
802	Cr_2F_4
803	WSSe
804	Cd_2Se_2
805	In_2Se_2
806	$Ge_2P_2S_6$
807	$Sn_2Cl_2N_2$
808	$Sc_2Cl_2Se_2$
809	Sn_2S_2
810	$Al_2Cl_2Se_2$
811	AsBrS
812	S_2Si_2
813	$Ga_2Cl_2S_2$
814	As_8Si_4
815	$Mo_2Br_4O_4$
816	BrSSb
817	BiClS
818	$Pd_2N_4O_{12}$
819	$Bi_2Br_2O_2$
820	SnS_2
821	Pt_2Se_4
822	$ZrSe_2$
823	Cu_2Cl_2
824	$SnCl_2$
825	MoSSe
826	GeO_2
827	ScO_2
828	BrSbSe
829	GeTe
830	$MnBr_2$
831	AsClTe
832	As_2
833	$Ga_2Br_2S_2$
834	CdI_2
835	$Al_2I_2Se_2$
836	Cu_2Br_2
837	AsBrSe
838	PbI_2
839	$Br_2Ge_2N_2$
840	WOS
841	AlSb

842	Cr_2Br_6
843	$Sc_2Br_2Se_2$
844	Sc_4S_6
845	Cd_2S_4
846	Cu_2Br_2
847	MoW_3S_8
848	$Mo_2W_2S_8$
849	PbSe
850	WS_2
851	Cu_2WS_4
852	$Al_2Br_2Se_2$
853	AsClS
854	P_8Si_4
855	$In_2I_2S_2$
856	HgI_2
857	$Mn_2Mo_2O_{12}Te_2$
858	In_2Cl_2
859	$NiCl_2O_8$
860	$Nb_2Br_4S_4$
861	Ga_2O_2
862	Mo_3WS_8
863	V_4O_{10}
864	$MnRe_2O_8$
865	$V_2O_{10}P_2$
866	Au_2CaF_{12}
867	Ir_2Br_6
868	PbH_2O_2
869	Ag_2Cl_2
870	CdF_2O_2
871	$HgBr_2$
872	$NiRe_2O_8$
873	PbI_2
874	MoS_2
875	SnTe
876	GaP
877	$Hf_2I_2N_2$
878	SnS_2
879	$MnBr_2$
880	Rh_2Cl_6
881	In_2I_6
882	$NiZrCl_6$
883	F_2Ge
884	In_2S_2
885	$Ag_8C_4N_8$
886	$Nb_2Cl_4S_4$
887	$Al_2I_2S_2$
888	$Zr_2Br_2N_2$
889	$HfNiCl_6$
890	Zn_2Se_2
891	$Cu_2PtC_6N_8$
892	In_2Se_2
893	$AgScP_2Se_6$
894	SnF_2

895	$MnZrBr_6$
896	In_4Br_8
897	Ga_2Se_2
898	$PbBr_2$
899	Tl_2Br_6
900	$Sc_2I_2S_2$
901	Hg_4I_8
902	ClSSb
903	ClSbSe
904	PtO_2
905	In_2S_2
906	Tl_2Cl_6
907	$HfSe_2$
908	PtS_2
909	$Li_2F_2S_2$
910	ZrO_2
911	Zn_2S_4
912	SnO
913	$MnCl_2$
914	Ge_2S_2
915	AsClSe
916	Ag_2Br_2
917	AsClS
918	$In_4I_4Te_4$
919	$Bi_2Cl_2O_2$
920	As_4Se_6
921	Cr_2Cl_6
922	$As_4Ge_4Se_4$
923	$MnF_{12}Sb_2$
924	Bi_2Br_6
925	$W_2O_{12}Sb_4$
926	Al_2Te_2
927	ZnI_2
928	$Pd_3P_2S_8$
929	Ga_2Se_2
930	Ag_2I_2
931	Al_8Te_{12}
932	$MnBr_2$
933	Cd_2S_2
934	Ga_2I_2
935	Cu_2I_2
936	In_2I_2
937	$Sc_4I_4O_4$
938	$MnCl_2$
939	$In_2Cl_2S_2$
940	PbO
941	Pt_2S_4
942	$Sc_2I_2O_2$
943	$Zr_2Br_2N_2$
944	PbS
945	$Zn_2H_8N_4Te_2$
946	Ir_2Cl_6
947	I_6Sb_2

948	Ag_2Br_2
949	$FeMn_2C_6N_6$
950	SnI_2
951	$Na_2F_2S_2$
952	$Zr_2Cl_2N_2$
953	Sc_2I_6
954	$Cl_2Ge_2N_2$
955	Sc_2I_6
956	Cu_2I_2
957	Ag_2I_2
958	GaN
959	$O_4S_8Sb_8$
960	$Cd_2P_2S_6$
961	Ti_4O_8
962	$Sc_2P_2S_8$
963	$In_2Br_2S_2$
964	Tl_2Cl_4
965	As_2I_6
966	$Zr_2Cl_2N_2$
967	SnI_2
968	ZrS_2
969	HfO_2
970	P_2
971	$Cs_2C_6N_6Se_6$
972	CF_2Si
973	$PbCl_2$
974	Ag_2WO_4
975	Bi_2Br_6
976	GeI_2
977	$Hf_2Br_2N_2$
978	Al_2Te_2
979	$Ga_2In_2S_6$
980	$HgBr_2$
981	Au_2Br_2
982	Al_2Se_2
983	Ag_2Cl_2
984	$PbBr_2$
985	$HgBr_2$
986	In_2Br_6
987	$AgScP_2S_6$
988	$In_4Br_4Te_4$
989	$MnCl_2$
990	V_4O_{10}
991	Zn_2Se_2
992	Al_2MgS_4
993	$Mg_2P_2Se_6$
994	Cu_2O_4S
995	In_2Br_2
996	V_4O_{10}
997	Tl_2I_2
998	$Hf_2Br_2N_2$
999	Mo_2O_6
1000	$HgCl_2$

1001	Ag_2MoO_4
1002	Al_2S_2
1003	$Zn_2P_2S_6$
1004	HgF_2
1005	Zn_2I_2
1006	Al_2I_6
1007	HfS_2
1008	$SnBr_2$
1009	SnO_2
1010	$Hf_2Cl_2N_2$
1011	$Sc_2Cl_2S_2$
1012	$Mn_2H_4O_8S_2$
1013	Ga_2Br_2
1014	$Sc_2Br_2S_2$
1015	GeO
1016	CdI_2
1017	Al_2Se_2
1018	Al_2S_2
1019	$Ga_2Cl_2Te_2$
1020	H_2Si_2
1021	$CdC_4Cl_2H_4N_2$
1022	SnSe
1023	Ga_2S_2
1024	Bi_2Cl_6
1025	$Hg_2V_2O_6$
1026	$W_2Cl_4O_4$
1027	GeSe
1028	$Al_2I_2O_2$
1029	Pb_2Br_4
1030	CdH_2O_2
1031	As_4S_6
1032	$Al_2Tl_2F_8$
1033	AlP
1034	CdH_2S_2
1035	$Al_2Br_2S_2$
1036	As_4S_6
1037	$PbBr_2$
1038	$Hg_4Mo_2O_8$
1039	$CsC_2I_3N_2$
1040	$Na_2Nb_2Cl_{12}$
1041	SnS
1042	$In_2Br_2O_2$
1043	In_2Cl_2
1044	Br_2Ge
1045	Ga_2S_2
1046	$SnCl_2$
1047	$Hf_2Cl_2N_2$
1048	Br_6Sb_2
1049	ZnH_2O_2
1050	$Al_2Cl_2S_2$
1051	CdI_2
1052	HgH_2S_2
1053	Bi_2Cl_6

1054	$PbCl_2$
1055	$CdBr_2$
1056	$Na_4O_8S_4$
1057	Ga_2Cl_2
1058	Tl_2I_2
1059	Pb_2O_2
1060	$ZnBr_2$
1061	Tl_2Br_2
1062	Tl_2Cl_6
1063	ZnI_2
1064	$HgCl_2$
1065	GeS
1066	Cu_2MoO_4
1067	Ti_2O_6
1068	$HgCl_2$
1069	As_2Br_6
1070	Sn_2O_2
1071	$SnBr_2$
1072	Al_2Br_6
1073	$Hg_4W_2O_8$
1074	$Cu_2C_2Cl_2O_2$
1075	MgF_2S_2
1076	$Ga_2Br_2O_2$
1077	CdClHO
1078	Ga_2Cl_6
1079	Br_2Ge
1080	Zn_2S_2
1081	$Mo_2Ta_2O_{11}$
1082	MgI_2
1083	Y_2I_6
1084	$H_4O_{12}Te_4$
1085	PbF_2
1086	Ga_2Br_6
1087	Hg_2GeO_4
1088	$In_2Cl_2O_2$
1089	Pb_4O_4
1090	Cl_2Ge
1091	$Li_2H_4N_2O_6$
1092	Au_2MoO_4
1093	Sc_2Br_6
1094	$K_2C_6H_6O_6$
1095	$Ga_2F_4H_{10}N_4$
1096	Tl_2Cl_2
1097	O_8Te_4
1098	SnO_2
1099	TiO_2
1100	$Bi_4Sr_2O_8$
1101	PbF_4
1102	$PbWO_4$
1103	$Sr_2Cl_4O_8$
1104	$Zn_2Ge_2O_6$
1105	In_2Br_6
1106	$SnCl_2$

1107	Y_2I_6
1108	$PbCl_2$
1109	$InLiI_4O_{12}$
1110	$Na_2Ta_2Cl_{12}$
1111	$Mg_2P_2S_6$
1112	$Na_2H_2O_2$
1113	$Li_2H_4N_2$
1114	$InNaI_4O_{12}$
1115	$Na_2F_2O_2$
1116	$Ca_2Cl_4O_8$
1117	$AlLiP_2S_6$
1118	CaF_2O_2
1119	$Tl_2O_6Sb_2$
1120	$Li_2PtH_6O_6$
1121	$Na_2PtH_6O_6$
1122	$Bi_2Cd_2Cl_2O_4$
1123	Ti_2O_4
1124	SrF_2O_2
1125	In_2Cl_6
1126	$Bi_4B_4O_{12}$
1127	$CdPb_2Cl_2O_2$
1128	AlN
1129	Cu_2WO_4
1130	$Li_2F_2O_2$
1131	$Mo_2Zn_2O_8$
1132	$CdBr_2$
1133	CaI_2
1134	Cl_2Ge
1135	Au_2WO_4
1136	MgF_2O_2
1137	Sc_2Br_6
1138	GeO_2
1139	$BiHO_6Se_2$
1140	Sn_2O_2
1141	Tl_2Br_2
1142	$CdBr_2$
1143	$CdCl_2$
1144	$Mo_2Zn_2O_{12}Te_2$
1145	C_2F_2
1146	$K_2N_2O_6$
1147	$Mg_2Mo_2O_{12}Te_2$
1148	$Sc_2O_{13}Te_5$
1149	$O_{14}S_2Te_4$
1150	Mo_2ZrO_8
1151	$Sc_2Br_2O_2$
1152	As_4O_8
1153	Sc_2Cl_6
1154	$LiC_5H_5N_2O_5$
1155	$Li_4O_8Sb_4$
1156	$Zn_2Cl_4O_6Sb_4$
1157	$Hg_4K_2Cl_6O_6S_2$
1158	$ZnBr_2$
1159	MgI_2
1160	$Hg_2K_4Cl_8$
1161	BaI_2
1162	$Li_2Cl_2O_4$
1163	$Mg_3H_4O_9Si_2$
1164	MgH_2O_2
1165	$ZnBr_2$
1166	MgH_2O_2
1167	$Bi_2Ge_3O_9$
1168	$As_2O_8Sb_2$
1169	$As_2H_2O_{10}Te_2$
1170	$Zn_2O_6Si_2$
1171	$Ag_2C_8N_6$
1172	SrI_2
1173	Li_4CO_4
1174	S_8Si_4
1175	$ZnCl_2$
1176	C_2H_2
1177	$V_4F_{12}O_4$
1178	Hf_2O_6
1179	TiO_2
1180	$Rb_2Br_2F_8$
1181	Y_2Br_6
1182	$Na_2H_2O_2$
1183	MgH_2S_2
1184	$Hg_3B_2O_6$
1185	$FeSn_2C_6N_6$
1186	CaI_2
1187	$Na_2H_2S_2$
1188	$MgBr_2$
1189	Zr_2O_6
1190	$Na_2H_8I_2O_4$
1191	$Zn_2As_4O_8$
1192	O_6Sb_4
1193	$CdCl_2$
1194	Tl_2Cl_2
1195	GeO_2
1196	$Ga_2Cl_2O_2$
1197	SrH_2O_2
1198	CaH_2O_2
1199	Rb_2I_2
1200	$Bi_2O_9Si_3$
1201	In_2Cl_6
1202	$Ge_3O_9Sb_2$
1203	CH_2Si
1204	As_4O_6
1205	CdF_2
1206	SrH_2S_2
1207	CaH_2S_2
1208	Ga_2Cl_6
1209	Al_2Cl_6
1210	$CdCl_2$
1211	BaI_2
1212	As_4O_6
1213	K_2I_2
1214	Al_2Br_6
1215	SrI_2
1216	Sc_2Cl_6
1217	$Ca_2Sn_4F_{12}$
1218	$Li_2H_2O_2$
1219	$Na_2SnH_6O_6$
1220	$FeZn_2C_6N_6$
1221	BaI_2
1222	Re_2ZnO_8
1223	$Li_2H_2S_2$
1224	$Ca_4O_{12}Te_4$
1225	$As_2O_6Sb_2$
1226	CaI_2
1227	SrI_2
1228	$Sn_2F_2O_6P_2$
1229	$Sn_2C_2H_6O_6P_2$
1230	$Li_6H_2O_8Te_2$
1231	Cs_2Br_2
1232	SnF_4
1233	Y_2Br_6
1234	$Cd_2H4O_8Se_2$
1235	$HfNa_2H_6O_6$
1236	$Na_2C_2N_2S_2$
1237	$CaBr_2$
1238	$Al_2Br_2O_2$
1239	Cs_2F_2
1240	$BaBr_2$
1241	Rb_2Br_2
1242	$Ca_2Br_2H_2$
1243	$ZnCl_2$
1244	$Sr_2F_2I_2$
1245	$Ba_2H_8O_6$
1246	$Sc_2Cl_2O_2$
1247	As_4O_6
1248	$ZrH_2O_6P_2$
1249	$Ga_2H_2O_8Se_2$
1250	$Sn_2H_2O_6P_2$
1251	$SrBr_2$
1252	Bi_2F_6
1253	$Na_4As_4O_8$
1254	$Sr_2Br_2H_2$
1255	$As_2O_8P_2$
1256	ZrO_2
1257	$O_8P_2Sb_2$
1258	K_2Br_2
1259	$Sn_2O_8S_2$
1260	$Y_2Cl_2O_2$
1261	$Sr_2H_8O_6$
1262	Y_2Cl_6
1263	ZnF_2
1264	ZrO_2
1265	$Zn_2H_4O_8Se_2$

1266	$ZnCl_2$
1267	$MgNa_2H_4O_8S_2$
1268	$As_4O1_2S_2$
1269	Cs_2Cl_2
1270	$K_2C_2H_2O_6$
1271	HfO_2
1272	Mg_2Cl_4
1273	$As_4H_2O_{12}P_2$
1274	Rb_2F_2
1275	$BaBr_2$
1276	$SrBr_2$
1277	$MgBr_2$
1278	Rb_2Cl_2
1279	BN
1280	$K_2C_4H_6O_6$
1281	$Na_2B_2H_8O_8$
1282	$CaBr_2$
1283	$BaCl_2$
1284	$MgCl_2$

1285	$CaCl_2$
1286	HfO_2
1287	$Na_2C_2H_6N_8O_2$
1288	$CaBr_2$
1289	K_2Cl_2
1290	$BaBr_2$
1291	$SrBr_2$
1292	$SrCl_2$
1293	K_2F_2
1294	$BaF_{12}Sb_2$
1295	$O_{10}P_4$
1296	ZnC_4N_6
1297	$Sr_2O_{12}P_4$
1298	Y_2Cl_6
1299	$ZnB_2C_8N_8$
1300	$BaCl_2$
1301	$SrCl_2$
1302	$MgCl_2$
1303	$K_2Cl_2O_6$

1304	$H_4O_{10}Si_4$
1305	Al_2Cl_6
1306	$CaCl_2$
1307	$Cs_2F_2H_6O_6P_2$
1308	$BaCl_2$
1309	$Cs_2C_2F_6O_6S_2$
1310	BaF_2
1311	$Ca_2Cl_4H_8O_4$
1312	$Al_2Cl_2O_2$
1313	$SrCl_2$
1314	$Rb_2C_2F_6O_6S_2$
1315	$CaCl_2$
1316	$MgCl_2$
1317	$BeH_4O_4P_2$
1318	SrF_2
1319	MgB_2H_8
1320	CaF_2

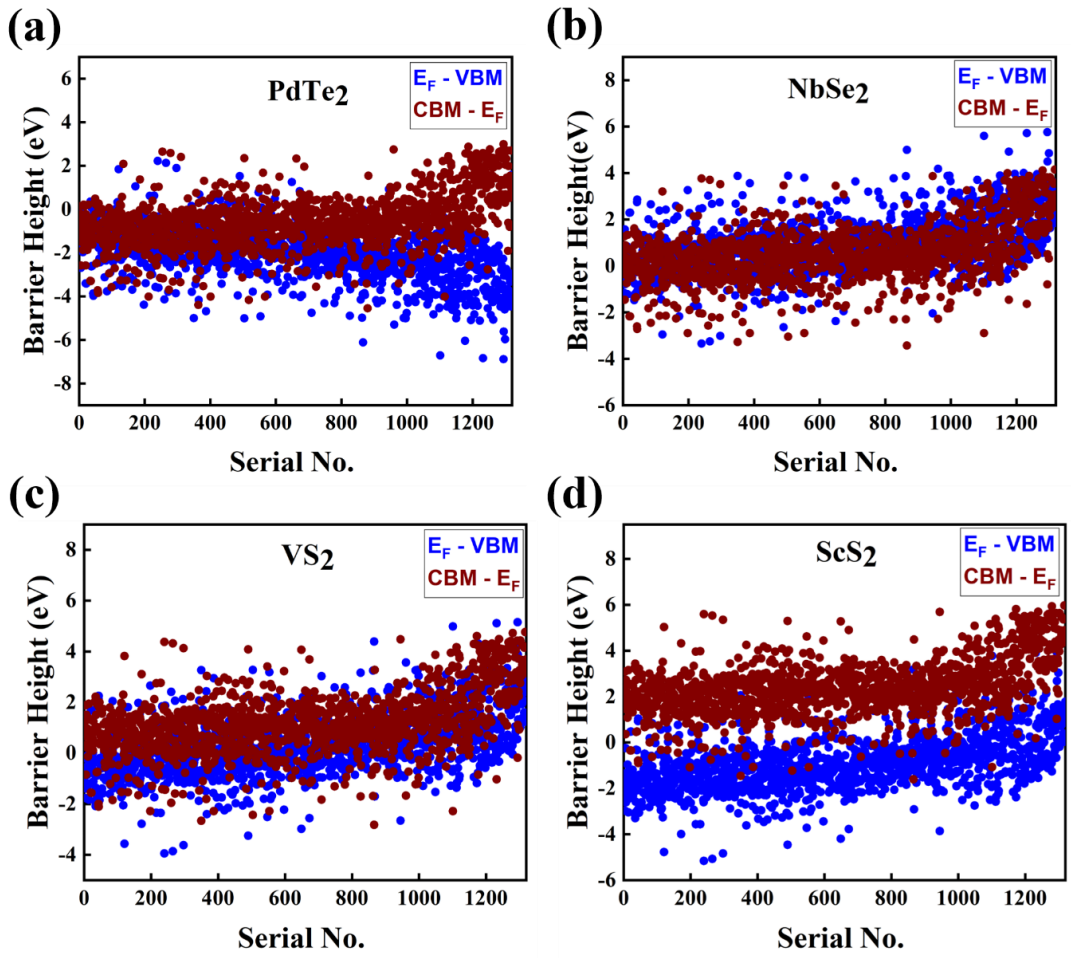

FIG S2. Barrier heights of various 2D monolayers obtained from the C2DB database with 2D metals: (a) $PdTe_2$, (b) $NbSe_2$, (c) VS_2 and (d) ScS_2.

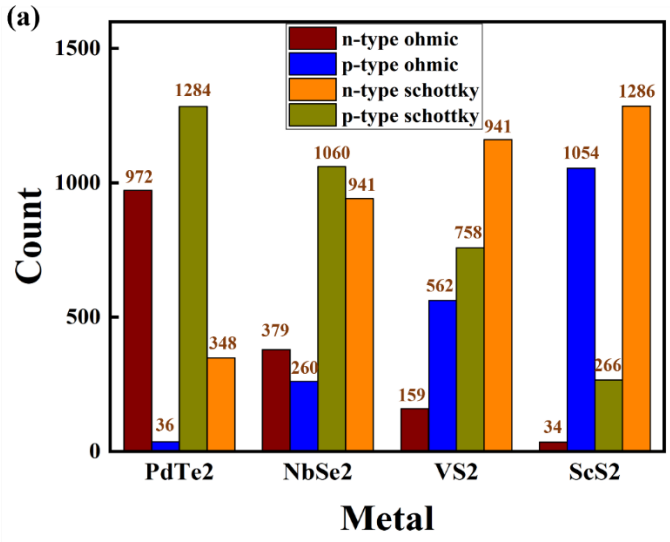

FIG S3. Count of various types of contacts formed by monolayers with metals, as obtained from PBE energy levels

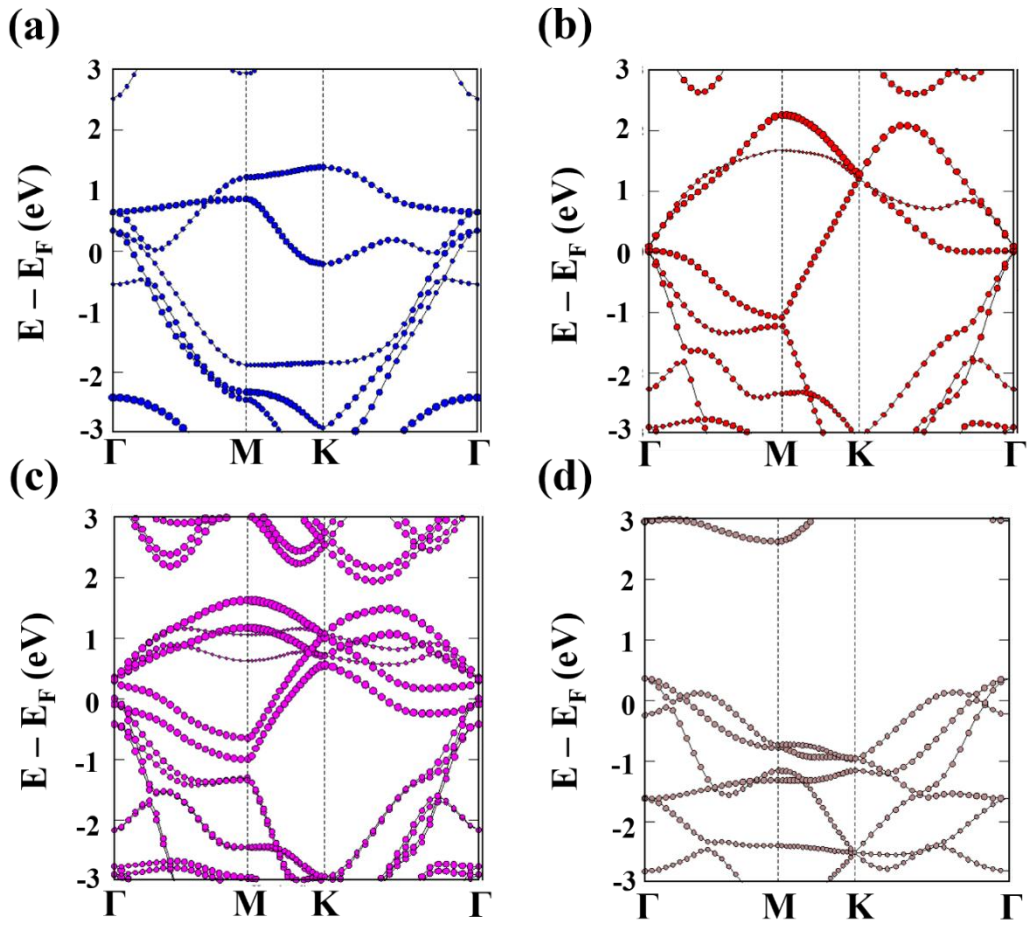

FIG S4. Band structure (PBE) of metal monolayers: (a) $PdTe_2$ (b) $NbSe_2$ (c) VS_2 and (d)ScS_2

Table – S2 List of monolayers selected for forming actual vdW heterostructures with $PdTe_2$, $NbSe_2$, and ScS_2 metal monolayers, including space group, prototype, lattice constant, lattice mismatch, barrier height obtained from the database, and predicted type of contact based on barrier height.

Metal	Semiconductors	Space group	Prototype	Lattice constant	Lattice mismatch (%)	Barrier height (from database) eV	Type of contact predicted
$PdTe_2$ P3m1 4.04 AB2	BiClS	P3m1	ABC	4.229	4.68	-1.68	Ohmic (n)
	BiClSe	P3m1	ABC	4.146	2.62	-1.55	Ohmic (n)
	PbS_2	P3m1	ABC	3.848	4.75	-2.02	Ohmic (n)
	Tl_2S_2	P-6m2	AB	4.057	0.42	-1.71	Ohmic (n)
	Tl_2Se_2	P-6m2	AB	4.229	4.68	-1.41	Ohmic (n)
	$HgBr_2$	P-6m2	AB2	3.976	1.58	-1.27	Ohmic (n)
	YI_2	P-6m2	AB2	4.105	1.69	-0.46	Ohmic (p)
	ScI_2	P-6m2	AB2	3.979	1.51	-0.31	Ohmic (p)
$NbSe_2$ P-3m1 3.48 AB2	PbO_2	P-3m1	AB2	3.402	2.24	-2.26	Ohmic (n)
	GeS_2	P-3m1	AB2	3.444	1.03	-0.87	Ohmic (n)
	ZrSSe	P3m1	ABC	3.637	4.51	-0.52	Ohmic (n)
	HfS_2	P-6m2	AB2	3.543	1.81	-0.04	Ohmic (n)
	ZrS_2	P-6m2	AB2	3.571	2.61	-0.10	Ohmic (n)
	In_2O_2	P-6m2	AB	3.440	1.15	-1.32	Ohmic (n)
	$ZrBr_2$	P-6m2	AB2	3.560	2.30	-1.02	Ohmic (p)
	$HfBr_2$	P-6m2	AB2	3.500	0.57	-1.20	Ohmic (p)
	$TiBr_2$	P-6m2	AB2	3.472	0.23	-1.14	Ohmic (p)
	HfBrI	P3m1	ABC	3.644	4.72	-1.34	Ohmic (p)
	TiBrI	P3m1	ABC	3.633	4.40	-1.29	Ohmic (p)
	HfClI	P3m1	ABC	3.578	2.82	-1.13	Ohmic (p)
	TiClI	P3m1	ABC	3.552	2.07	-1.06	Ohmic (p)
ScS_2	HfBrI	P3m1	ABC	3.644	2.57	-3.82	Ohmic (p)

P3m1 3.74 AB2	ZrBrI	P3m1	ABC	3.703	0.99	-3.65	Ohmic (p)
	TiBrI	P3m1	ABC	3.633	2.86	-3.77	Ohmic (p)
	HfI_2	P-6m2	AB2	3.773	0.88	-4.01	Ohmic (p)
	TiI_2	P-6m2	AB2	3.769	0.78	-3.95	Ohmic (p)
	ZrI_2	P-6m2	AB2	3.829	2.38	-3.83	Ohmic (p)

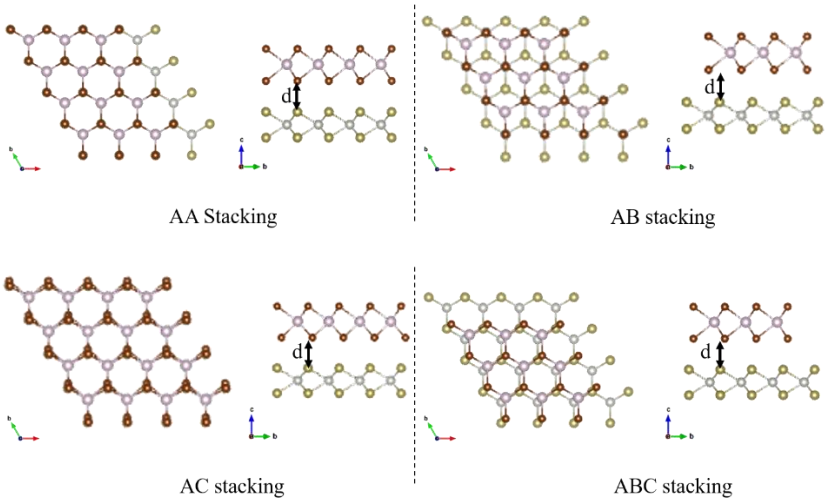

FIG S5. Optimized geometries of $PdTe_2/HgBr_2$ with different stacking order.

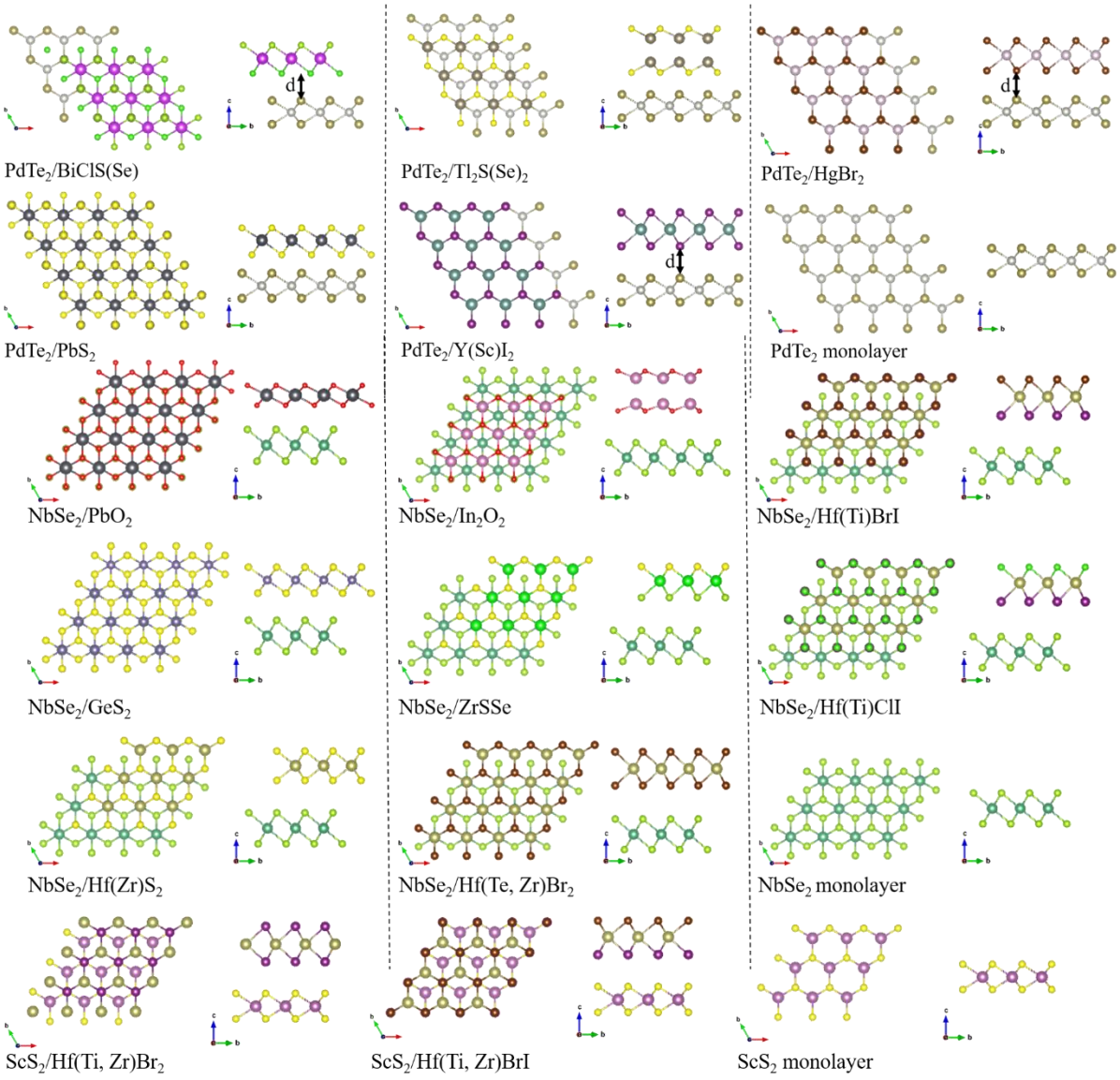

FIG S6. Optimized geometries of all vdW heterostructures formed with selected monolayers, including the structures of the metal monolayers.

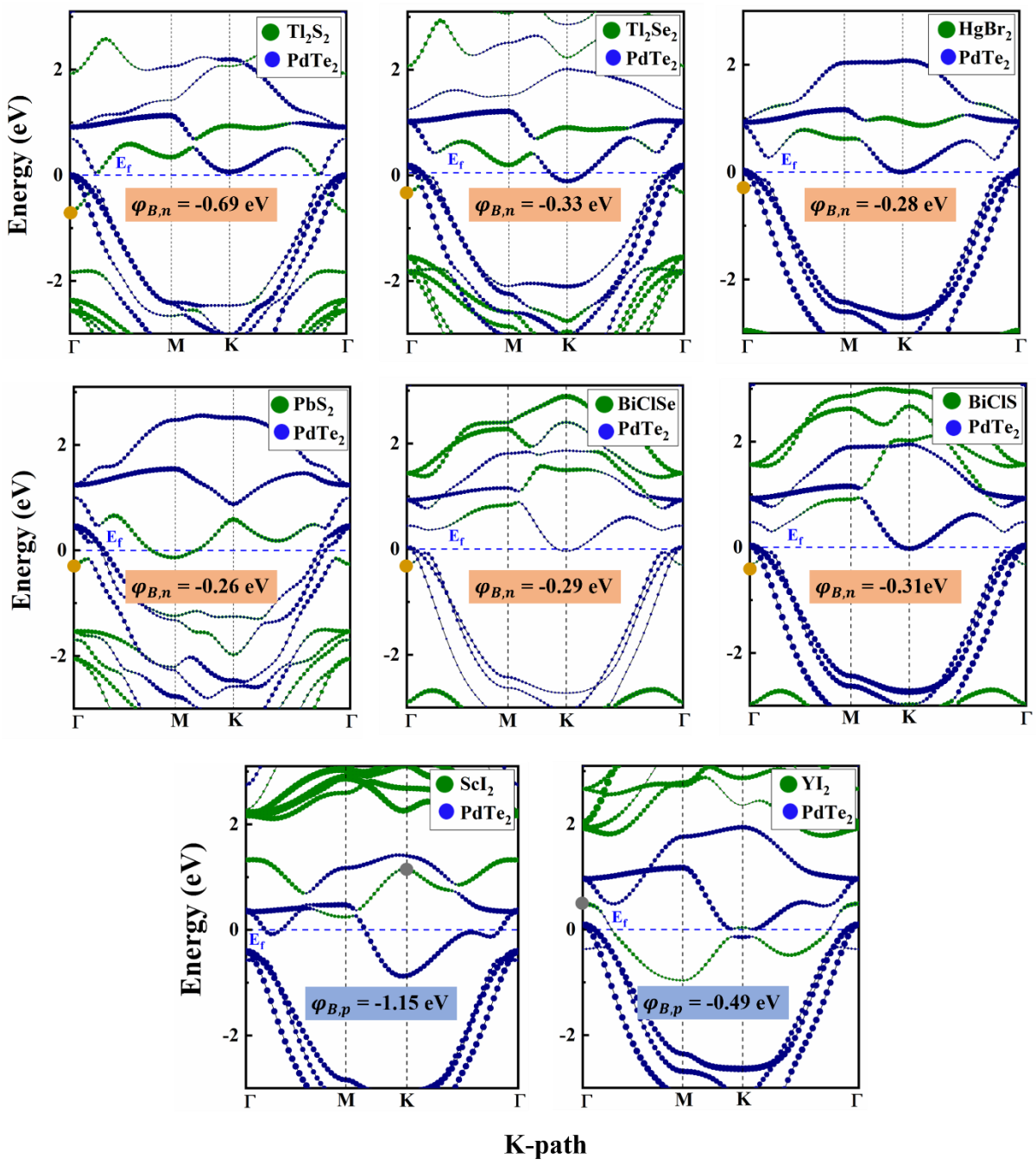

FIG S7. Band structure (HSE06) of selected vdWHs formed with $PdTe_2$ metal monolayer. Blue and green bubbles represent the contributions of $PdTe_2$, and the chosen materials (Tl_2S_2, Tl_2Se_2, $HgBr_2$, PbS_2, BiClSe, BiClS, ScI_2, and YI_2) to the band structure, respectively. The orange and grey bubbles represent the CBM and VBM respectively of the semiconducting monolayers.

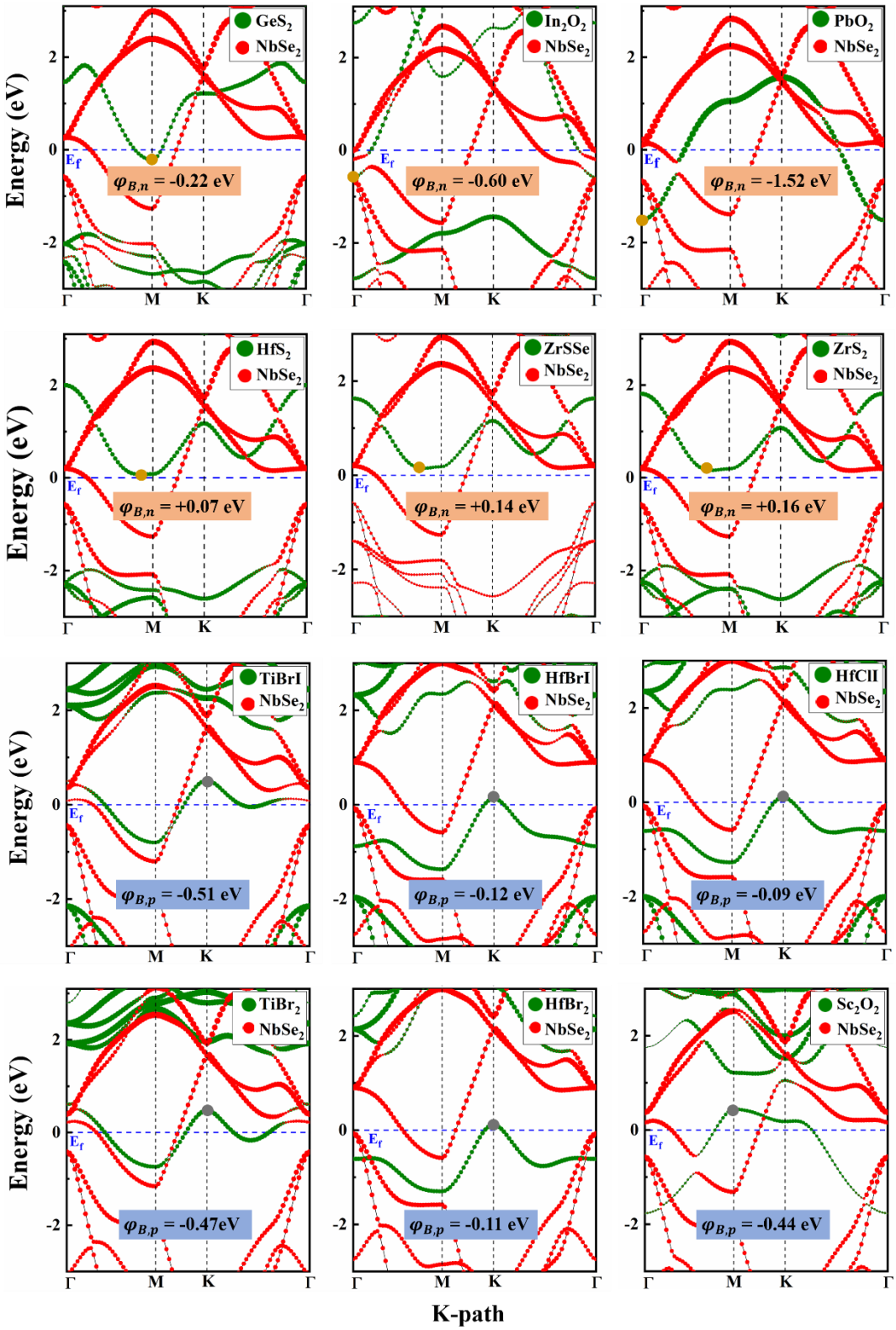

FIG S8. Band structure (HSE06) of selected vdW heterostructures formed with the $NbSe_2$ metal monolayer. Red and green bubbles represent the contributions of $NbSe_2$, and the chosen materials, both n-type (GeS_2, In_2O_2, PbO_2, HfS_2, ZrS_2, and ZrSSe) and p-type ($HfBr_2$, $TiBr_2$,

$ZrBr_2$, HfBrI, TiBrI and HfClI) to the band structure, respectively. The orange and grey bubbles represent the CBM and VBM respectively of the semiconducting monolayers.

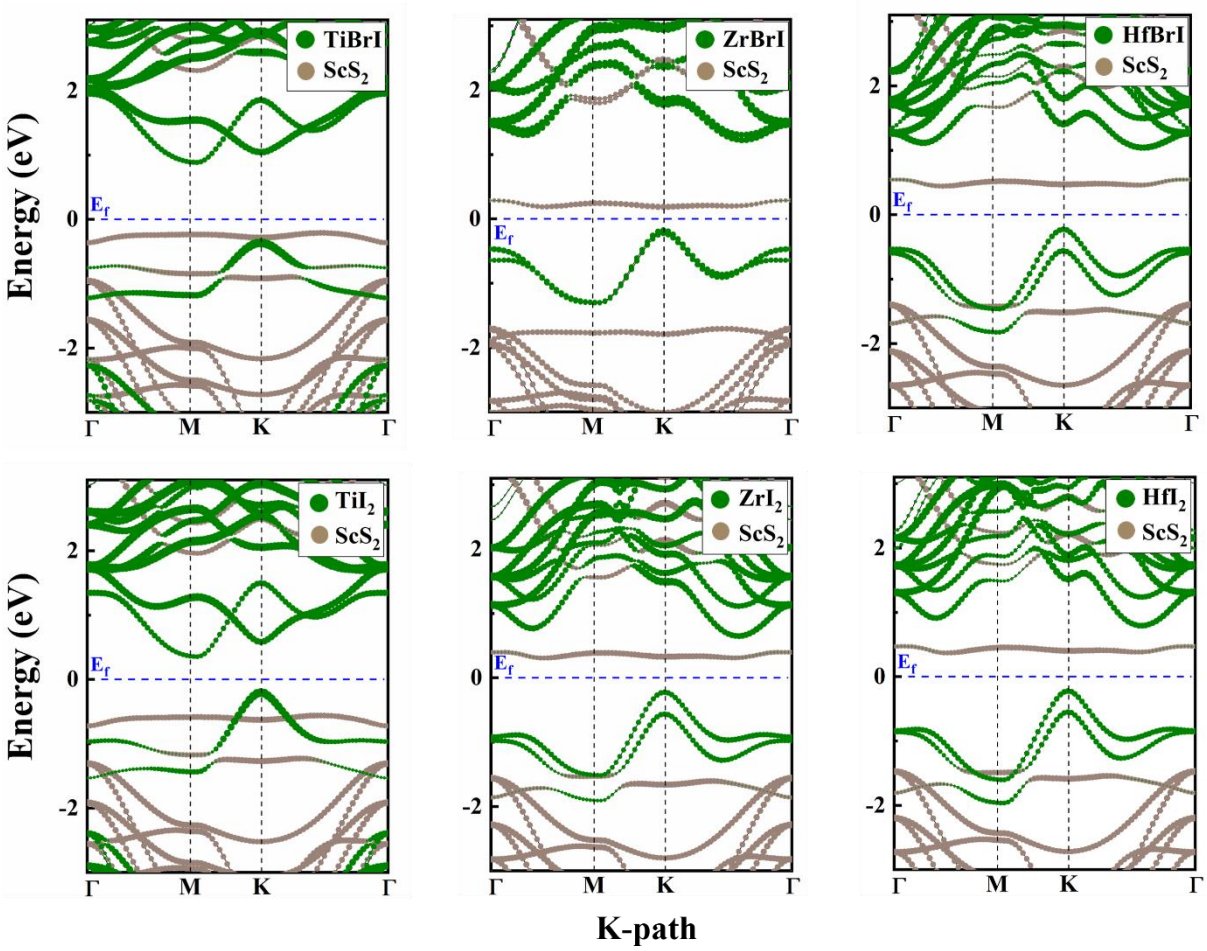

FIG S9. Band structure (HSE06) of selected vdW heterostructures formed with ScS_2 metal monolayer. Brown and green bubbles represent the contributions of ScS_2 and the chosen materials ($HfBr_2$, $TiBr_2$, $ZrBr_2$, HfBrI, TiBrI and HfClI) predicted to form p-type contact with ScS_2, to the band structure, respectively.

Table – S3. Formation energy, lattice mismatch, barrier height, and contact type for the optimized geometries of actual van der Waals heterostructures with $PdTe_2$, $NbSe_2$ and ScS_2 metal monolayers.

vdWHs	Formation Energy (eV)	Stacking type	Lattice mismatch (%)	Barrier height (Actual vdWHs) (eV)	Type of contact (From calculation)
$PdTe_2/BiClS$	-0.51	ABC	0.52	-0.31	Ohmic (n)
$PdTe_2/BiClSe$	-0.49	ABC	1.8	-0.29	Ohmic (n)
$PdTe_2/PbS_2$	-1.93	ABC	3.3	-0.26	Ohmic (n)
$PdTe_2/Tl_2S_2$	-1.64	AB	0.34	-0.69	Ohmic (n)
$PdTe_2/Tl_2Se_2$	-1.63	AB	3	-0.33	Ohmic (n)
$PdTe_2/HgBr_2$	-0.34	AA	1	-0.28	Ohmic (n)
$PdTe_2/YI_2$	-1.36	AA	1.1	-0.49	Ohmic (p)
$PdTe_2/ScI_2$	-1.43	AA	0.98	-1.15	Ohmic (p)
$NbSe_2/PbO_2$	-0.41	AC	2.30	-1.52	Ohmic (n)
$NbSe_2/GeS_2$	-0.26	ABC	1.09	-0.22	Ohmic (n)
$NbSe_2/ZrSSe$	-0.21	AA	4.45	+0.14	Schottky (n)
$NbSe_2/HfS_2$	-0.20	AA	2.56	+0.07	nearly Ohmic(n) < 0.1 eV
$NbSe_2/ZrS_2$	-0.20	AA	1.75	+0.16	Schottky (n)
$NbSe_2/In_2O_2$	-0.22	AB	1.20	-0.60	Ohmic (n)
$NbSe_2/ZrBr_2$	-1.27	AA	2.29	-0.06	Ohmic (p)
$NbSe_2/HfBr_2$	-0.22	AA	0.52	-0.11	Ohmic (p)
$NbSe_2/TiBr_2$	-0.19	AA	0.29	-0.47	Ohmic (p)
$NbSe_2/HfBrI$	-1.37	AA	4.65	-0.12	Ohmic (p)
$NbSe_2/TiBrI$	-1.32	AA	4.34	-0.51	Ohmic (p)
$NbSe_2/HfClI$	-1.31	AA	2.76	-0.09	Ohmic (p)
$NbSe_2/TiClI$	-1.29	AA	2.01	-0.91	Ohmic (p)

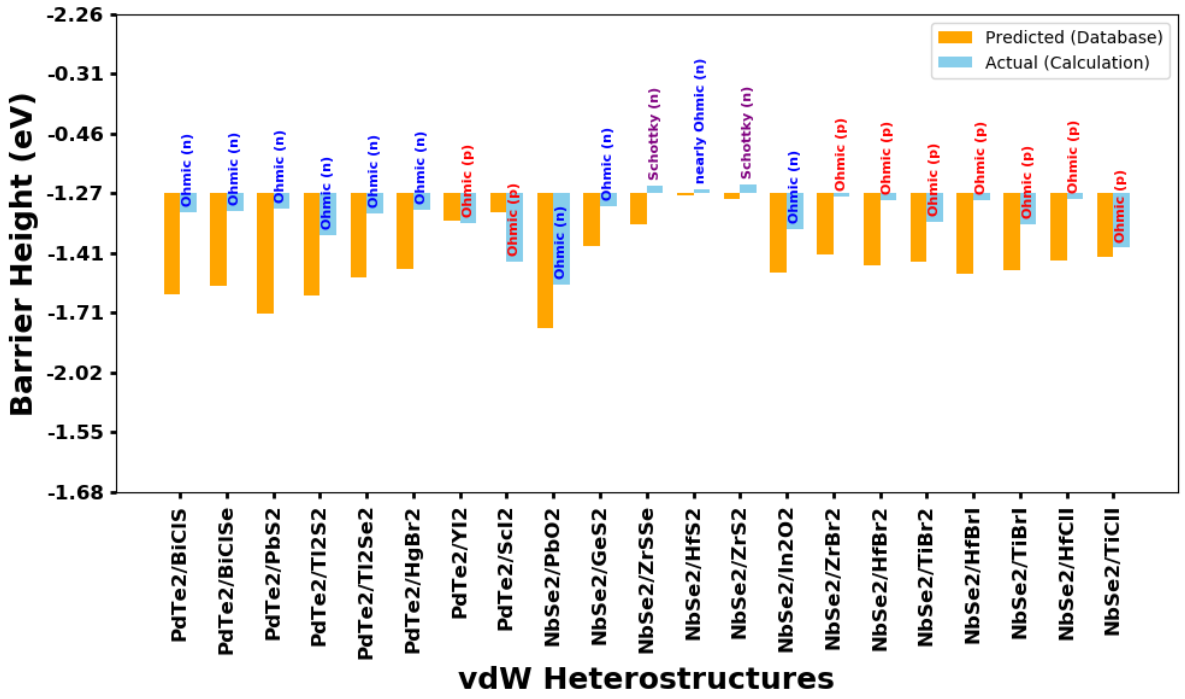

FIG S10. Comparison of barrier height and contact type in actual van der Waals heterostructures of selected monolayers with predictions from the C2DB database.

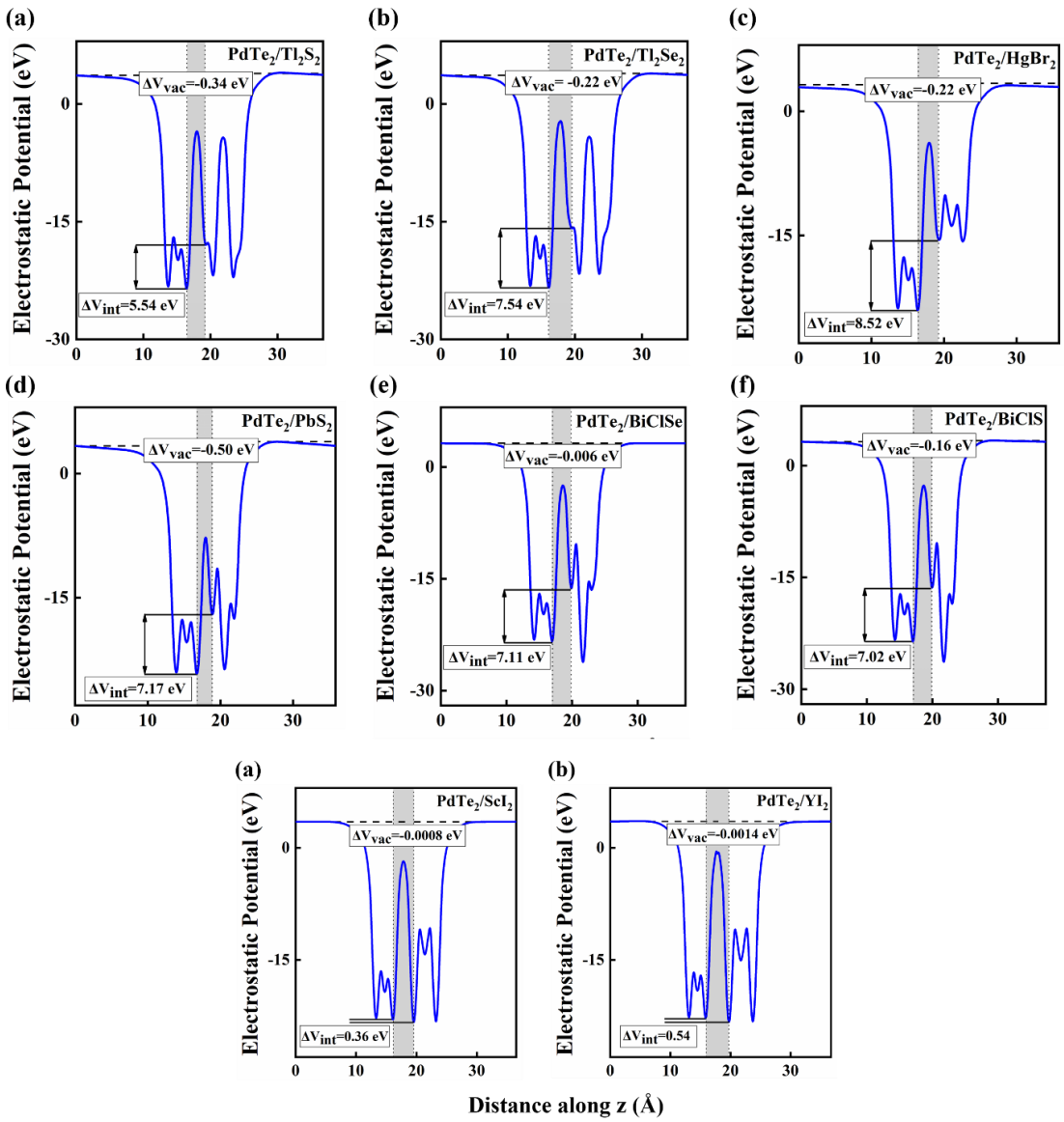

FIG S11. In-plane averaged out-of-plane electrostatic potential of vdWHs formed with $PdTe_2$ metal monolayer and selected materials (Tl_2S_2, Tl_2Se_2, $HgBr_2$, PbS_2, BiClSe, BiClS, ScI_2, and YI_2). The grey shaded region represents metal-semiconductor interface.

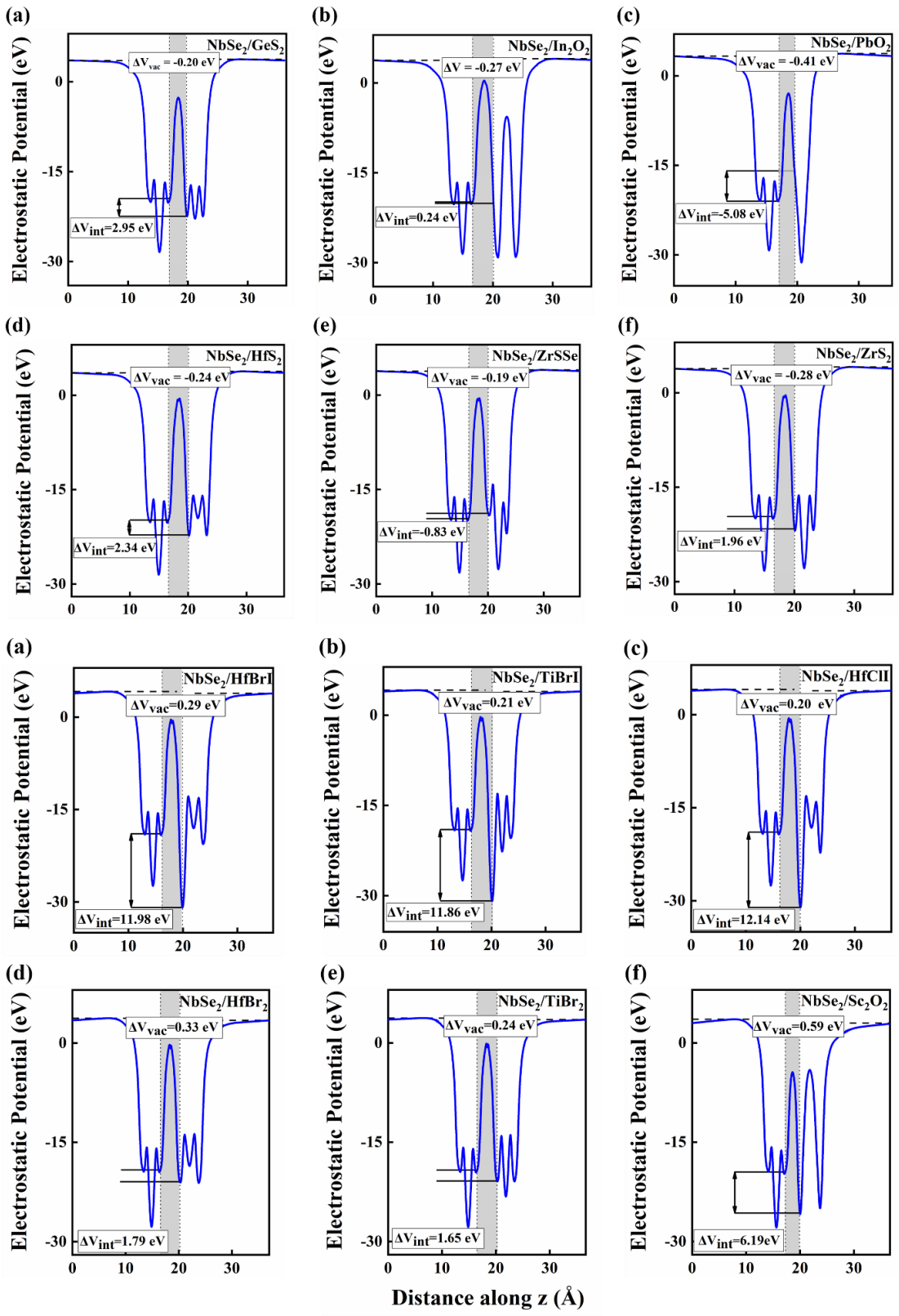

FIG S12. The in-plane averaged out-of-plane electrostatic potential of $NbSe_2$ metal monolayer and selected materials of both n-type (GeS_2, In_2O_2, PbO_2, HfS_2, ZrS_2, and ZrSSe) and p-type ($HfBr_2$, $TiBr_2$, $ZrBr_2$, HfBrI, TiBrI and HfClI). The grey shaded region represents metal-semiconductor interface.

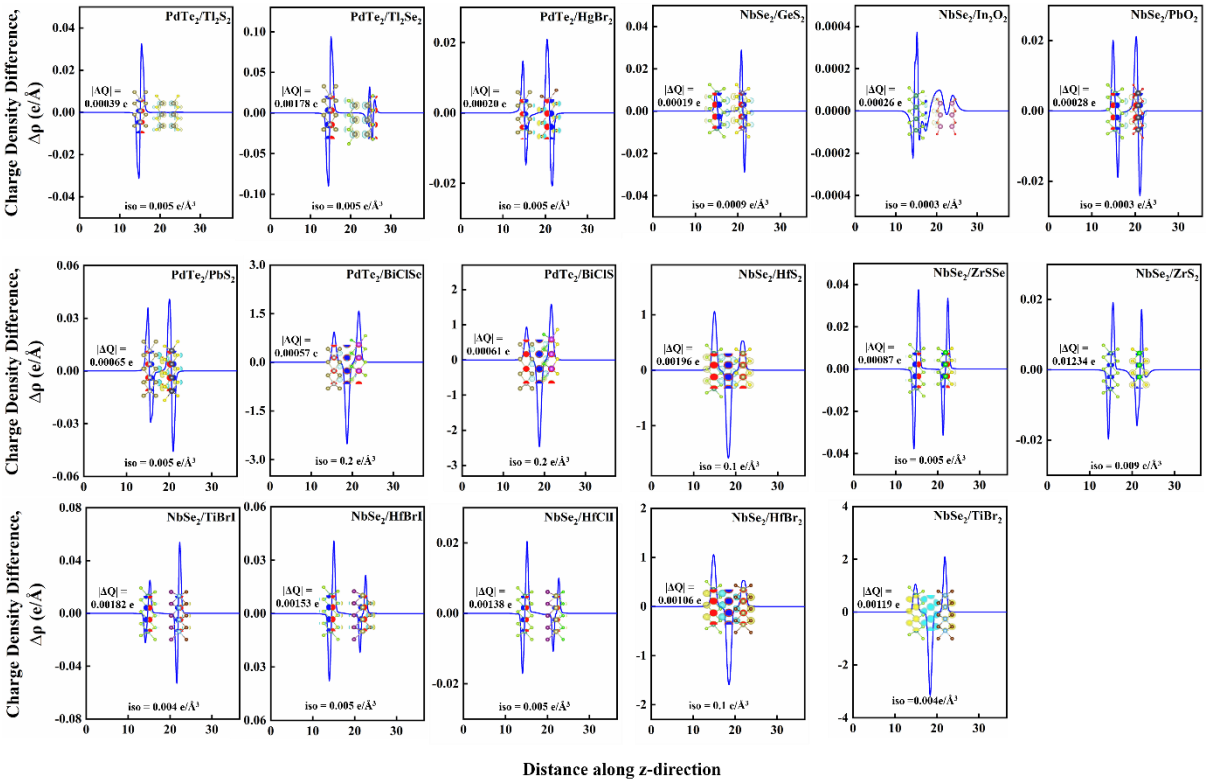

FIG S13. Charge density difference plot for all vdW heterostructures.

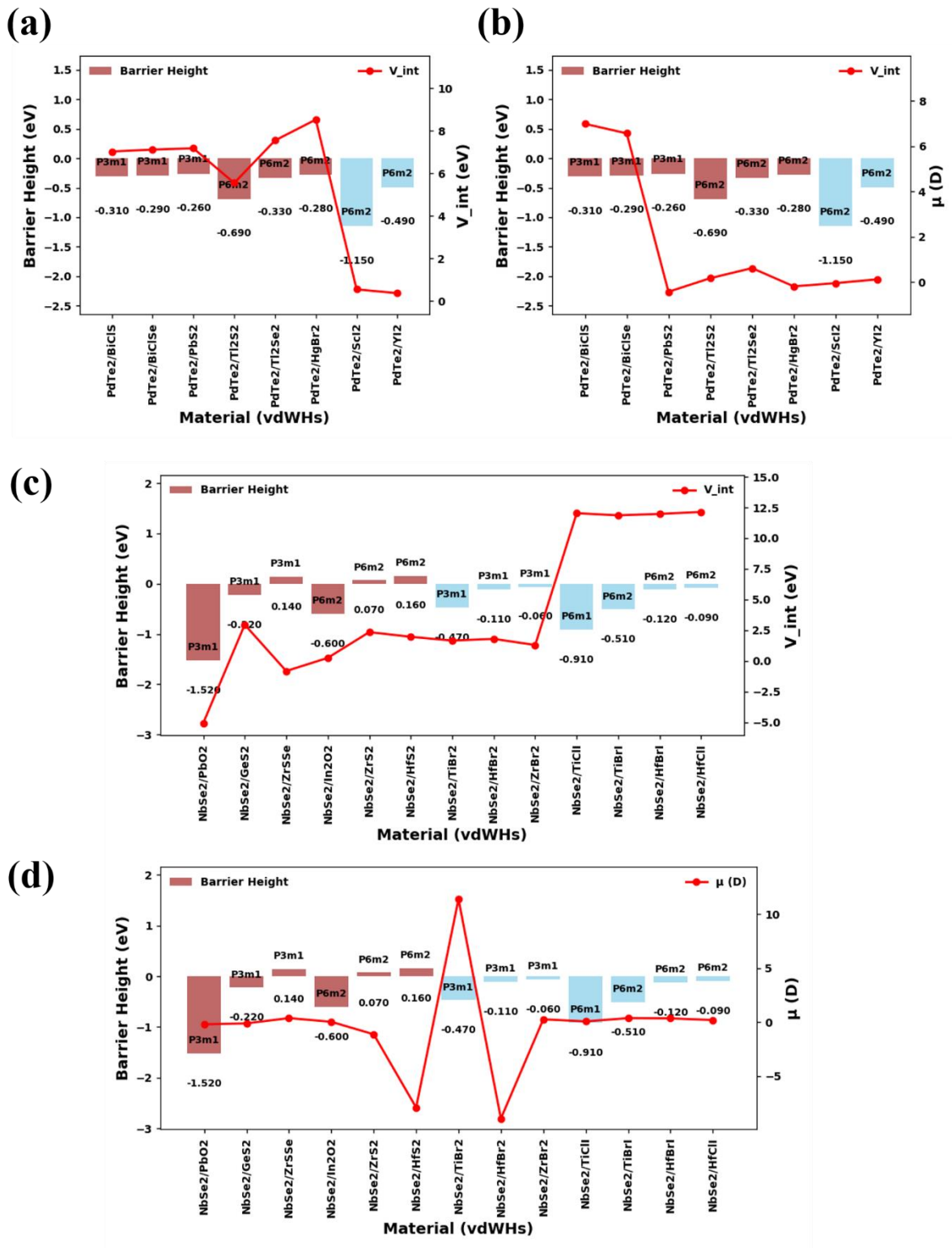

FIG S14. Trend of barrier height ($\varphi_{B,n}/\varphi_{B,p}$), electrostatic potential difference at the interface (ΔV_{int}), and interfacial dipole moment, (μ) for actual vdW heterostructures.

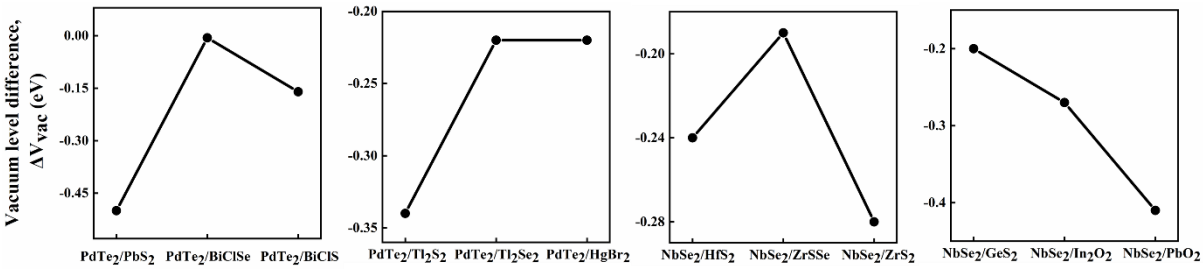

FIG S15. Trend of vacuum level difference, (ΔV_{vac}) in the electrostatic potential for various vdW heterostructures.

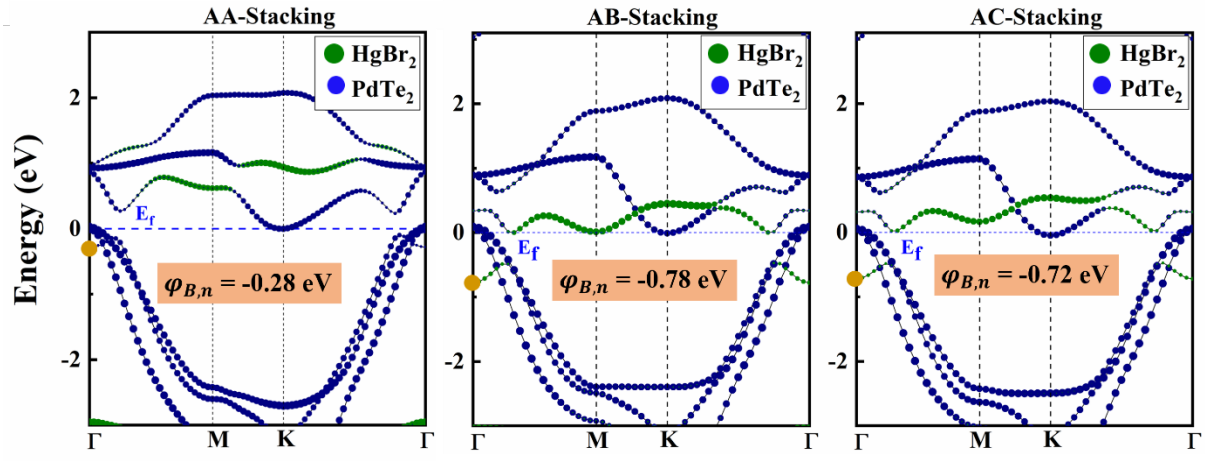

FIG S16. Band structure (HSE06) of $PdTe_2/HgBr_2$ vdW heterostructures with different stacking order. The orange bubble represents the CBM the semiconducting monolayers.

Table – S4. Comparison of Schottky barrier height, interfacial charge, and interfacial dipole moment of $PdTe_2/HgBr_2$ vdW heterostructures with different stacking orders

Stacking	Schottky barrier height ($e\ V$)	Interfacial charge induced $\Delta Q\ (e)$	Interfacial dipole moment $\mu\ (D)$
AA	-0.28	0.002162	-11.18
AB	-0.79	-0.000085	-1.86
AC	-0.72	0.000045	-1.82