

1 Primitive cell: Convergence tests

Table 1: Volumes of primitive cell for c-BN.

Structure	a (Å)	Volume
Perfect	2.56	11.958
Increase	2.58	12.240
Decrease	2.54	11.681

$$E_{dec}^{rel} = |E_{perf} - E_{dec}| \quad (1)$$

$$E_{inc}^{rel} = |E_{perf} - E_{inc}| \quad (2)$$

$$\Delta E_{dec}^{rel} = |E_{dec}^{rel}[i+1] - E_{dec}^{rel}[i]| \quad (3)$$

$$\Delta E_{inc}^{rel} = |E_{inc}^{rel}[i+1] - E_{inc}^{rel}[i]| \quad (4)$$

Table 2: Energy cutoff: Convergence test of primitive cell for c-BN. Criteria is 1 meV.

ENCUT (eV)	E_{perf} (eV)	E_{dec} (eV)	E_{inc} (eV)	E_{dec}^{rel} (meV)	E_{inc}^{rel} (meV)	ΔE_{dec}^{rel} (meV)	ΔE_{inc}^{rel} (meV)
200	-17.0024	-16.9378	-17.0416	64.6290	39.1838	–	–
250	-17.5246	-17.5200	-17.5383	4.6243	13.7043	60.0047	25.4795
300	-17.4699	-17.4620	-17.4607	7.8421	9.1176	3.2178	4.5867
350	-17.4260	-17.4170	-17.4157	8.9417	10.1970	1.0996	1.0794
400	-17.4490	-17.4468	-17.4407	2.1904	8.2843	6.7513	1.9127
450	-17.4542	-17.4483	-17.4452	5.9543	9.0336	3.7639	0.7493
500	-17.4513	-17.4455	-17.4420	5.7687	9.2785	0.1856	0.2449
550	-17.4517	-17.4461	-17.4424	5.6772	9.3078	0.0915	0.0293
600	-17.4545	-17.4488	-17.4450	5.6520	9.4998	0.0252	0.1920
650	-17.4567	-17.4512	-17.4472	5.5594	9.5653	0.0926	0.0655
700	-17.4582	-17.4527	-17.4487	5.5391	9.5108	0.0203	0.0545
750	-17.4591	-17.4535	-17.4496	5.5855	9.4552	0.0464	0.0556
800	-17.4597	-17.4540	-17.4503	5.6308	9.4063	0.0453	0.0489
850	-17.4599	-17.4543	-17.4505	5.6572	9.4013	0.0264	0.0050
900	-17.4600	-17.4543	-17.4506	5.6599	9.4011	0.0028	0.0001
950	-17.4601	-17.4544	-17.4507	5.6605	9.3973	0.0006	0.0038

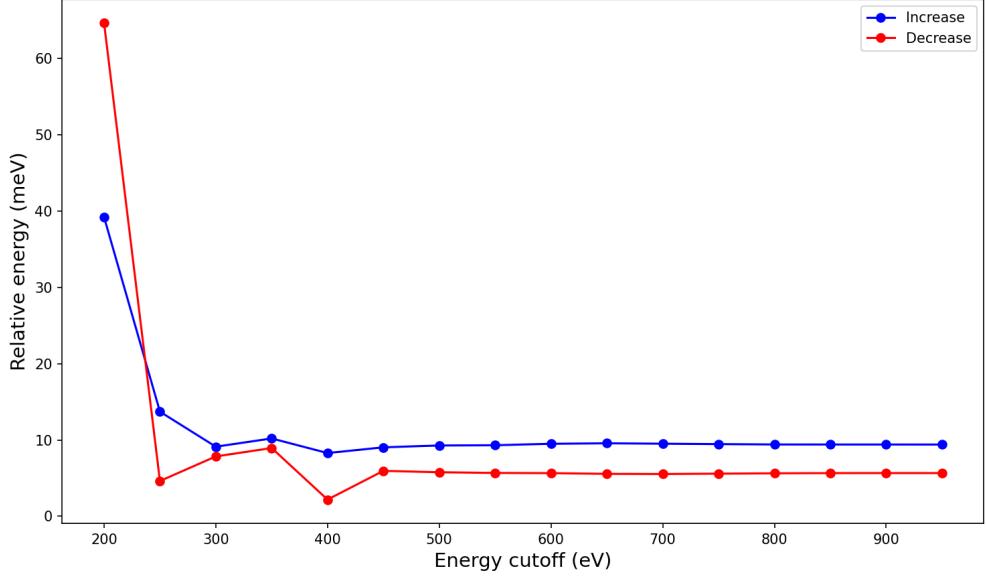


Figure 1: Convergence test of primitive cell for c-BN.

Table 3: K-density: Convergence test of primitive cell for c-BN. Criteria is 1 meV.

K-density (1/Å ³)	E_{perf} (eV)	E_{dec} (eV)	E_{inc} (eV)	E_{dec}^{rel} (meV)	E_{inc}^{rel} (meV)	ΔE_{dec}^{rel} (meV)	ΔE_{inc}^{rel} (meV)
2	-17.4348	-17.4288	-17.4259	6.0799	8.9643	—	—
3	-17.4510	-17.4452	-17.4418	5.8184	9.2433	0.2615	0.2790
4	-17.4513	-17.4455	-17.4420	5.7687	9.2785	0.0497	0.0352
5	-17.4513	-17.4455	-17.4420	5.7838	9.2641	0.0151	0.0144
6	-17.4513	-17.4455	-17.4420	5.7887	9.2551	0.0049	0.0090
7	-17.4513	-17.4455	-17.4420	5.7923	9.2623	0.0036	0.0072
8	-17.4513	-17.4455	-17.4420	5.7890	9.2603	0.0033	0.0020
9	-17.4513	-17.4455	-17.4420	5.7880	9.2638	0.0010	0.0034

Table 4: Kpoints mesh of primitive cell for c-BN

K-density (1/Å ³)	Kpoints mesh
2	$5 \times 5 \times 5$
3	$8 \times 8 \times 8$
4	$10 \times 10 \times 10$
5	$13 \times 13 \times 13$
6	$15 \times 15 \times 15$
7	$18 \times 18 \times 18$
8	$20 \times 20 \times 20$
9	$23 \times 23 \times 23$

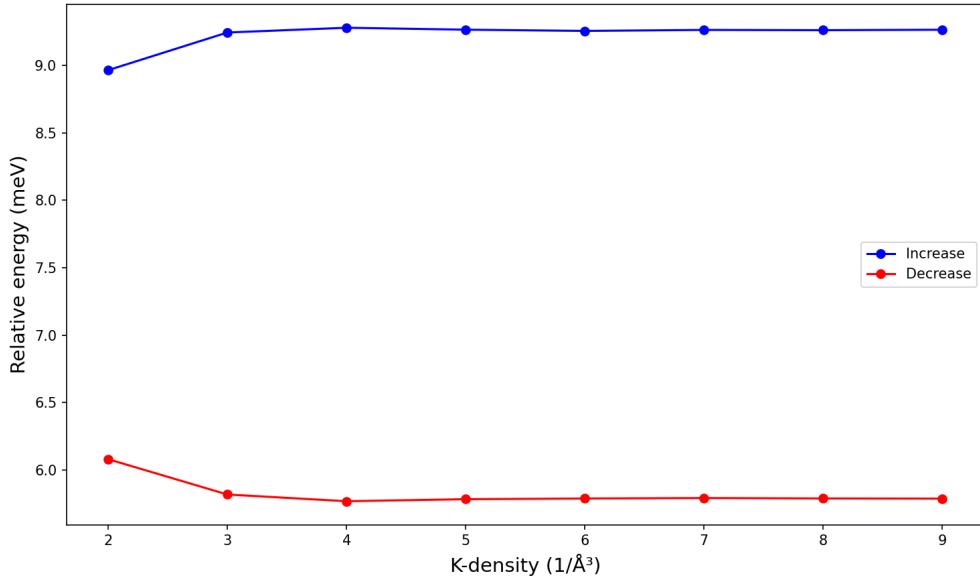


Figure 2: Convergence test of primitive cell for c-BN.

2 Convergence test: Stable phases

It also was calculated using the volumes, modifying the lattice parameters: $\Delta a = \pm 0.02$.

2.1 Boron

Table 5: Energy cutoff: Convergence test of boron. Criteria is 1 meV.

ENCUT (eV)	E_{perf} (eV)	E_{dec} (eV)	E_{inc} (eV)	E_{dec}^{rel} (meV)	E_{inc}^{rel} (meV)	ΔE_{dec}^{rel} (meV)	ΔE_{inc}^{rel} (meV)
200	-78.6696	-78.6207	-78.6963	48.8942	26.7108	—	—
250	-79.8598	-79.8543	-79.8489	5.4990	10.8634	43.3952	15.8474
300	-80.2543	-80.2398	-80.2543	14.4919	0.0024	8.9929	10.8610
350	-80.4190	-80.4018	-80.4173	17.1116	1.6907	2.6197	1.6883
400	-80.4372	-80.4209	-80.4352	16.3599	1.9767	0.7517	0.2860
450	-80.4363	-80.4199	-80.4342	16.3471	2.0519	0.0128	0.0752
500	-80.4404	-80.4243	-80.4381	16.0692	2.3424	0.2779	0.2905
550	-80.4460	-80.4301	-80.4436	15.9086	2.4194	0.1606	0.0770
600	-80.4531	-80.4372	-80.4507	15.9103	2.3978	0.0017	0.0216
650	-80.4593	-80.4434	-80.4569	15.9044	2.4684	0.0059	0.0707
700	-80.4631	-80.4472	-80.4606	15.8750	2.4987	0.0294	0.0302
750	-80.4647	-80.4488	-80.4621	15.8515	2.5468	0.0234	0.0481
800	-80.4651	-80.4493	-80.4625	15.8085	2.5706	0.0431	0.0238
850	-80.4652	-80.4494	-80.4626	15.7976	2.5815	0.0109	0.0109
900	-80.4654	-80.4496	-80.4628	15.7855	2.5935	0.0121	0.0120
950	-80.4659	-80.4501	-80.4633	15.7921	2.5953	0.0067	0.0018

Table 6: K-density: Convergence test of boron. Criteria is 1 meV.

K-density (1/Å ³)	E_{perf} (eV)	E_{dec} (eV)	E_{inc} (eV)	E_{dec}^{rel} (meV)	E_{inc}^{rel} (meV)	ΔE_{dec}^{rel} (meV)	ΔE_{inc}^{rel} (meV)
2	-80.4923	-80.4760	-80.4898	16.2435	2.4457	—	—
3	-80.4276	-80.4113	-80.4255	16.3307	2.0707	0.0873	0.3750
4	-80.4342	-80.4199	-80.4354	16.3471	2.0519	0.0163	0.0188
5	-80.4375	-80.4212	-80.4355	16.3470	2.0716	0.0001	0.0198
6	-80.4375	-80.4212	-80.4355	16.3368	2.0831	0.0102	0.0114
7	-80.4375	-80.4212	-80.4355	16.3522	2.0772	0.0154	0.0059
8	-80.4375	-80.4212	-80.4355	16.3443	2.0709	0.0079	0.0064
9	-80.4375	-80.4212	-80.4355	16.3380	2.0667	0.0063	0.0042

Table 7: Kpoints mesh for boron (mp-160).

K-density (1/Å ³)	Kpoints mesh
2	$3 \times 3 \times 3$
3	$4 \times 4 \times 4$
4	$5 \times 5 \times 5$
5	$7 \times 7 \times 7$
6	$8 \times 8 \times 8$
7	$9 \times 9 \times 9$
8	$10 \times 10 \times 10$
9	$12 \times 12 \times 12$

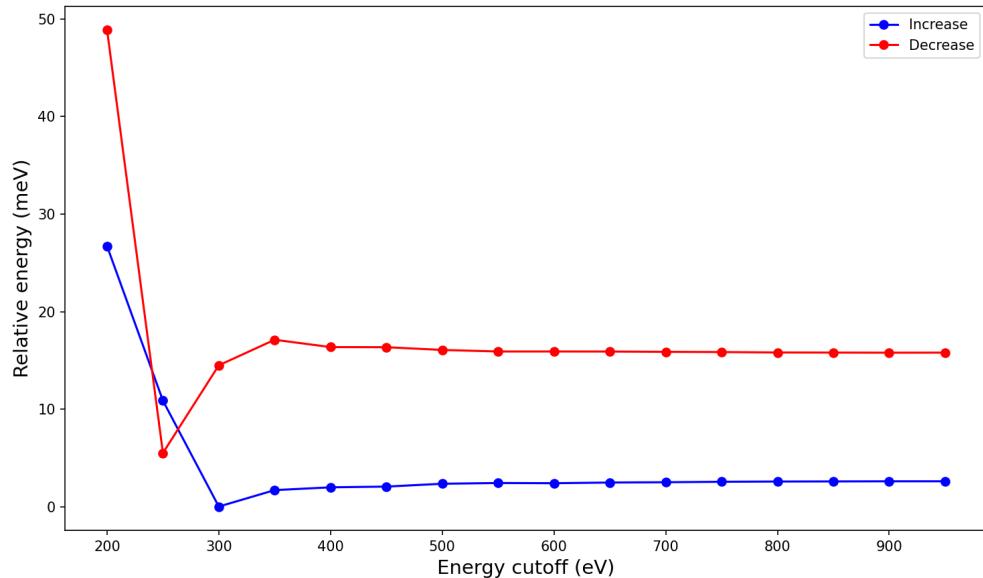


Figure 3: Convergence test of boron.

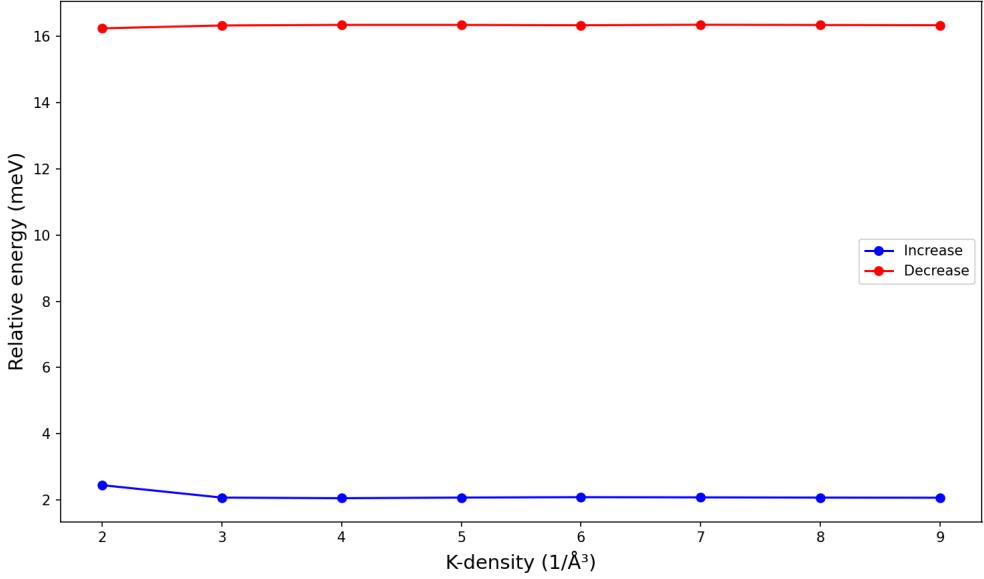


Figure 4: Convergence test of boron.

2.2 Nitrogen

Table 8: Energy cutoff: Convergence test of nitrogen. Criteria is 1 meV.

ENCUT (eV)	E_{perf} (eV)	E_{dec} (eV)	E_{inc} (eV)	E_{dec}^{rel} (meV)	E_{inc}^{rel} (meV)	ΔE_{dec}^{rel} (meV)	ΔE_{inc}^{rel} (meV)
200	-17.2558	-17.2318	-17.2195	24.0068	36.2361	—	—
250	-16.6474	-16.6301	-16.6489	17.3020	1.4754	6.7049	34.7608
300	-16.4950	-16.4872	-16.4993	7.7920	4.3531	9.5100	2.8778
350	-16.5192	-16.5103	-16.5228	8.8587	3.5650	1.0667	0.7882
400	-16.5906	-16.5837	-16.5946	6.8461	3.9972	2.0126	0.4322
450	-16.6146	-16.6101	-16.6188	4.4686	4.2182	2.3775	0.2210
500	-16.6232	-16.6188	-16.6267	4.3515	3.5494	0.1171	0.6688
550	-16.6285	-16.6243	-16.6318	4.1817	3.3163	0.1699	0.2331
600	-16.6332	-16.6291	-16.6363	4.0529	3.1872	0.1288	0.1292
650	-16.6366	-16.6326	-16.6398	3.9907	3.1911	0.0622	0.0040
700	-16.6389	-16.6350	-16.6421	3.9576	3.1518	0.0331	0.0394
750	-16.6399	-16.6359	-16.6430	3.9074	3.1653	0.0502	0.0135
800	-16.6406	-16.6367	-16.6437	3.9270	3.1215	0.0196	0.0438
850	-16.6410	-16.6371	-16.6441	3.9195	3.1240	0.0076	0.0025
900	-16.6413	-16.6374	-16.6444	3.8977	3.1113	0.0217	0.0127
950	-16.6417	-16.6378	-16.6448	3.8852	3.1017	0.0126	0.0095

Table 9: K-density: Convergence test of nitrogen. Criteria is 1 meV. We can note that gases are independent of the kdensity or kpoints mesh. The Γ -point only calculation is sufficient.

K-density (1/ \AA^3)	E_{perf} (eV)	E_{dec} (eV)	E_{inc} (eV)	E_{dec}^{rel} (meV)	E_{inc}^{rel} (meV)	ΔE_{dec}^{rel} (meV)	ΔE_{inc}^{rel} (meV)
1	-16.6233	-16.6193	-16.6267	4.0180	3.3979	—	—
2	-16.6233	-16.6188	-16.6268	4.4684	3.5690	0.4504	0.1711
4	-16.6232	-16.6188	-16.6267	4.3515	3.5494	0.1169	0.0196
5	-16.6231	-16.6188	-16.6267	4.3198	3.5666	0.0318	0.0172
7	-16.6232	-16.6188	-16.6267	4.3258	3.5164	0.0061	0.0502
8	-16.6232	-16.6188	-16.6267	4.3391	3.5305	0.0133	0.0141

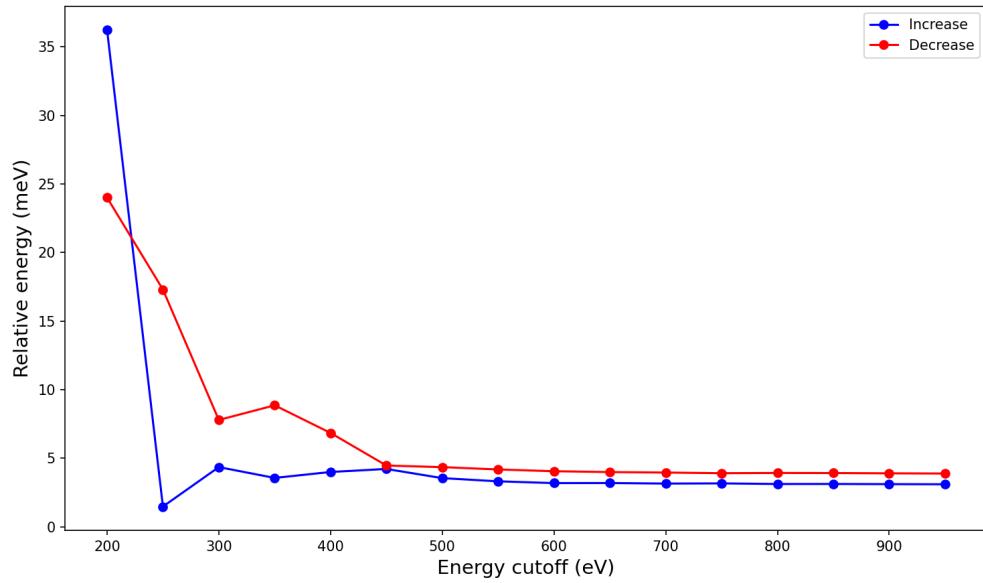


Figure 5: Convergence test of nitrogen.

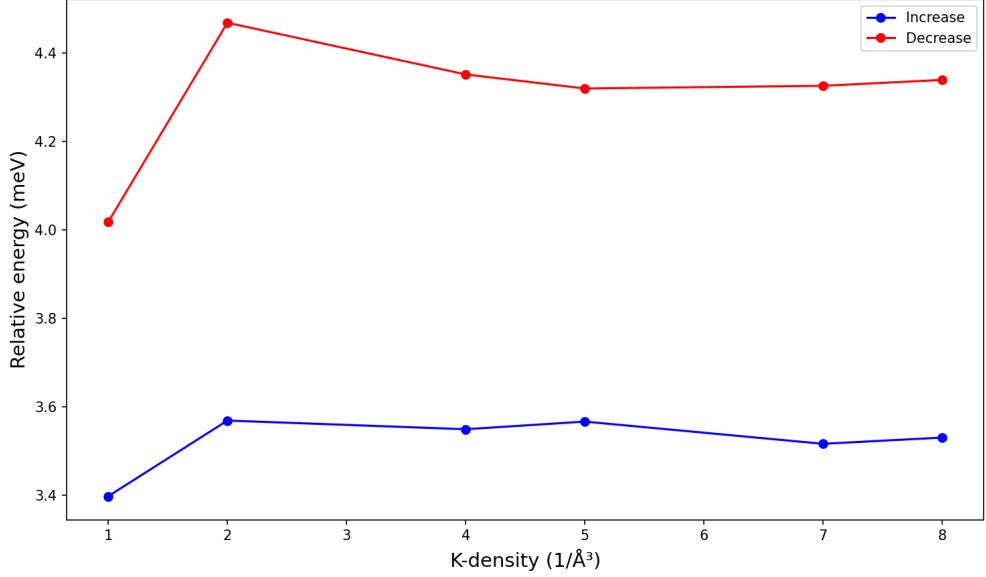


Figure 6: Convergence test of nitrogen.

3 Chemical potentials: Stable phases

Table 10: Boron and nitrogen structures.

Species	Total energy (eV)	Number of atoms	$\mu_i^{elemental}$ (eV)
Boron	-80.43	12	-6.70
Nitrogen	-16.63	2	-8.31

4 Convergence for supercell size

$$E_{form}^{q=0} = E_{def}^{q=0} - E_{perf} + \mu_i^{elemental} \quad (5)$$

Table 11: Convergence test of supercell size for c-BN.

N	E_{perf} (eV)	$E_{def}[V_B]$ (eV)	$E_{def}[V_N]$ (eV)	$E_{form}[V_B]$ (eV)	$E_{form}[V_N]$ (eV)
64	-558.450	-542.435	-542.054	9.311	8.071
216	-1884.780	-1868.495	-1868.242	9.581	8.212
512	-4467.653	-4451.32	-4451.095	9.628	8.232
1000	-8725.994	-8709.647	-8709.423	9.643	8.245
1728	-15078.619	-15062.268	-15062.042	9.647	8.251

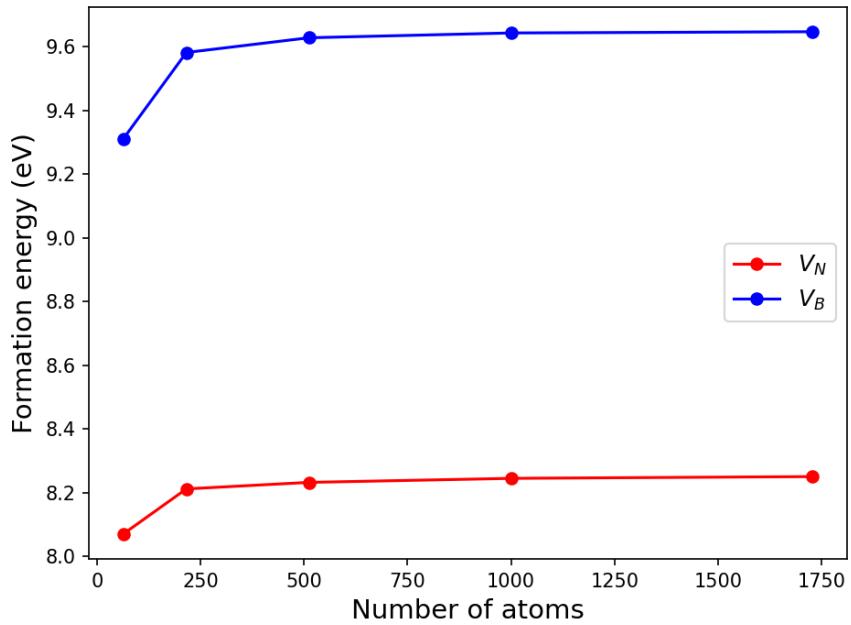


Figure 7: Convergence test on supercell size for native vacancies.

5 Supercell: Convergence tests

Using supercell with 216 atoms for nitrogen vacancy (V_N^0). Keep in mind the Eq. 5.

Table 12: Energy cutoff: Convergence test of supercell for nitrogen vacancy (V_N^0)

ENCUT (eV)	E_{perf} (eV)	$E_{def}[V_N^0]$ (eV)	E_{form} (eV)	ΔE_{form} (meV)
200	-1834.115	-1818.842	6.963	–
250	-1893.042	-1876.577	8.155	1.192
300	-1886.670	-1870.314	8.046	0.109
350	-1881.787	-1865.501	7.976	0.070
400	-1884.291	-1867.965	8.016	0.040
450	-1884.546	-1868.208	8.028	0.012
500	-1884.225	-1867.889	8.026	0.002
550	-1884.296	-1867.959	8.026	0.001
600	-1884.593	-1868.255	8.029	0.002
650	-1884.875	-1868.535	8.030	0.002
700	-1885.008	-1868.667	8.031	0.001
750	-1885.077	-1868.736	8.031	0.000
800	-1885.177	-1868.834	8.032	0.001
850	-1885.182	-1868.840	8.032	0.000
900	-1885.194	-1868.852	8.032	0.000
950	-1885.243	-1868.901	8.033	0.000

 Table 13: K-density: Convergence test of supercell for nitrogen vacancy (V_N^0).

K-density (1/ \AA^3)	E_{perf} (eV)	$E_{def}[V_N^0]$ (eV)	E_{form} (eV)	ΔE_{form} (meV)
1	-1884.225	-1867.889	8.026	–
2	-1884.766	-1868.411	8.045	0.019
4	-1884.765	-1868.409	8.046	0.001
6	-1884.765	-1868.409	8.046	0.000
7	-1884.764	-1868.409	8.046	0.000
9	-1884.765	-1868.409	8.046	0.000

Table 14: Kpoints mesh for supercell.

K-density (1/Å ³)	Kpoints mesh
1	$1 \times 1 \times 1$
2	$2 \times 2 \times 2$
3	$2 \times 2 \times 2$
4	$3 \times 3 \times 3$
5	$3 \times 3 \times 3$
6	$4 \times 4 \times 4$
7	$5 \times 5 \times 5$
8	$5 \times 5 \times 5$
9	$6 \times 6 \times 6$

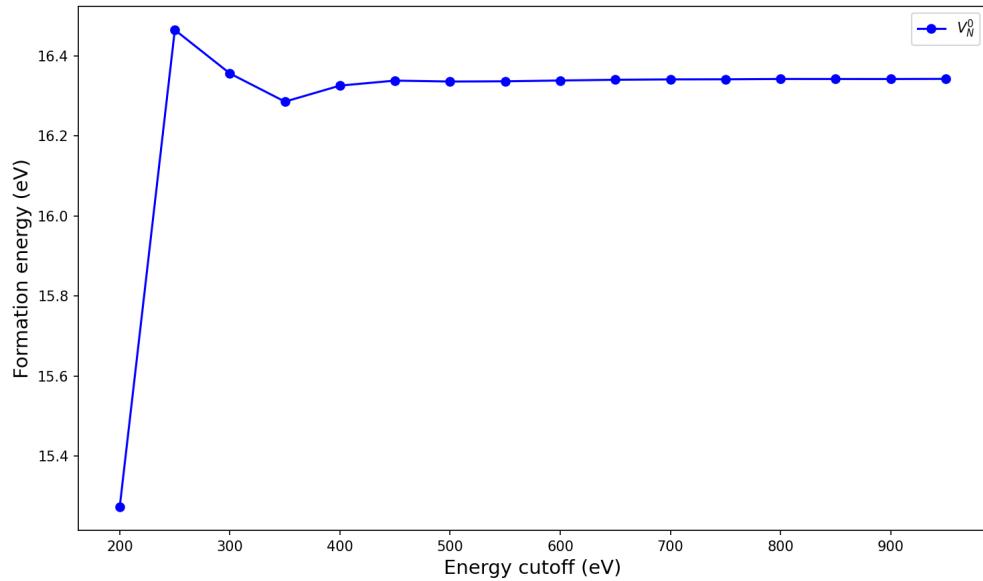


Figure 8: Convergence test of supercell for nitrogen vacancy (V_N^0).

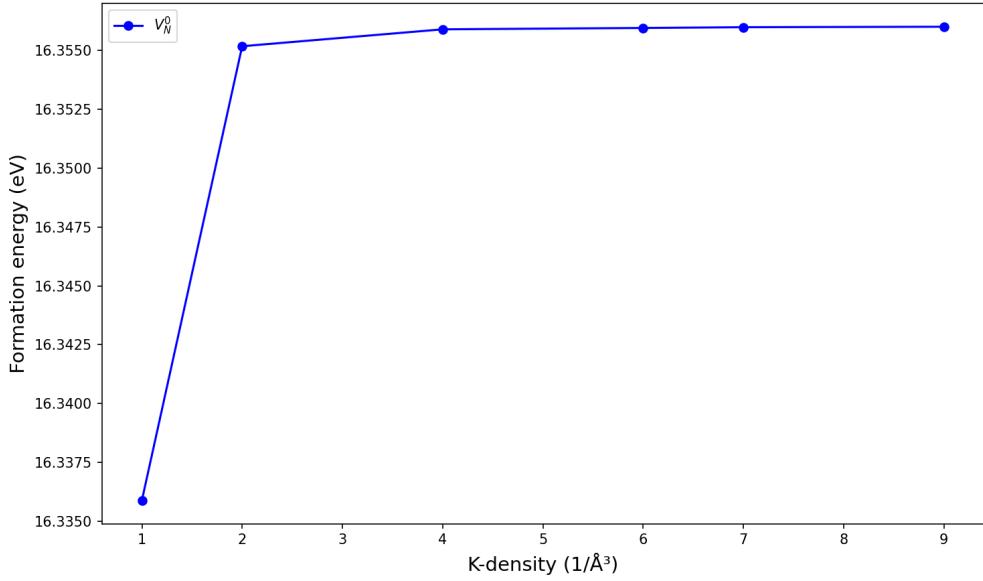


Figure 9: Convergence test of supercell for nitrogen vacancy (V_N^0).

6 Defects: post-analysis

The post-analysis was performed using [LSPD](#).

Table 15: Boron and nitrogen vacancies.

Defect	Charge	Magnetization (μ_B)	Spin
V_B	-4	0	0
	-3	0	0
	-2	1	1/2
	-1	2	1
	0	3	3/2
	+1	2.0056144	1
	+2	1.2317604	0.616
V_N	-1	2	1
	0	1	1/2
	+1	0	0
	+2	0.0015205	0
	+3	0	0
	+4	0	0

Table 16: Antisite vacancies.

Defect	Charge	Magnetization (μ_B)	Spin
	-4	0	0
	-3	0	0
	-2	0	0
	-1	1	1/2
B_N	0	2	1
	+1	3	3/2
	+2	2	1
	+3	1	1/2
	+4	0	0
	-4	0.0003541	0.00017705
	-3	-0.0028135	-0.00140675
	-2	0	0
	-1	1	1/2
N_B	0	0	0
	+1	1	1/2
	+2	0	0
	+3	0	0
	+4	0	0

Table 17: complex

Defect	Charge	Magnetization (μ_B)	Spin
	-3	0	0
	-2	0	0
	-1	1	1/2
$V_B - C_B$	0	2	1
	+1	3	3/2
	+2	2.0525509	1
	-4	0	0
	-3	1	1/2
	-2	2	1
	-1	1	1/2
$V_N - C_N$	0	0	0
	+1	0.0001228	0
	+2	0	0
	+3	0	0
	+4	0	0

Table 18: di-vac

Defect	Charge	Magnetization (μ_B)	Spin
	-4	1	1/2
	-3	2	1
	-2	-1.9289678	-0.9644839
	-1	0.9753022	0.4876511
$B_N - V_B$	0	4.9822933	2.49114665
	+1	2	1
	+2	3	3/2
	+3	0	0
	+4	0	0
	-4	1	1/2
	-3	0	0
	-2	1	1/2
	-1	0	0
$N_B - V_N$	0	1	1/2
	+1	0	0
	+2	1	1/2
	+3	0	0
	+4	0	0
	-4	2	1
	-3	1	1/2
	-2	0	0
	-1	1	1/2
$V_B - V_N$	0	2	1
	+1	3	3/2
	+2	2	1
	+3	3	3/2
	+4	2.0668582	1.0334291

Table 19: di-vacancy

Defect	Charge	Magnetization (μ_B)	Spin
	-4	0	0
	-3	0	0
	-2	0	0
	-1	1	1/2
$C_B - V_N$	0	2	1
	+1	1	1/2
	+2	0	0
	+3	-0.0020650	-0.0010325
	+4	0	0
	-4	0	0
	-3	1	1/2
	-2	2	1
	-1	3	3/2
$C_N - V_B$	0	2	1
	+1	1.2781017	0.63905085
	+2	1.1623836	0.5811918
	+3	0.8318067	0.41590335
	+4	0.7033280	0.351664

Table 20: Fig-4

Defect	Charge	Magnetization (μ_B)	Spin
C_B	-2	0	0
	-1	0	0
	0	0	0
	+1	0	0
	+2	0	0
C_N	-2	0	0
	-1	0	0
	0	0	0
	+1	0	0
	+2	0	0
O_B	-2	3	$3/2$
	-1	2	1
	0	1	$1/2$
	+1	0	0
	+2	0.8724211	0.43621055
O_N	-2	0	0
	-1	0	0
	0	0	0
	+1	0	0
	+2	0	0

Table 21: Fig-5

Defect	Charge	Magnetization (μ_B)	Spin
$V_B - O_N$	-3	0	0
	-2	0	0
	-1	1	1/2
	0	2	1
	+1	1.0390702	0.5195351
	+2	0.4850163	0.24250815
$V_B - Si_B$	-3	0	0
	-2	0	0
	-1	1	1/2
	0	2	1
	+1	3	3/2
	+2	2.0549873	1.02749365

Table 22: C-dimer

Defect	Charge	Magnetization (μ_B)	Spin
	-4	0	0
	-3	0	0
	-2	0	0
	-1	0	0
$C_B - C_N$	0	0	0
	+1	0	0
	+2	0	0
	+3	0	0
	+4	0	0
	-4	0	0
	-3	0	0
	-2	0	0
	-1	0	0
$C_B - C_B$	0	0	0
	+1	0	0
	+2	0	0
	+3	0	0
	+4	0	0
	-4	0	0
	-3	0	0
	-2	0	0
	-1	0	0
$C_N - C_N$	0	0	0
	+1	0	0
	+2	0	0
	+3	0	0
	+4	0	0

Table 23: Summary: Spin state information

Defect Charge	-4	-3	-2	-1	0	+1	+2	+3	+4
V_B	0	0	1/2	1	3/2	1	0.616	–	–
V_N	–	–	–	1	1/2	0	0	0	0
B_N	0	0	0	1/2	1	3/2	1	1/2	0
N_B	0	0	0	1/2	0	1/2	0	0	0
$V_B - C_B$	–	0	0	1/2	1	3/2	1	–	–
$V_N - C_N$	0	1/2	1	1/2	0	0	0	0	0
$B_N - V_B$	1/2	1	-0.964	0.488	2.491	1	3/2	0	0
$N_B - V_N$	1/2	0	1/2	0	1/2	0	1/2	0	0
$V_B - V_N$	1	1/2	0	1/2	1	3/2	1	3/2	1.033
$C_B - V_N$	0	0	0	1/2	1	1/2	0	0	0
$C_N - V_B$	0	1/2	1	3/2	1	0.639	0.581	0.416	0.352
C_B	–	–	0	0	0	0	0	–	–
C_N	–	–	0	0	0	0	0	–	–
O_B	–	–	3/2	1	1/2	0	0.436	–	–
O_N	–	–	0	0	0	0	0	–	–
$V_B - O_N$	–	0	0	1/2	1	0.520	0.243	–	–
$V_B - Si_B$	–	0	0	1/2	1	3/2	1.0275	–	–
$C_B - C_N$	0	0	0	0	0	0	0	0	0
$C_B - C_B$	0	0	0	0	0	0	0	0	0
$C_N - C_N$	0	0	0	0	0	0	0	0	0

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6.1 Vacancy: V_B^0

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Table 24: V_B^0

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
		430	149	0.346	Yes
Down	1	431	122	0.294	Yes
		432	175, 202	0.221, 0.221	Yes

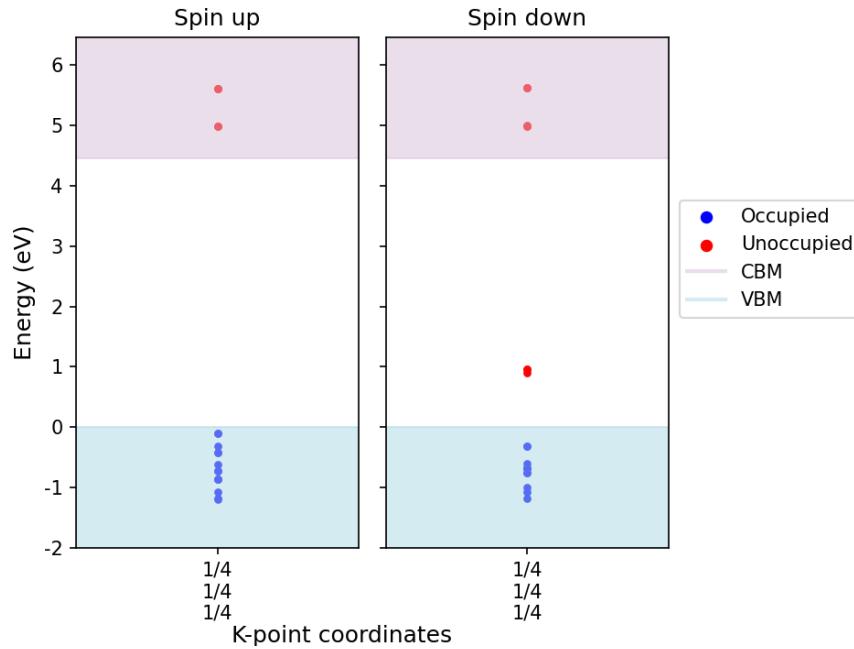


Figure 10: Kohn-Sham states.

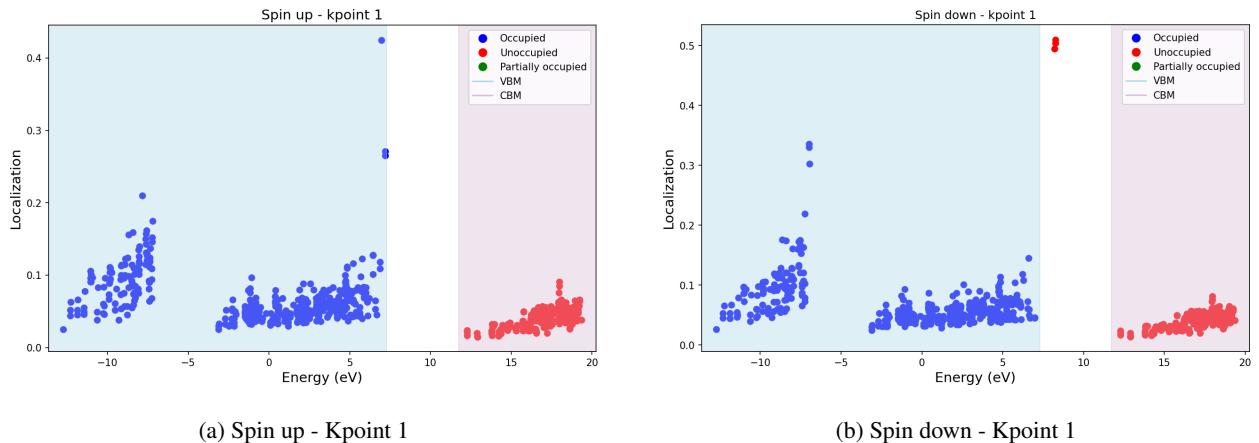


Figure 11: Localization factor using projected orbitals (s, p and d).

6.2 Vacancy: V_B^{+1}

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Table 25: V_B^{+1}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
Down	1	430	149	0.341	Yes
		431	122	0.283	Yes
		432	175, 202	0.213, 0.213	Yes

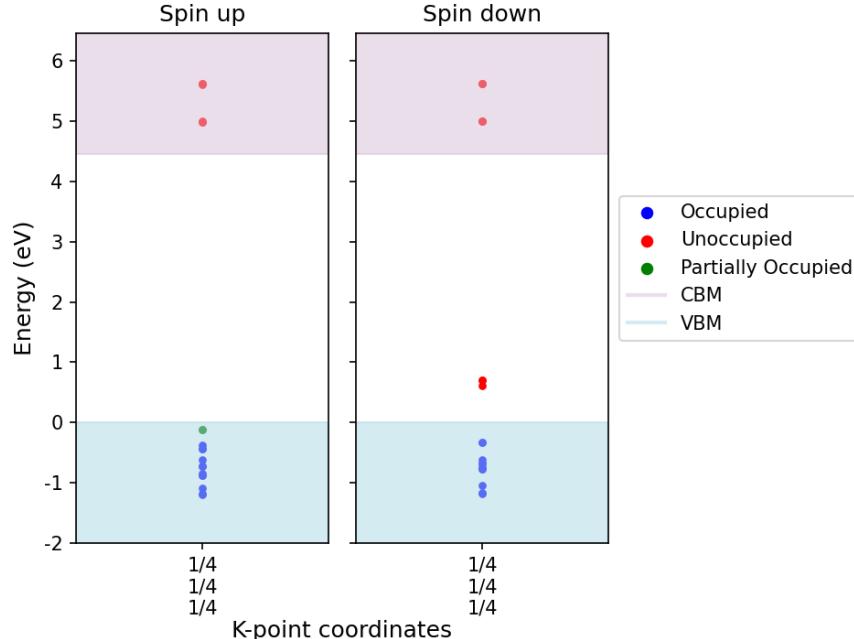


Figure 12: Kohn-Sham states.

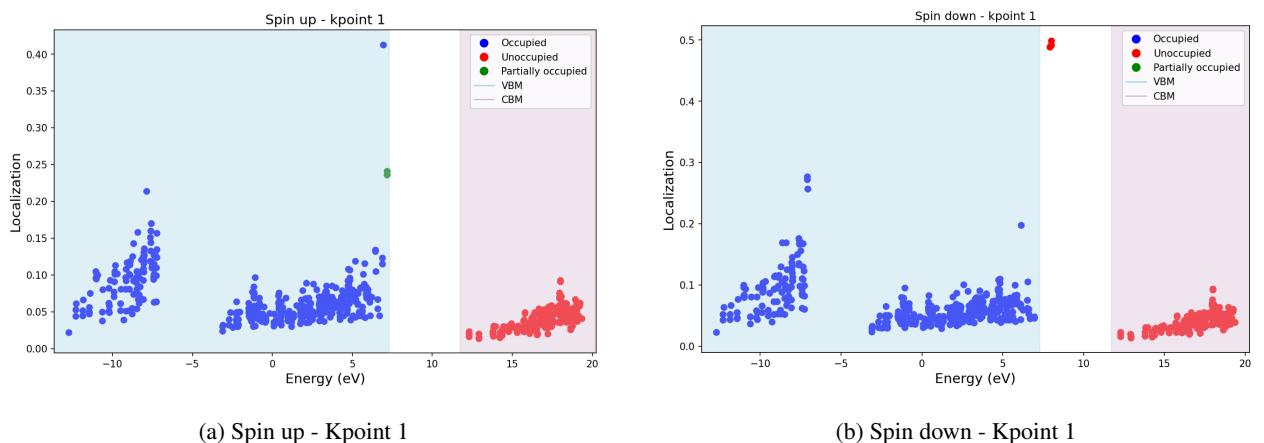


Figure 13: Localization factor using projected orbitals (s, p and d).

6.3 Vacancy: V_B^{+2}

[Go back to the Table 23](#)

Table 26: V_B^{+2}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
Down	1	430	149	0.334	Yes
		431	122	0.270	Yes
		432	175, 202	0.203, 0.203	Yes

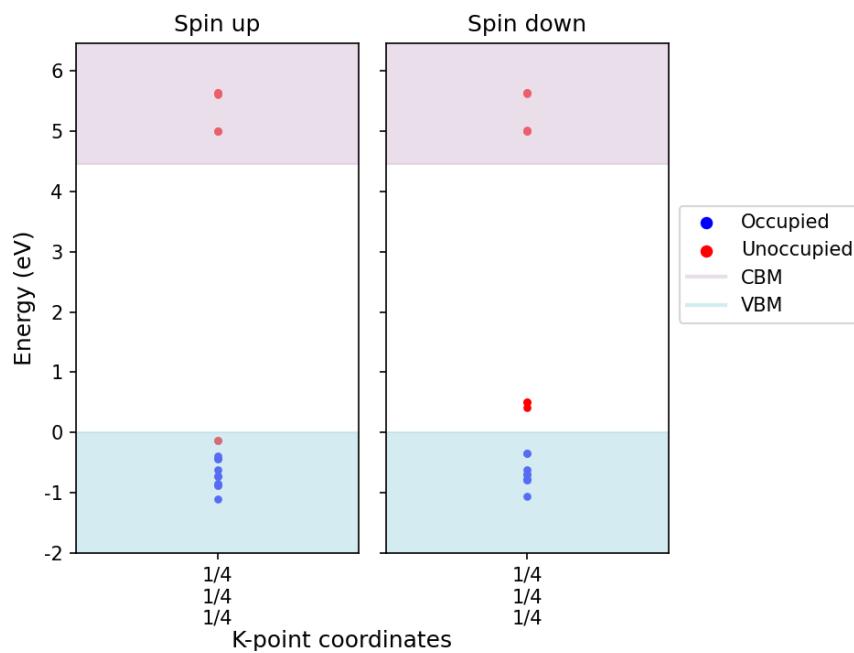


Figure 14: Kohn-Sham states.

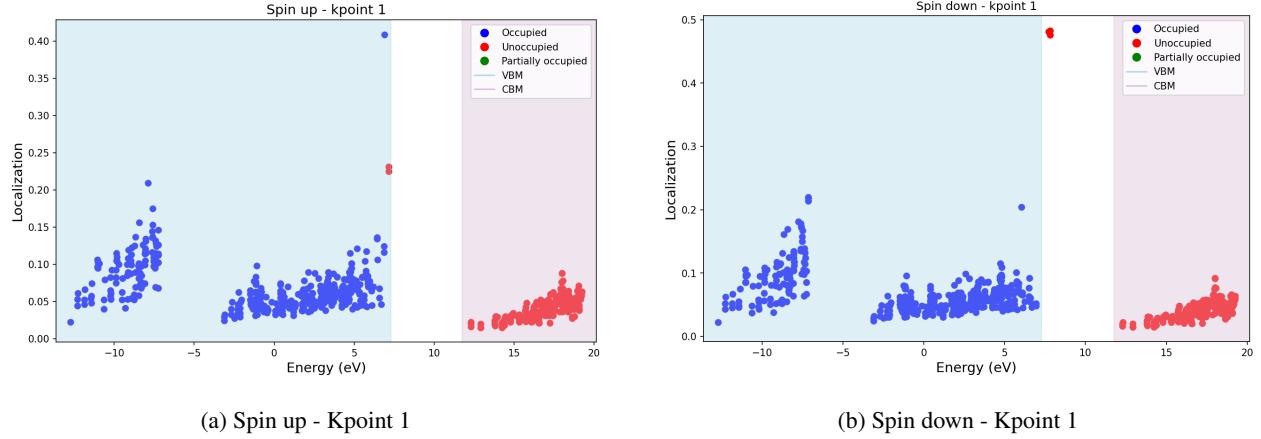


Figure 15: Localization factor using projected orbitals (s, p and d).

6.4 Vacancy: V_B^{-1}

[Go back to the Table 23](#)

Table 27: V_B^{-1}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	430	149	0.328	Yes
		431	122	0.260	Yes
		432	175, 202	0.196, 0.196	Yes
Down	1	430	149	0.349	Yes
		431	122	0.300	Yes
		432	175, 202	0.226, 0.225	Yes

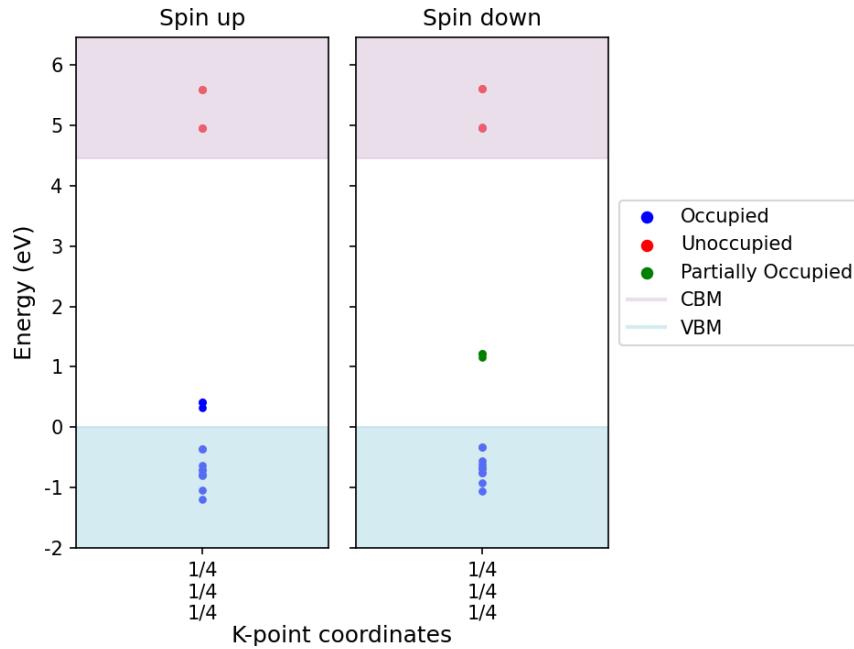


Figure 16: Kohn-Sham states.

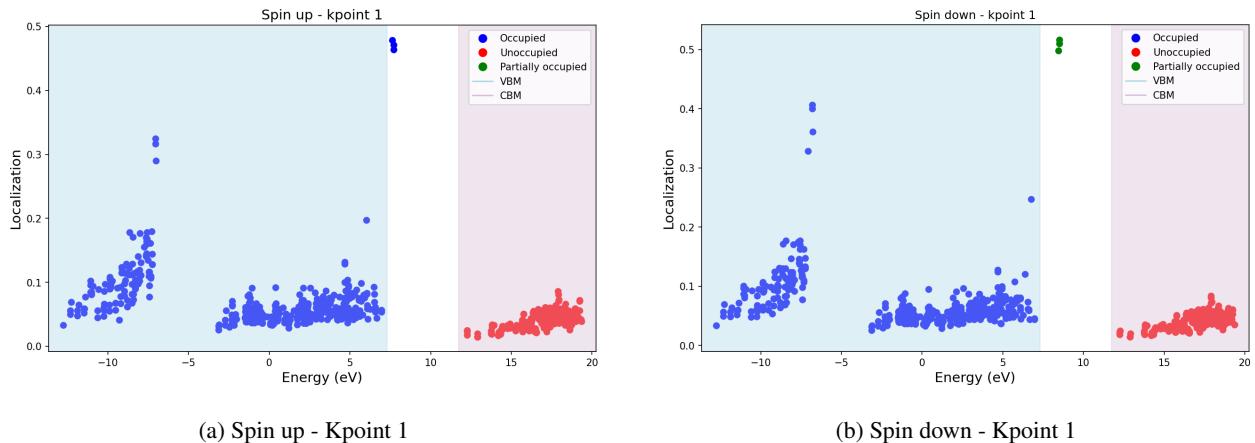


Figure 17: Localization factor using projected orbitals (s, p and d).

6.5 Vacancy: V_B^{-2}

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Table 28: V_B^{-2}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	430	149	0.347	Yes
		431	122	0.296	Yes
		432	175, 202	0.223, 0.223	Yes
Down	1	430	149	0.350	Yes
		431	122	0.303	Yes
		432	175, 202	0.228, 0.228	Yes

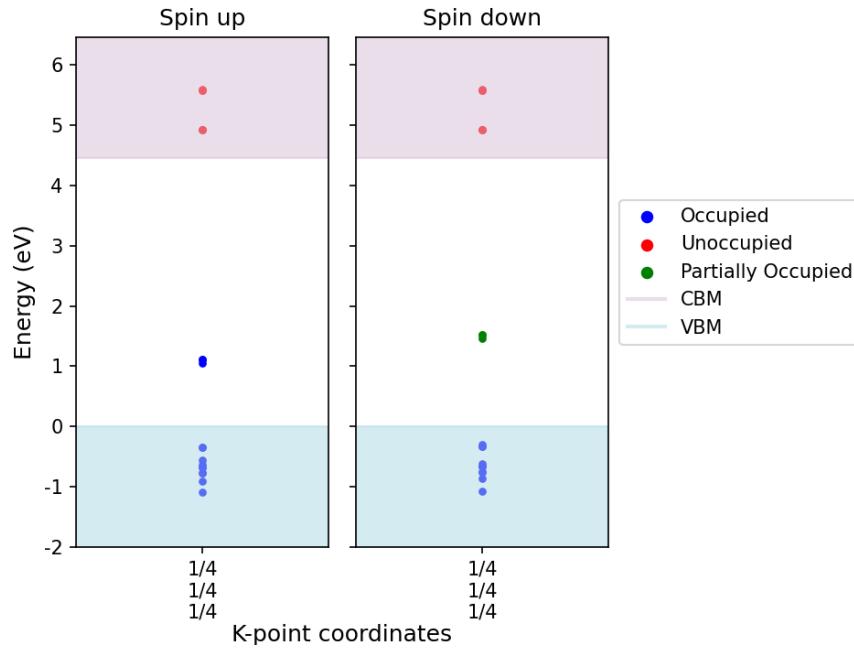


Figure 18: Kohn-Sham states.

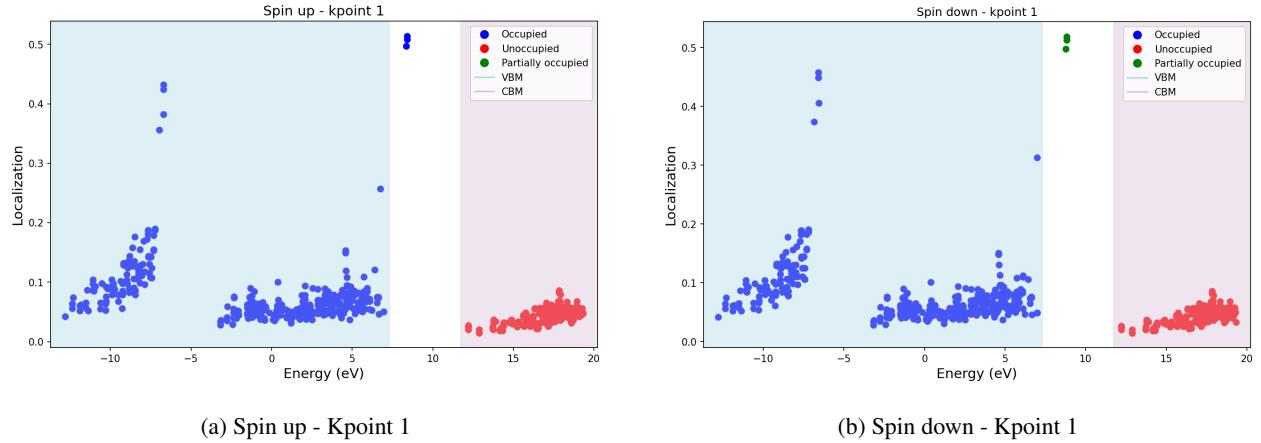


Figure 19: Localization factor using projected orbitals (s, p and d).

6.6 Vacancy: V_B^{-3}

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Table 29: V_B^{-3}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	430	149	0.347	Yes
		431	122	0.302	Yes
		432	175, 202	0.227, 0.227	Yes
Down	1	430	149	0.347	Yes
		431	122	0.302	Yes
		432	175, 202	0.227, 0.227	Yes

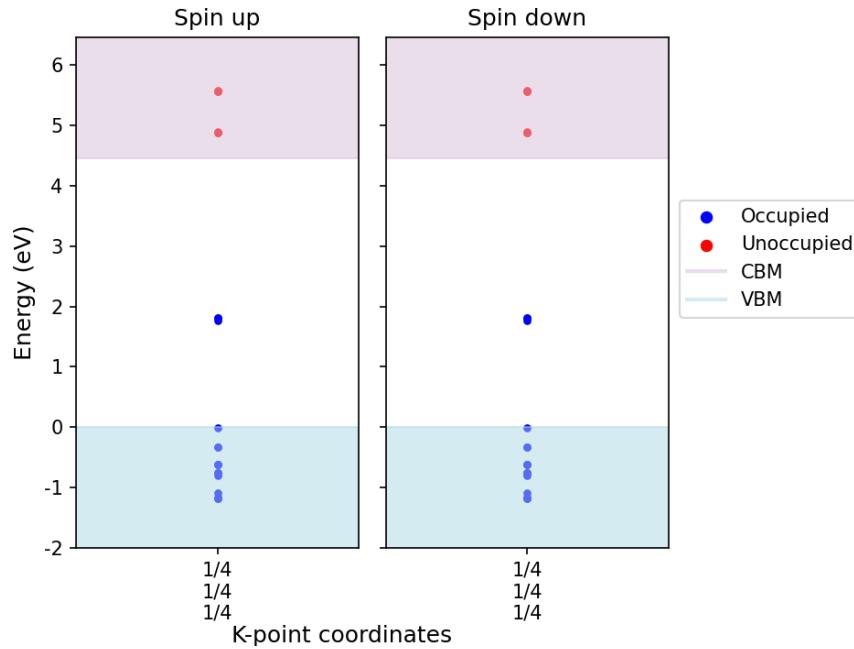


Figure 20: Kohn-Sham states.

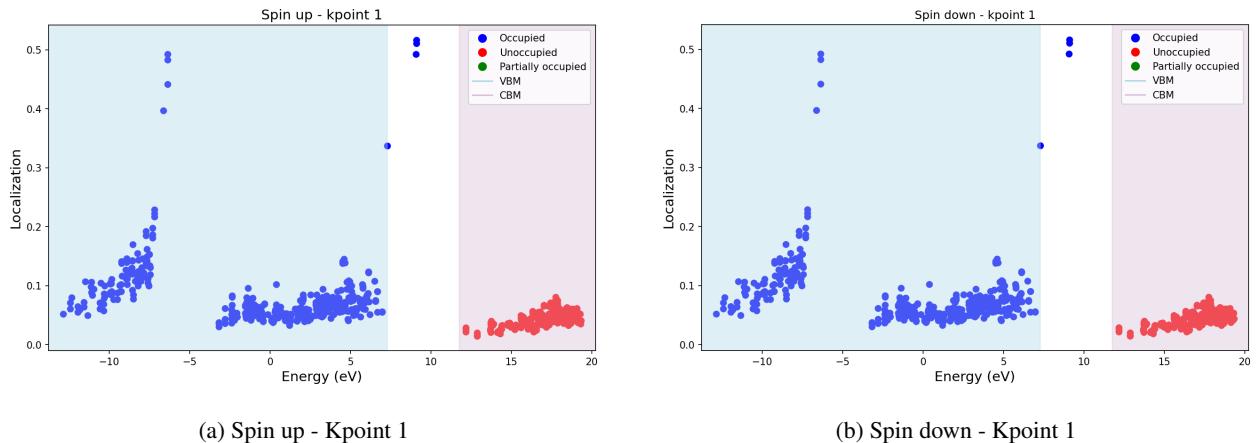


Figure 21: Localization factor using projected orbitals (s, p and d).

6.7 Vacancy: V_B^{-4}

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Table 30: V_B^{-4}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	430	149	0.347	Yes
		431	122	0.302	Yes
		432	175, 202	0.227, 0.227	Yes
Down	1	430	149	0.347	Yes
		431	122	0.302	Yes
		432	175, 202	0.227, 0.227	Yes

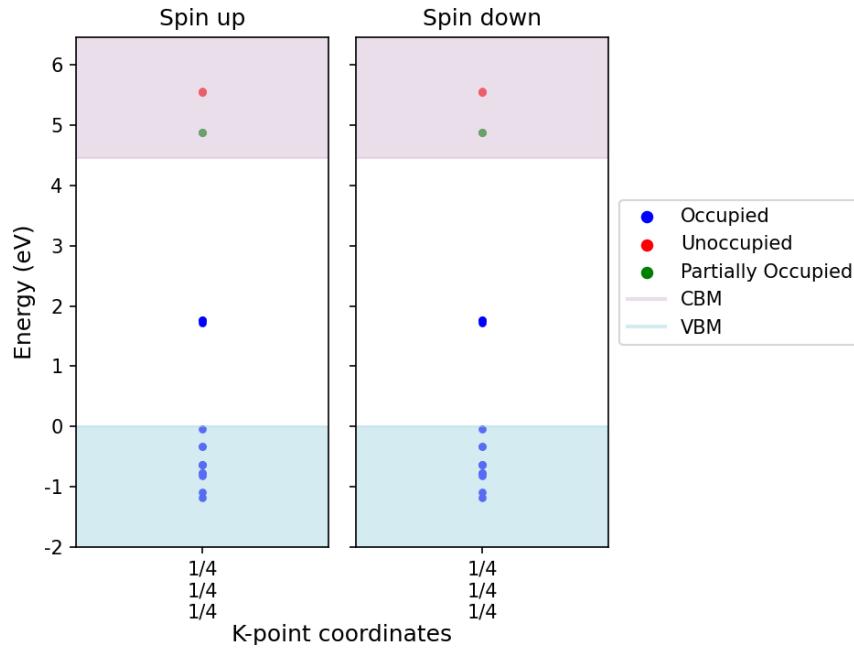


Figure 22: Kohn-Sham states.

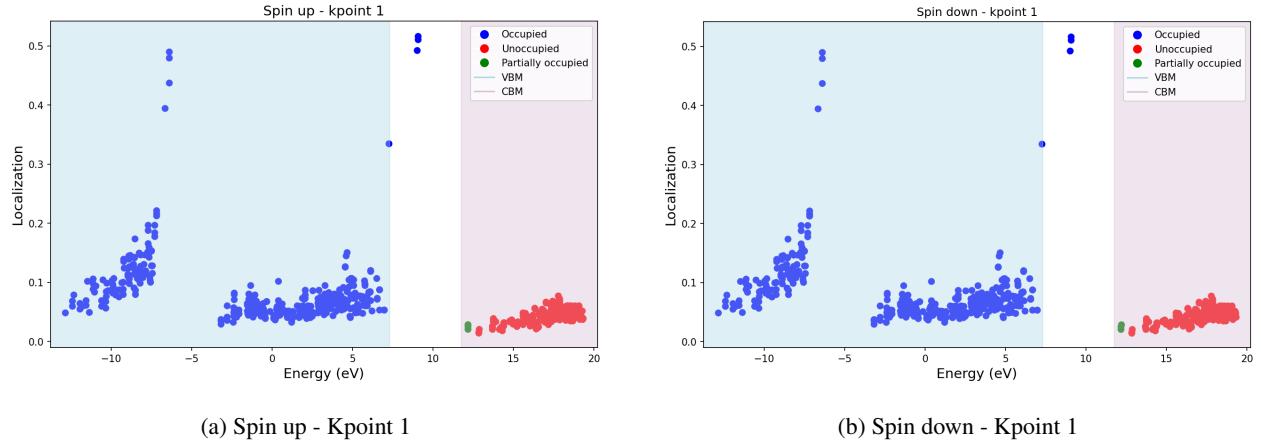


Figure 23: Localization factor using projected orbitals (s, p and d).

6.8 Vacancy: V_N^0

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Table 31: V_N^0

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	430	41	0.259	Yes
		431	71, 104	0.184, 0.184	Yes
		432	26	0.227, 0.245	Yes
Down	1	429	-	< 0.1	-

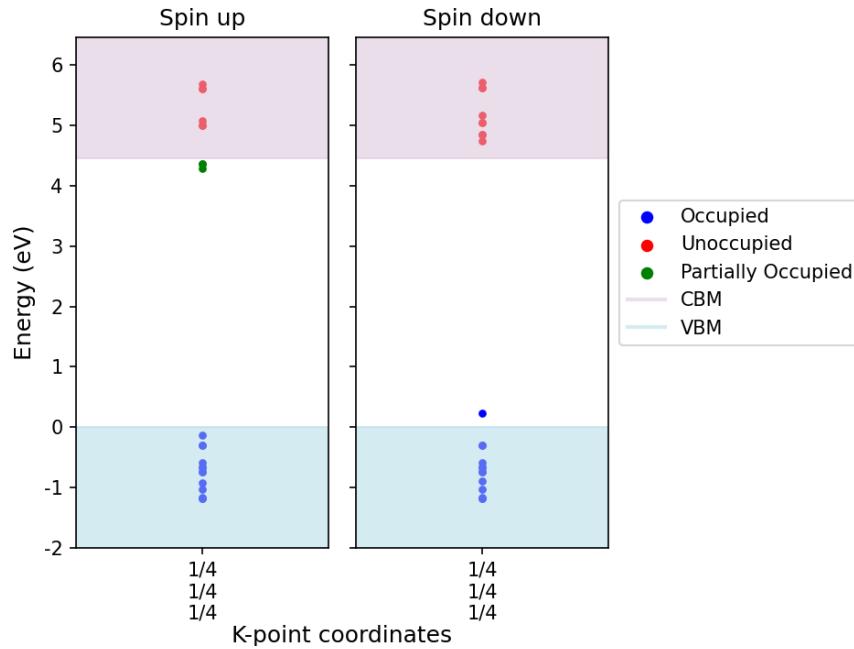


Figure 24: Kohn-Sham states.

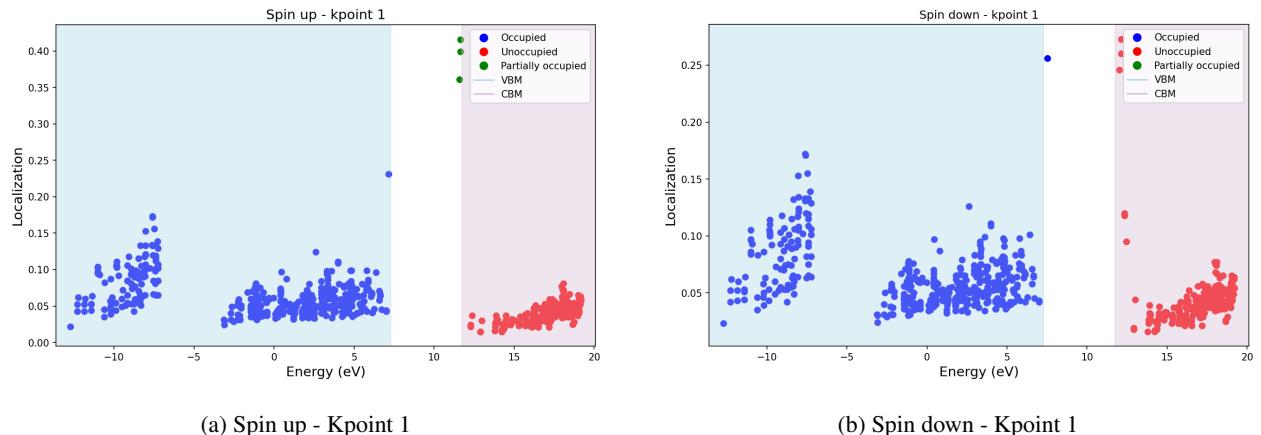


Figure 25: Localization factor using projected orbitals (s, p and d).

6.9 Vacancy: V_N^{+1}

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Table 32: V_N^{+1}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	430	41	0.267	Yes
		431	71, 104	0.187, 0.187	Yes
		432	26	0.249	Yes
Down	1	430	41	0.267	Yes
		431	71, 104	0.187, 187	Yes
		432	26	0.249	Yes

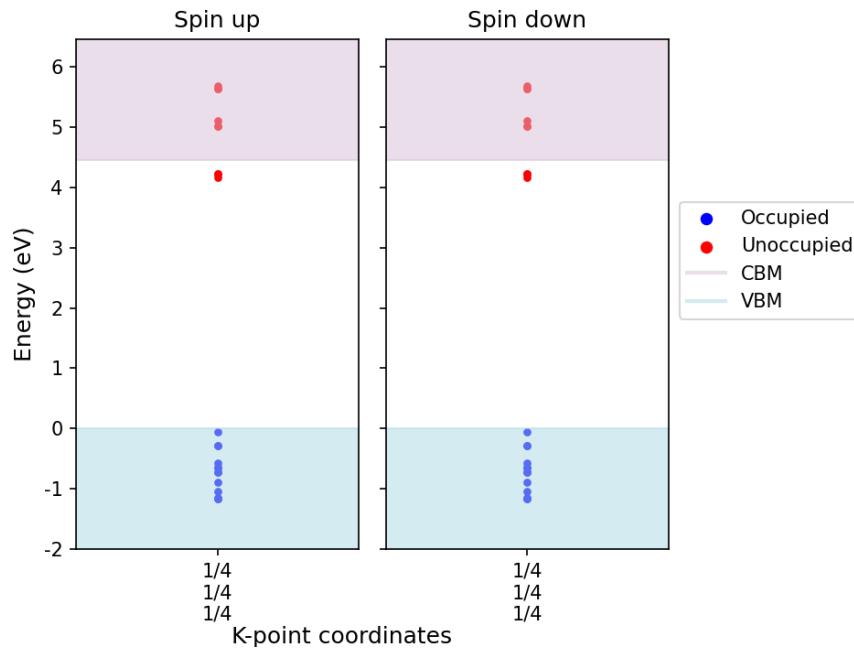


Figure 26: Kohn-Sham states.

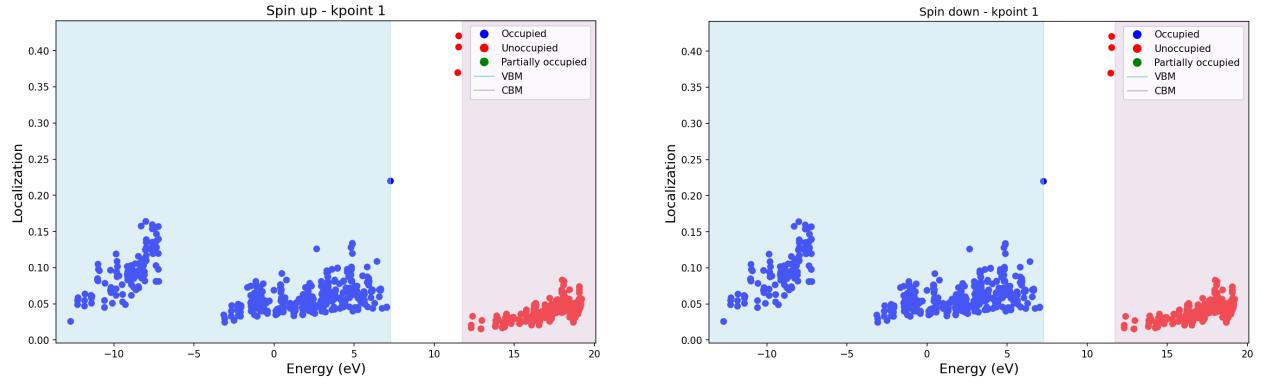


Figure 27: Localization factor using projected orbitals (s, p and d).

6.10 Vacancy: V_N^{+2}

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Table 33: V_N^{+2}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	429	—	< 0.1	—
		430	41	0.261	Yes
		431	26	0.245	Yes
		432	71, 104	0.184, 0.184	Yes
		429	—	< 0.1	—
Down	1	430	41	0.261	Yes
		431	26	0.245	Yes
		432	71, 104	0.184, 184	Yes

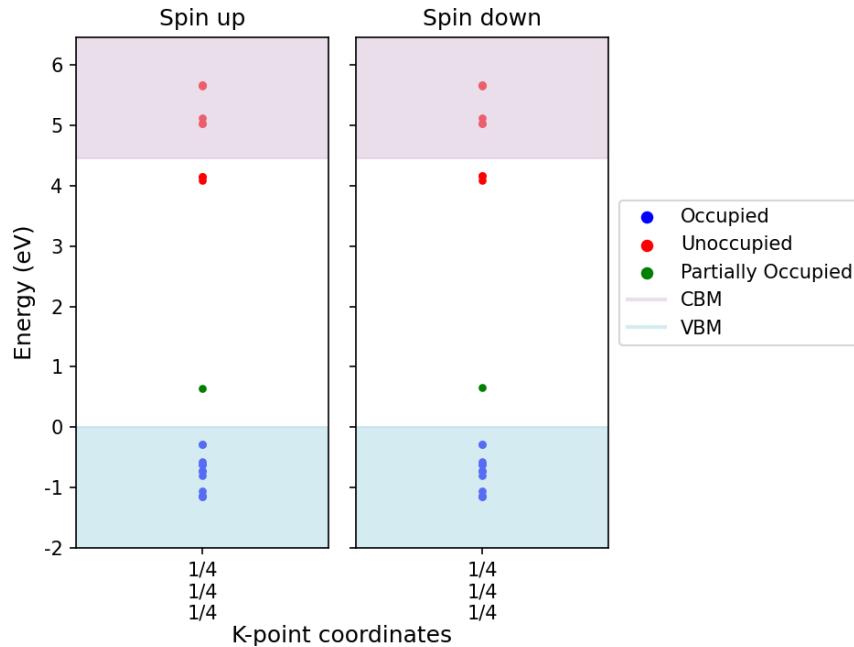


Figure 28: Kohn-Sham states.

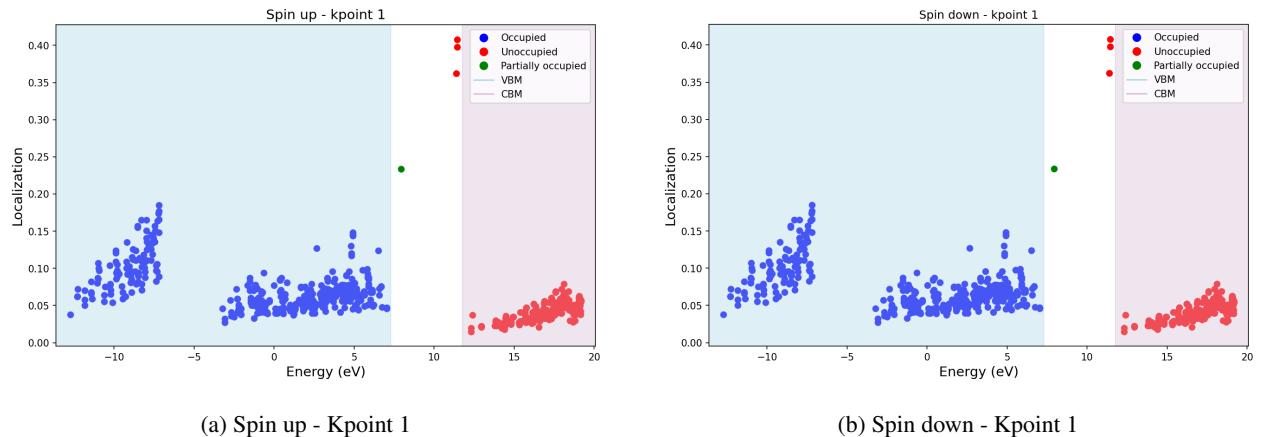


Figure 29: Localization factor using projected orbitals (s, p and d).

6.11 Vacancy: V_N^{+3}

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Table 34: V_N^{+3}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	429	—	< 0.1	—
		430	41	0.247	Yes
	431	71, 104	0.174, 0.174	Yes	Yes
	432	26	0.232	Yes	Yes
Down	1	429	—	< 0.1	—
		430	41	0.247	Yes
	431	71, 104	0.174, 0.174	Yes	Yes
	432	26	0.232	Yes	Yes

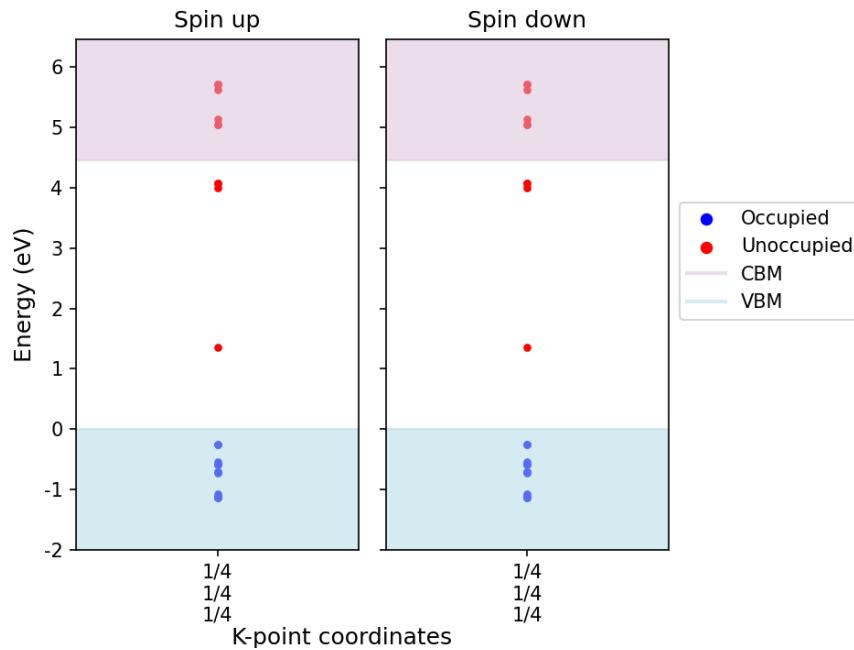
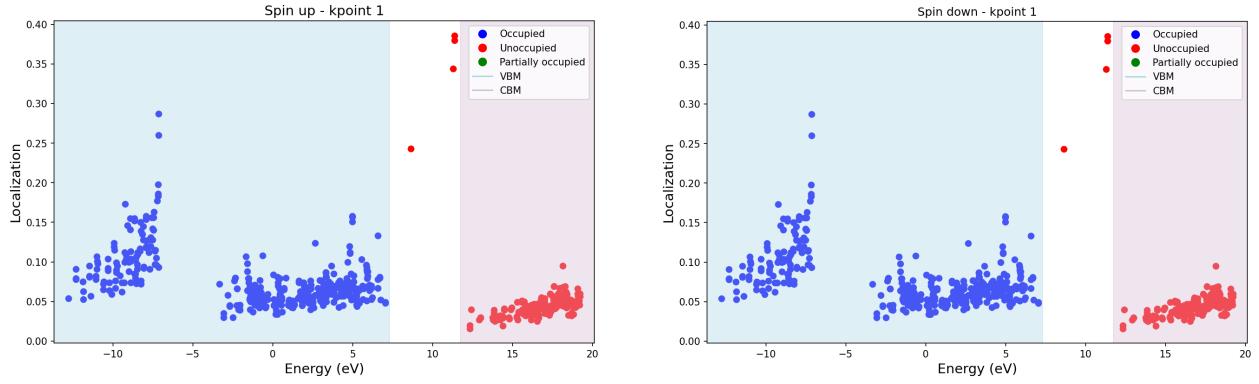


Figure 30: Kohn-Sham states.



(a) Spin up - Kpoint 1

(b) Spin down - Kpoint 1

Figure 31: Localization factor using projected orbitals (s, p and d).

6.12 Vacancy: V_N^{+4}

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Table 35: V_N^{+4}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	429	—	< 0.1	—
		430	41	0.247	Yes
		431	71, 104	0.174, 0.174	Yes
		432	26	0.232	Yes
		429	—	< 0.1	—
Down	1	430	41	0.247	Yes
		431	71, 104	0.174, 0.174	Yes
		432	26	0.232	Yes

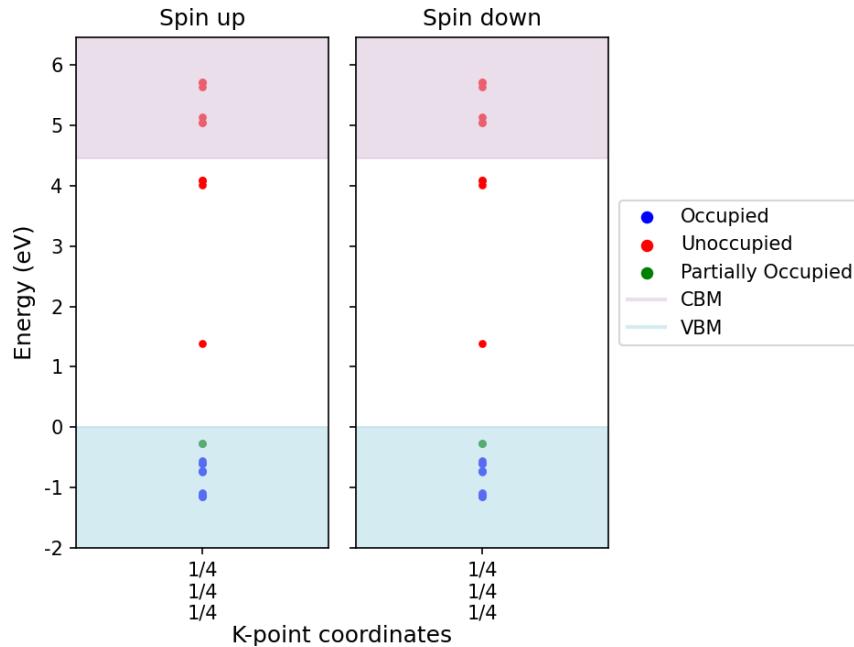


Figure 32: Kohn-Sham states.

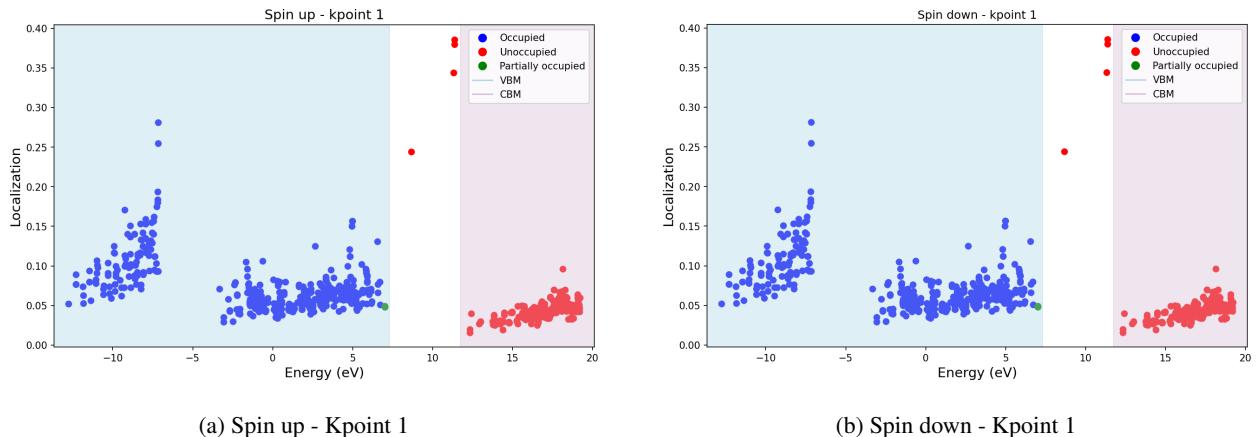


Figure 33: Localization factor using projected orbitals (s, p and d).

6.13 Vacancy: V_N^{-1}

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Table 36: V_N^{-1}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
Down	1	429	-	< 0.1	-

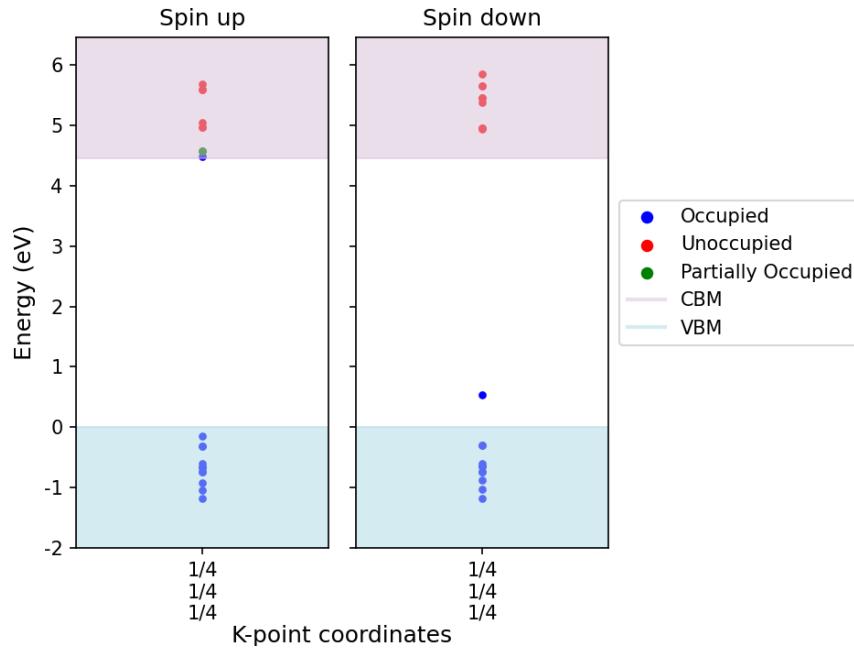


Figure 34: Kohn-Sham states.

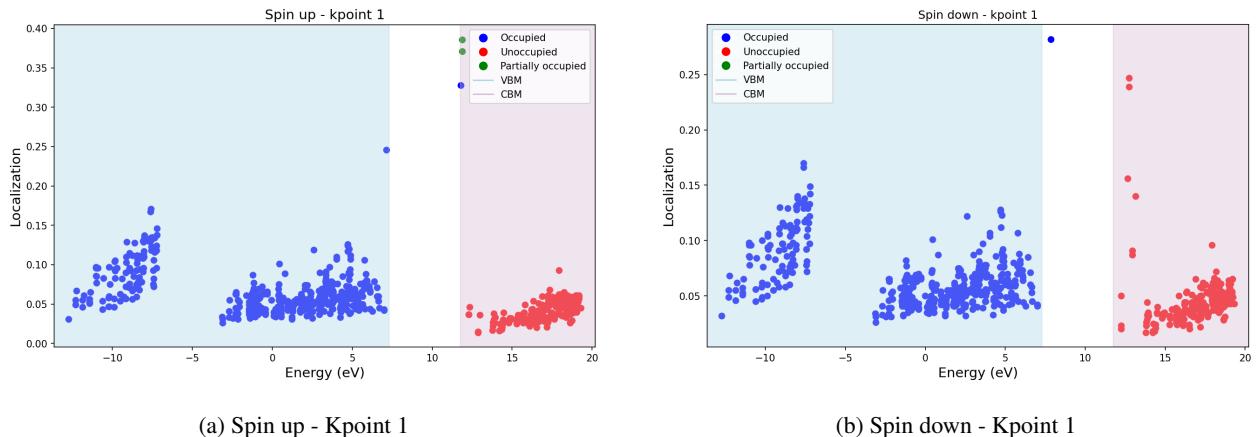


Figure 35: Localization factor using projected orbitals (s, p and d).

6.14 Antisite: B_N^0

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Table 37: B_N^0

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	430	41, 109	0.154, 0.220	Yes, *Defect*
		431	109	0.205	*Defect*
		432	26, 109	0.128, 0.205	Yes, *Defect*
Down	1	430	41, 109	0.178, 0.235	Yes, *Defect*
		431	71, 104, 109	0.116, 0.116, 0.230	Yes, Yes, *Defect*
		432	26, 109	0.154, 0.230	Yes, *Defect*

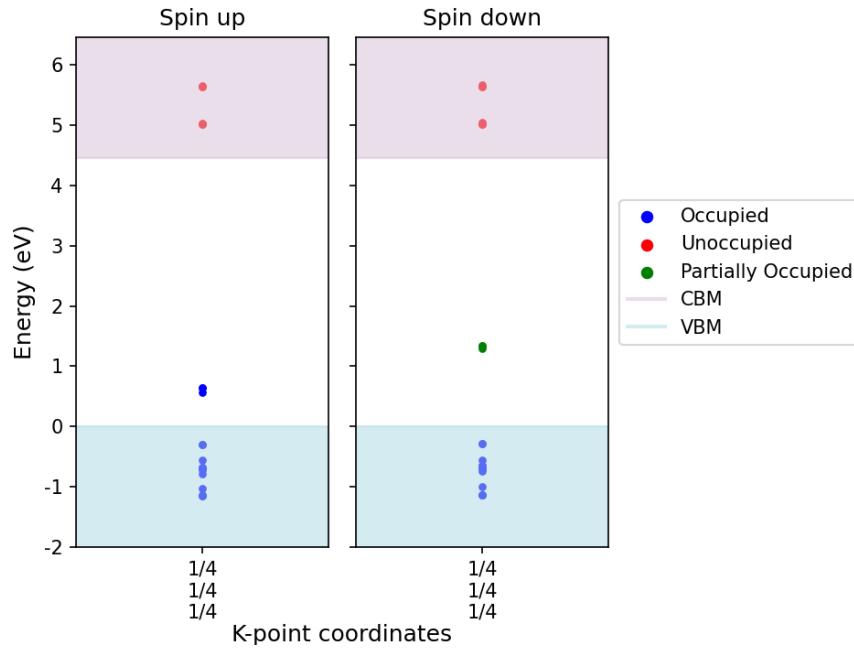


Figure 36: Kohn-Sham states.

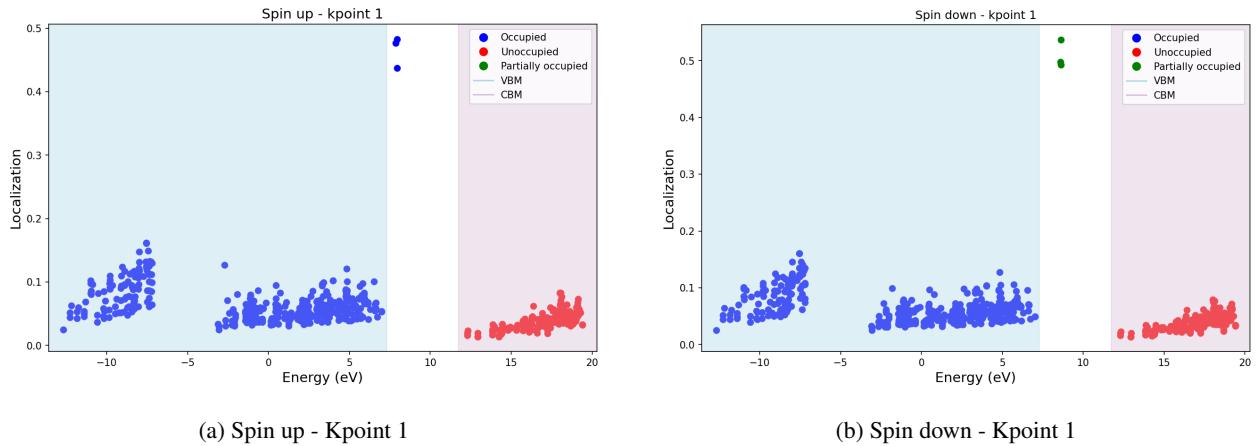


Figure 37: Localization factor using projected orbitals (s, p and d).

6.15 Antisite: B_N^{+1}

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Table 38: B_N^{+1}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	430	41, 109	0.109, 0.189	Yes, *Defect*
		431	109	0.150	*Defect*
		432	109	0.149	*Defect*
Down	1	430	41, 109	0.156, 0.227	Yes, *Defect*
		431	71, 104, 109	0.101, 0.101, 0.221	Yes, Yes, *Defect*
		432	26, 109	0.134, 0.221	Yes, *Defect*

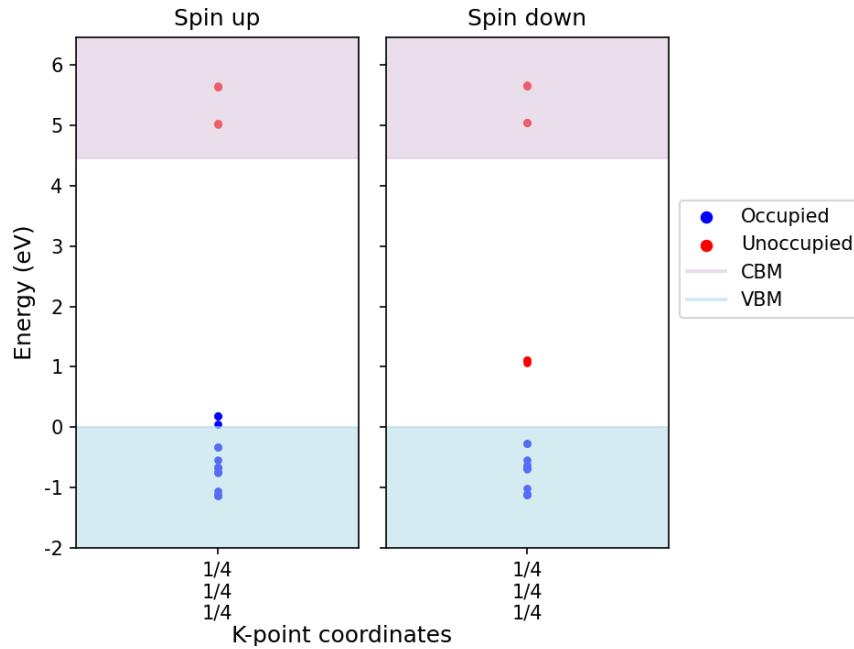


Figure 38: Kohn-Sham states.

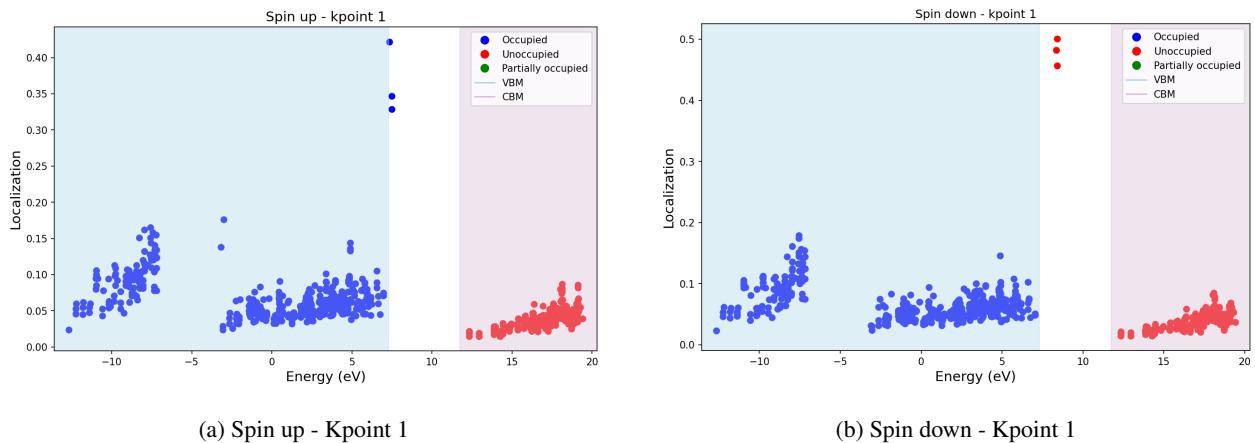


Figure 39: Localization factor using projected orbitals (s, p and d).

6.16 Antisite: B_N^{+2}

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Table 39: B_N^{+2}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	430	109	0.188	*Defect*
		431	109	0.148	*Defect*
		432	109	0.148	*Defect*
Down	1	430	41, 109	0.138, 0.222	Yes, *Defect*
		431	109	0.211	*Defect*
		432	26, 109	0.116, 0.211	Yes, *Defect*

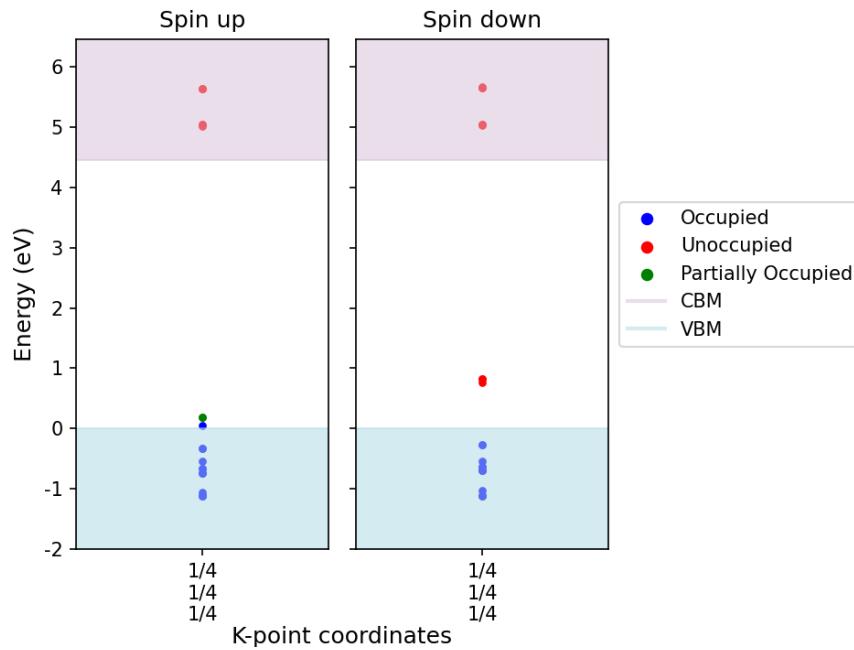


Figure 40: Kohn-Sham states.

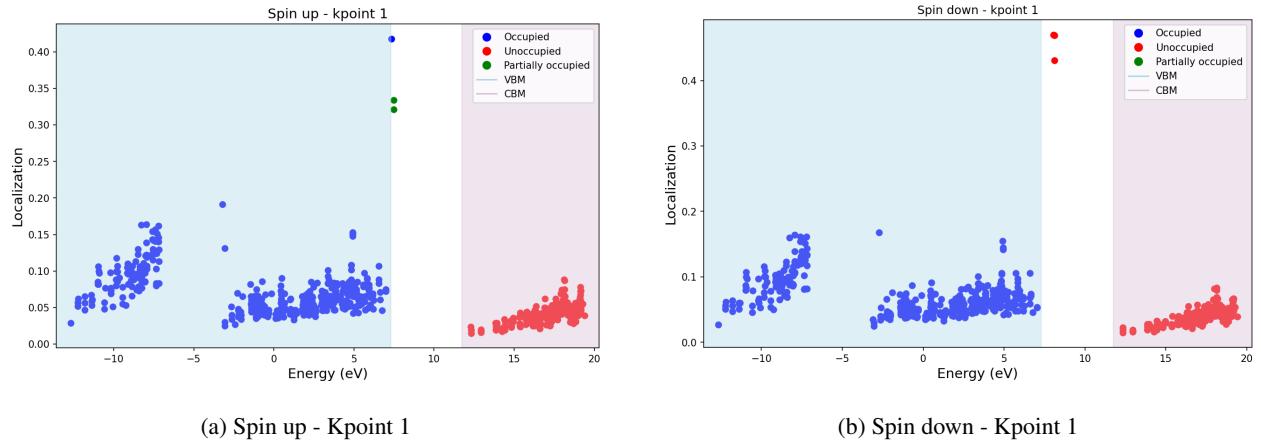


Figure 41: Localization factor using projected orbitals (s, p and d).

6.17 Antisite: B_N^{+3}

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Table 40: B_N^{+3}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	430	109	0.192	*Defect*
		431	109	0.155	*Defect*
		432	109	0.155	*Defect*
Down	1	430	41, 109	0.116, 0.214	Yes, *Defect*
		431	109	0.197	*Defect*
		432	109	0.197	*Defect*

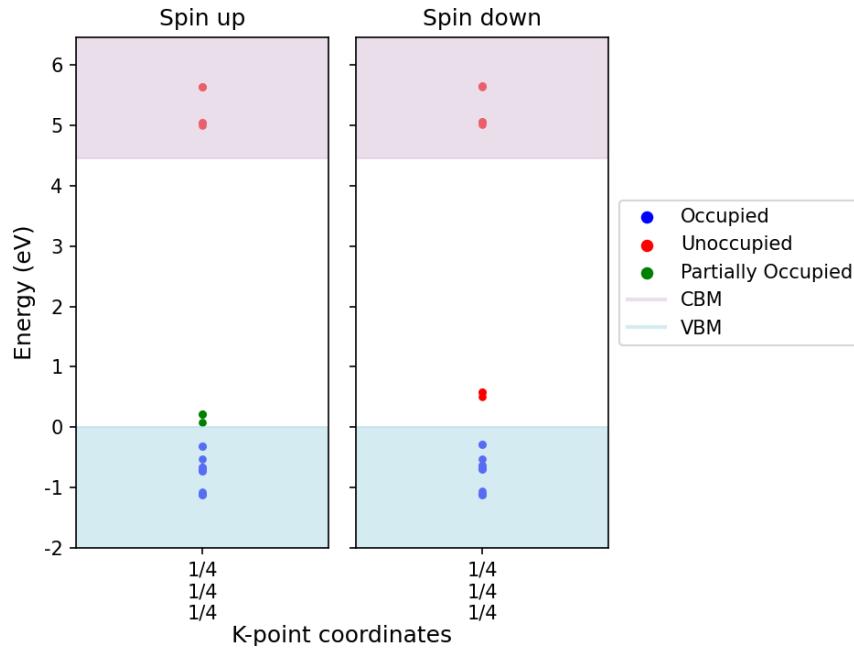


Figure 42: Kohn-Sham states.

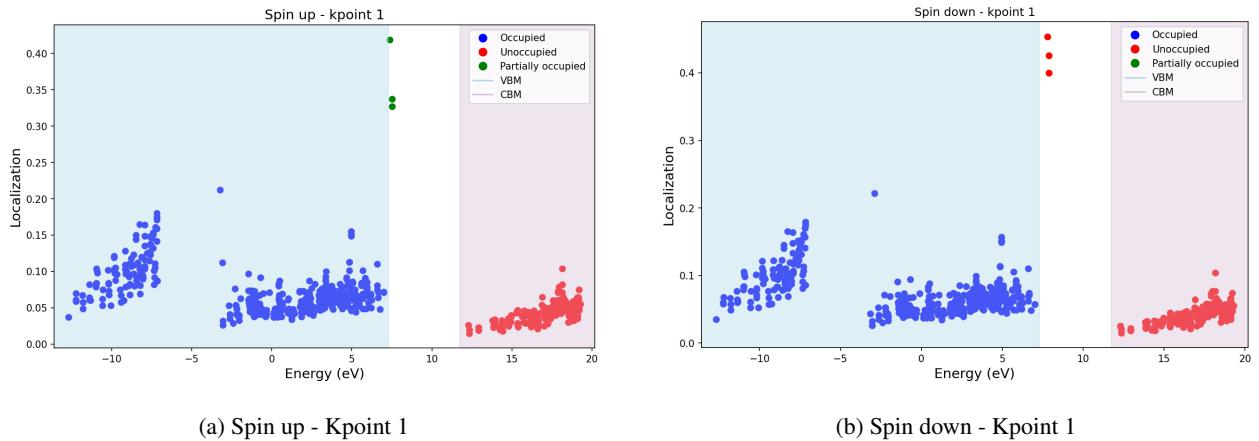


Figure 43: Localization factor using projected orbitals (s, p and d).

6.18 Antisite: B_N^{+4}

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Table 41: B_N^{+4}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	430	109	0.202	*Defect*
		431	109	0.171	*Defect*
		432	109	0.171	*Defect*
Down	1	430	109	0.202, 0.214	*Defect*
		431	109	0.171	*Defect*
		432	109	0.171	*Defect*

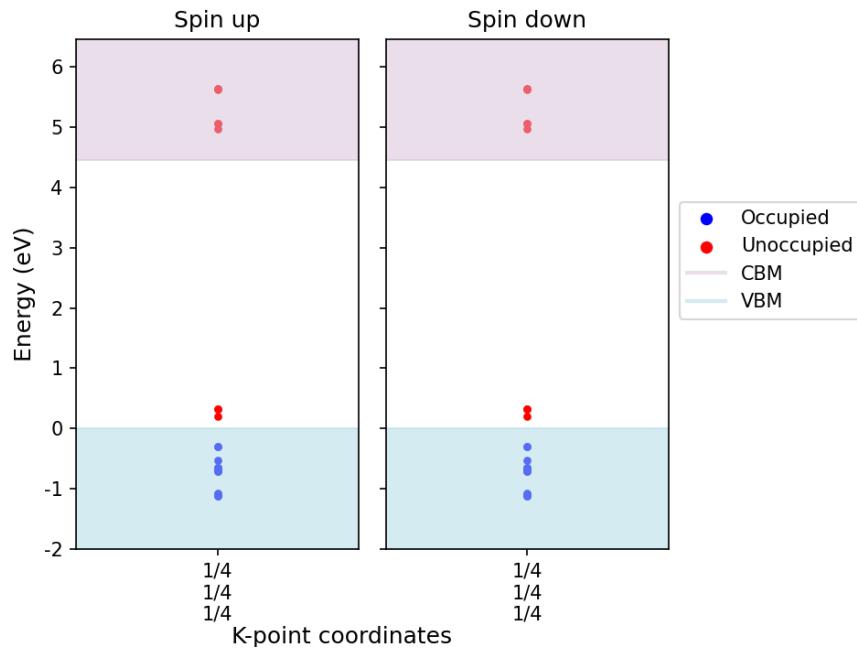


Figure 44: Kohn-Sham states.

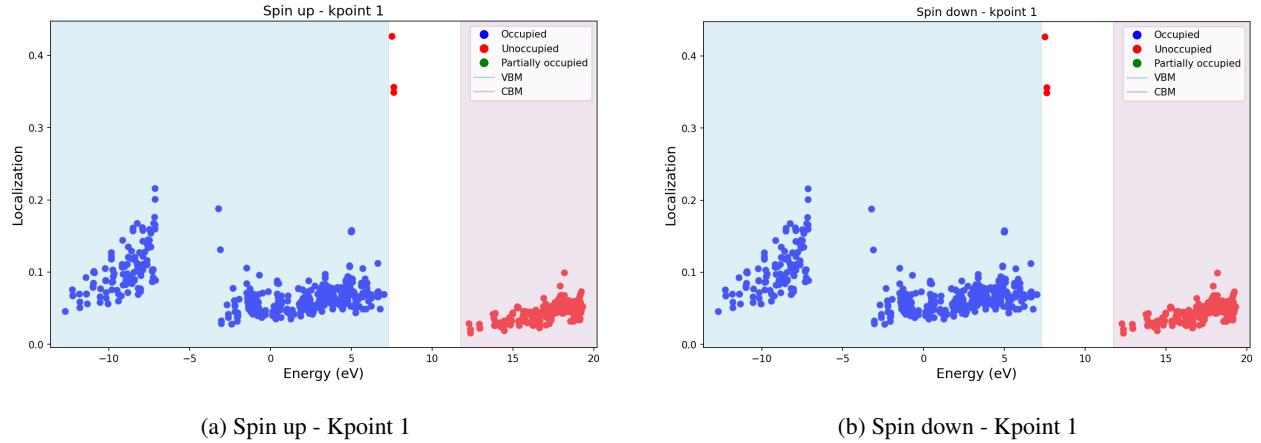


Figure 45: Localization factor using projected orbitals (s, p and d).

6.19 Antisite: B_N^{-1}

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Table 42: B_N^{-1}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	430	41, 109	0.192, 0.240	Yes, *Defect*
		431	71, 104, 109	0.125, 0.125, 0.235	Yes, Yes, *Defect*
		432	26, 109	0.167, 0.235	Yes, *Defect*
Down	1	430	41, 109	0.199, 0.243	Yes, *Defect*
		431	71, 104, 109	0.131, 0.131, 0.240	Yes, Yes, *Defect*
		432	26, 109	0.175, 0.240	Yes, *Defect*

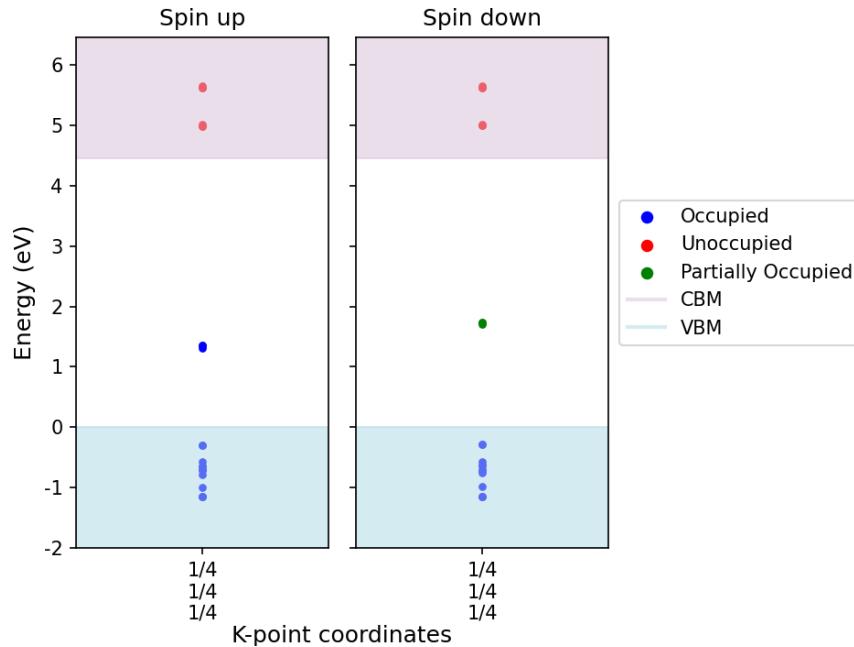


Figure 46: Kohn-Sham states.

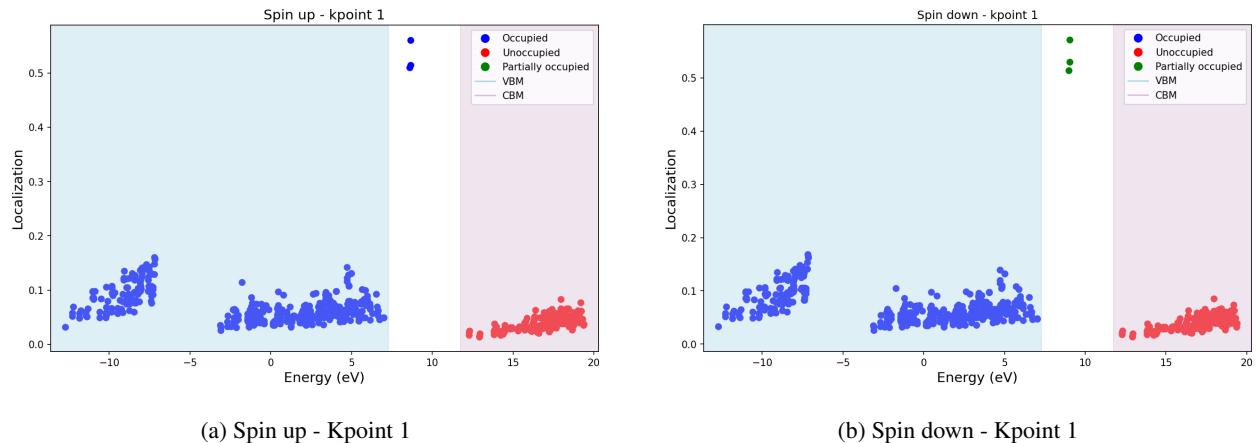


Figure 47: Localization factor using projected orbitals (s, p and d).

6.20 Antisite: B_N^{-2}

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Table 43: B_N^{-2}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	430	41, 109	0.217, 0.249	Yes, *Defect*
		431	71, 104, 109	0.144, 0.144, 0.249	Yes, Yes, *Defect*
		432	26, 109	0.192, 0.249	Yes, *Defect*
Down	1	430	41, 109	0.217, 0.249	Yes, *Defect*
		431	71, 104, 109	0.144, 0.144, 0.249	Yes, Yes, *Defect*
		432	26, 109	0.192, 0.249	Yes, *Defect*

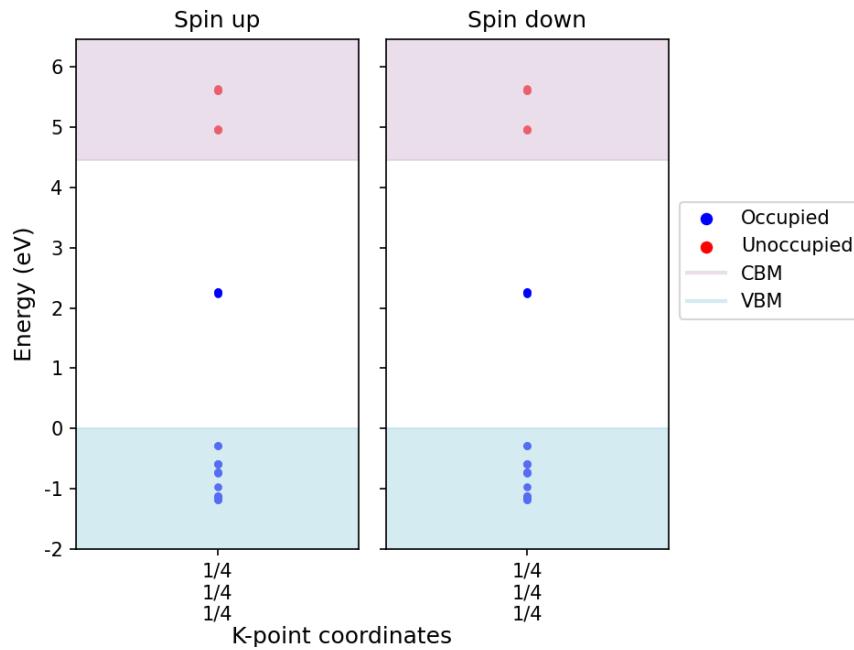


Figure 48: Kohn-Sham states.

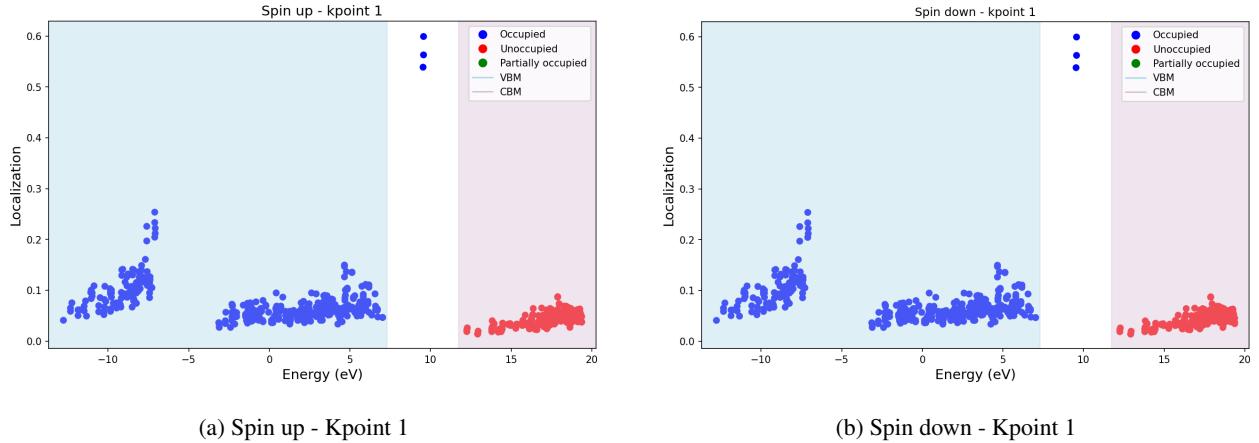


Figure 49: Localization factor using projected orbitals (s, p and d).

6.21 Antisite: B_N^{-3}

[Go back to the Table 23](#)

Table 44: B_N^{-3}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	430	41, 109	0.216, 0.249	Yes, *Defect*
		431	71, 104, 109	0.144, 0.144, 0.248	Yes, Yes, *Defect*
		432	26, 109	0.191, 0.248	Yes, *Defect*
Down	1	430	41, 109	0.216, 0.249	Yes, *Defect*
		431	71, 104, 109	0.144, 0.144, 0.248	Yes, Yes, *Defect*
		432	26, 109	0.191, 0.248	Yes, *Defect*

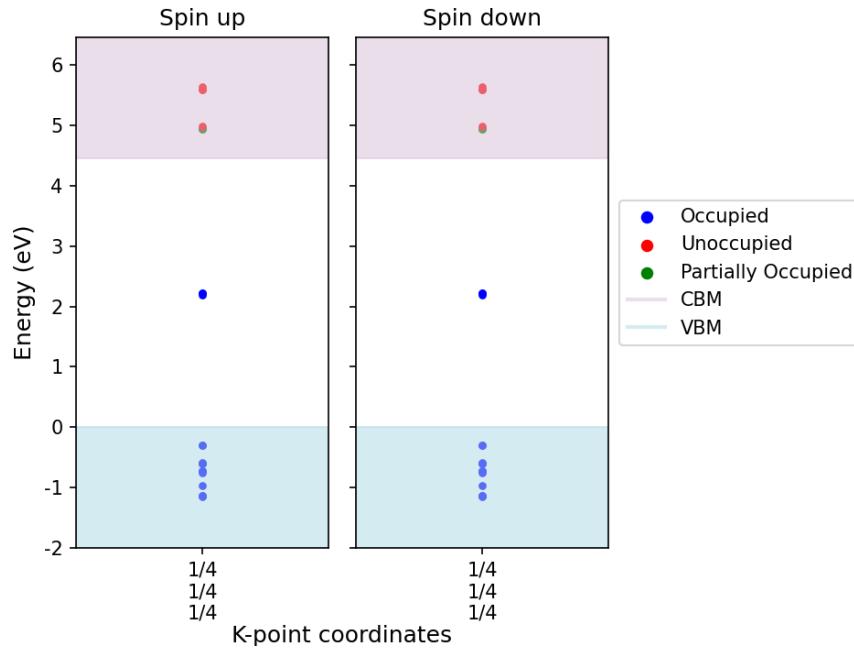


Figure 50: Kohn-Sham states.

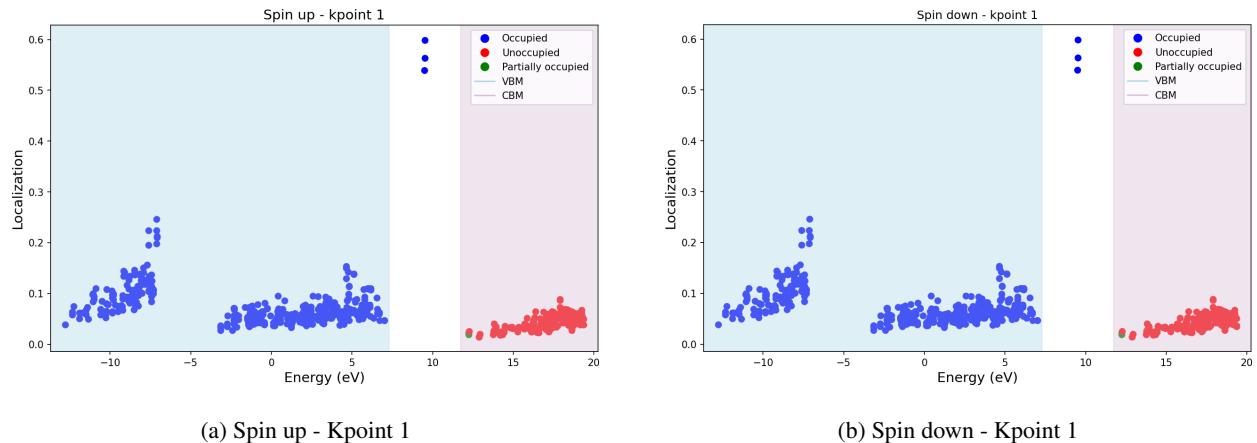


Figure 51: Localization factor using projected orbitals (s, p and d).

6.22 Antisite: B_N^{-4}

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Table 45: B_N^{-4}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	430	41, 109	0.216, 0.249	Yes, *Defect*
		431	71, 104, 109	0.143, 0.143, 0.248	Yes, Yes, *Defect*
		432	26, 109	0.191, 0.248	Yes, *Defect*
Down	1	430	41, 109	0.216, 0.249	Yes, *Defect*
		431	71, 104, 109	0.143, 0.143, 0.248	Yes, Yes, *Defect*
		432	26, 109	0.191, 0.248	Yes, *Defect*

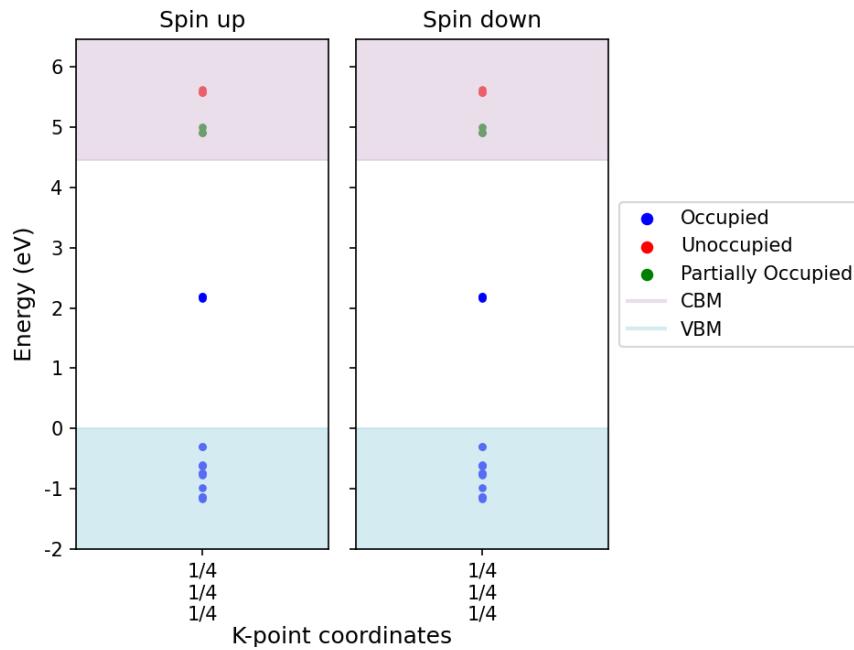


Figure 52: Kohn-Sham states.

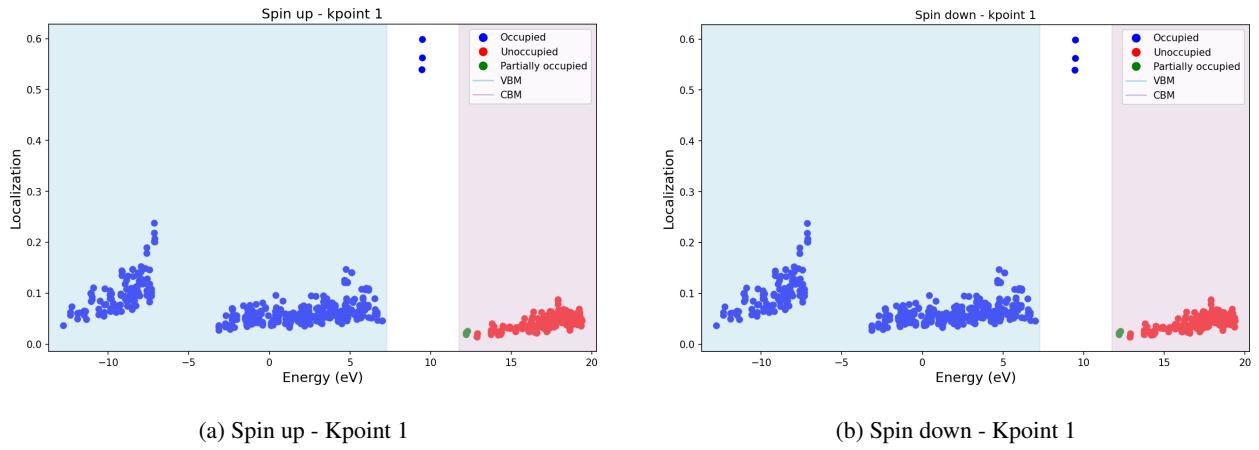


Figure 53: Localization factor using projected orbitals (s, p and d).

6.23 Antisite: N_B^0

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Table 46: N_B^0

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	433	108, 123, 150, 176, 203	0.149, 0.117, 0.114, 0.117, 0.117	*Defect*, Y, Y, Y, Y
		434	108, 150	0.301, 0.201	*Defect*, Y
		435	108, 176, 203	0.300, 0.132, 0.132	*Defect*, Y, Y
		436	108, 123	0.300, 0.175	*Defect*, Y
Down	1	433	108, 123, 150, 176, 203	0.149, 0.117, 0.114, 0.117, 0.117	*Defect*, Y, Y, Y, Y
		434	108, 150	0.301, 0.201	*Defect*, Y
		435	108, 176, 203	0.300, 0.132, 0.132	*Defect*, Y, Y
		436	108, 123	0.300, 0.175	*Defect*, Y

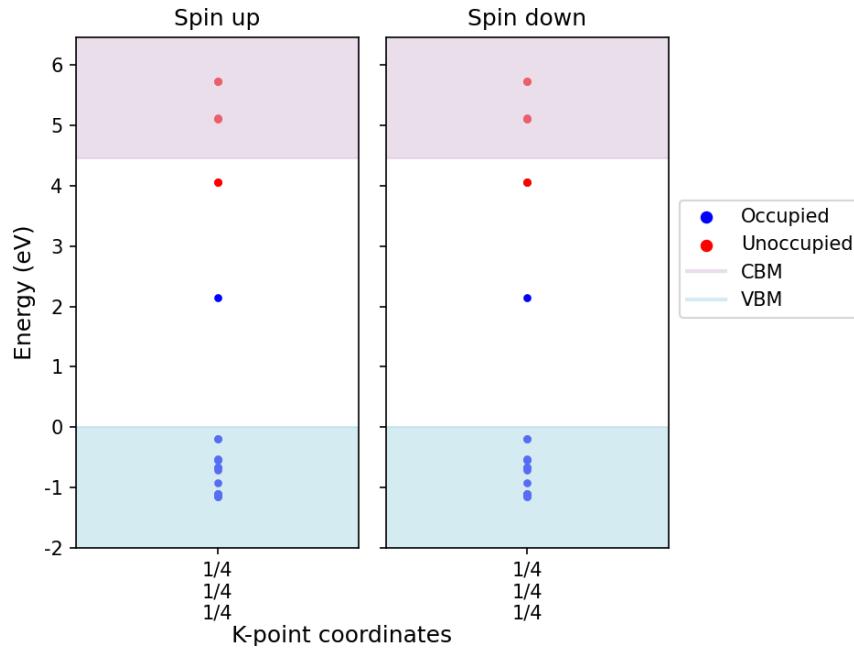


Figure 54: Kohn-Sham states.

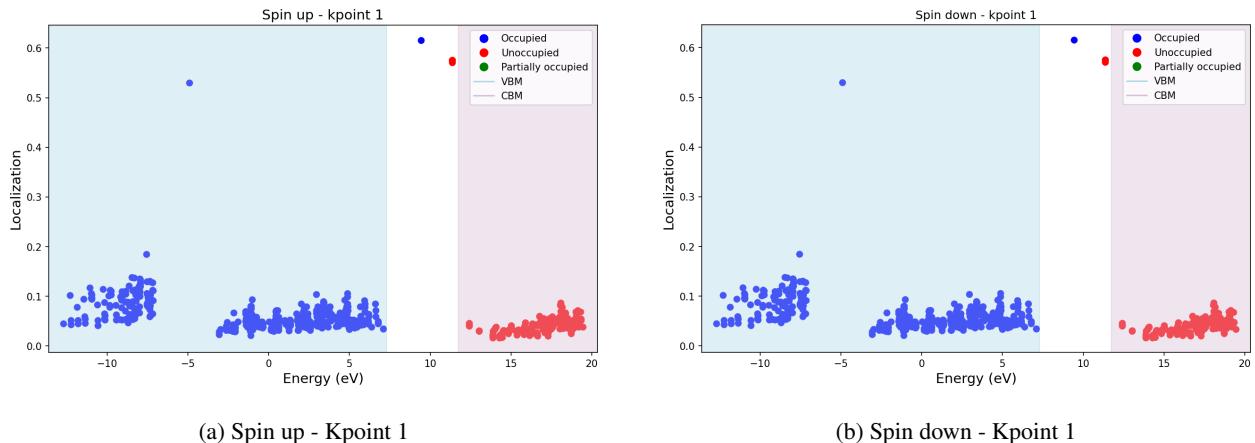


Figure 55: Localization factor using projected orbitals (s, p and d).

6.24 Antisite: N_B^{+1}

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Table 47: N_B^{+1}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	433	108, 123, 150, 176, 203	0.172, 0.116, 0.113, 0.116, 0.116	*Defect*, Y, Y, Y, Y
		434	108, 150	0.312, 0.209	*Defect*, Y
		435	108, 176, 203	0.311, 0.138, 0.138	*Defect*, Y, Y
		436	108, 123	0.311, 0.183	*Defect*, Y
Down	1	433	108, 123, 150, 176, 203	0.174, 0.112, 0.108, 0.112, 0.112	*Defect*, Y, Y, Y, Y
		434	108, 150	0.279, 0.198	*Defect*, Y
		435	108, 176, 203	0.278, 0.130, 0.130	*Defect*, Y, Y
		436	108, 123	0.278, 0.172	*Defect*, Y

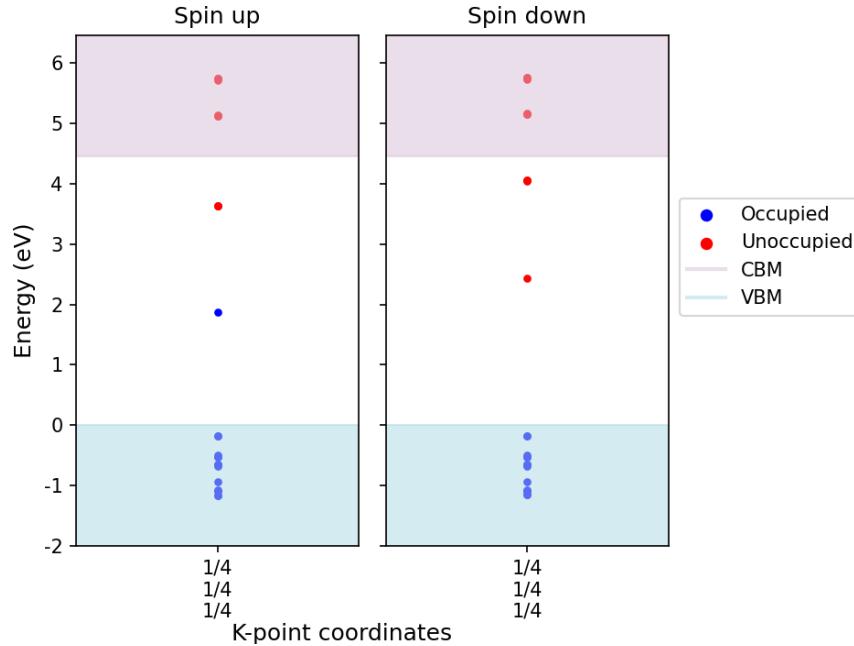


Figure 56: Kohn-Sham states.

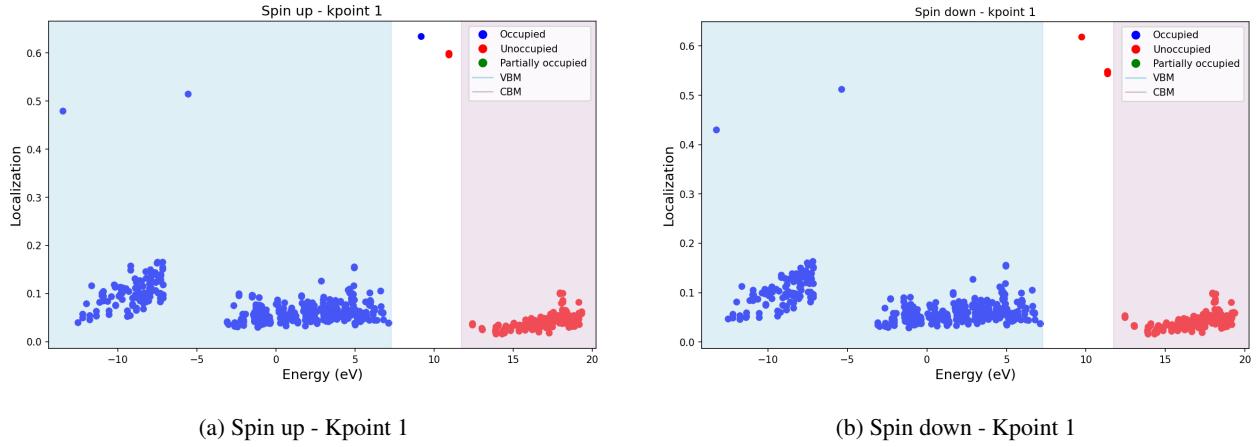


Figure 57: Localization factor using projected orbitals (s, p and d).

6.25 Antisite: N_B^{+2}

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Table 48: N_B^{+2}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	433	108	0.203	*Defect*
		434	108, 150	0.242, 0.177	*Defect*, Y
		435	108, 176, 203	0.242, 0.114, 0.114	*Defect*, Y, Y
		436	108, 123	0.242, 0.151	*Defect*, Y
Down	1	433	108	0.203	*Defect*
		434	108, 150	0.242, 0.177	*Defect*, Y
		435	108, 176, 203	0.242, 0.114, 0.114	*Defect*, Y, Y
		436	108, 123	0.242, 0.151	*Defect*, Y

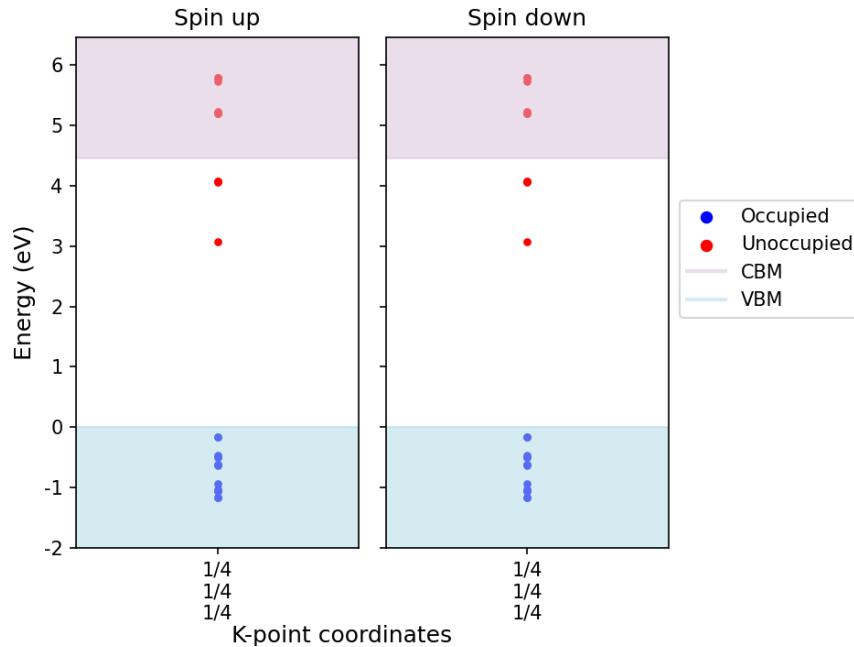


Figure 58: Kohn-Sham states.

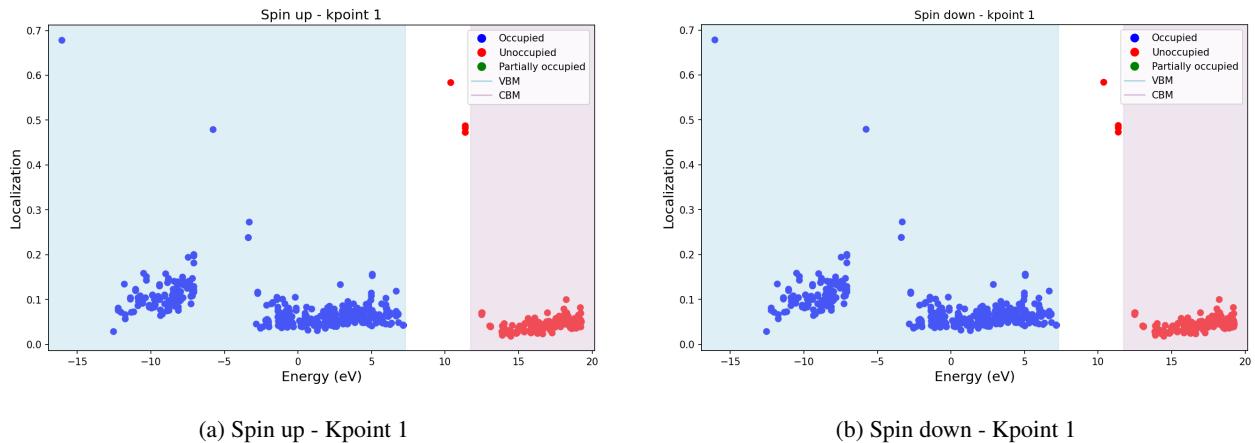


Figure 59: Localization factor using projected orbitals (s, p and d).

6.26 Antisite: N_B^{+3}

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Table 49: N_B^{+3}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	433	108	0.203	*Defect*
		434	108, 150	0.242, 0.177	*Defect*, Y
		435	108, 176, 203	0.242, 0.113, 0.113	*Defect*, Y, Y
		436	108, 123	0.242, 0.150	*Defect*, Y
Down	1	433	108	0.203	*Defect*
		434	108, 150	0.242, 0.177	*Defect*, Y
		435	108, 176, 203	0.242, 0.113, 0.113	*Defect*, Y, Y
		436	108, 123	0.242, 0.150	*Defect*, Y

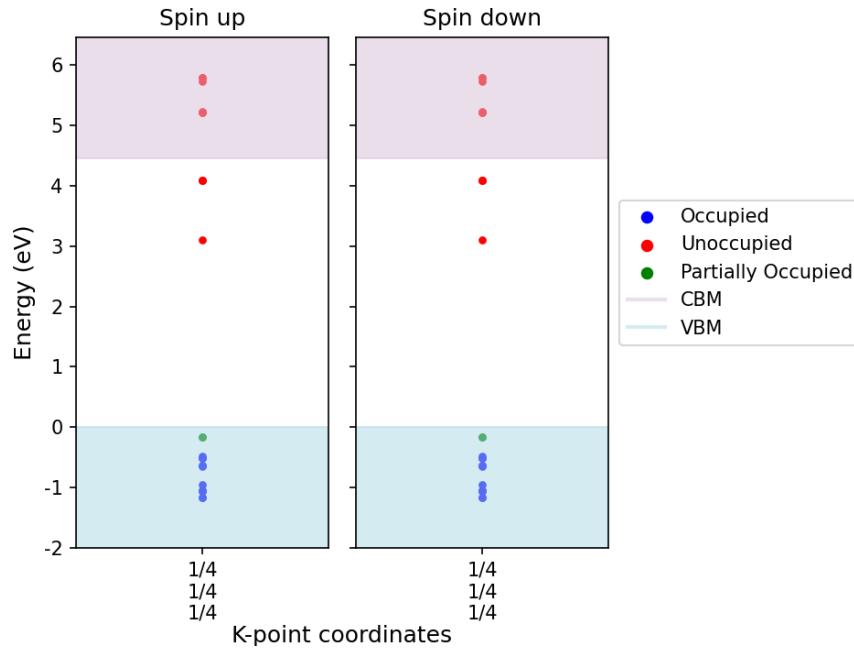


Figure 60: Kohn-Sham states.

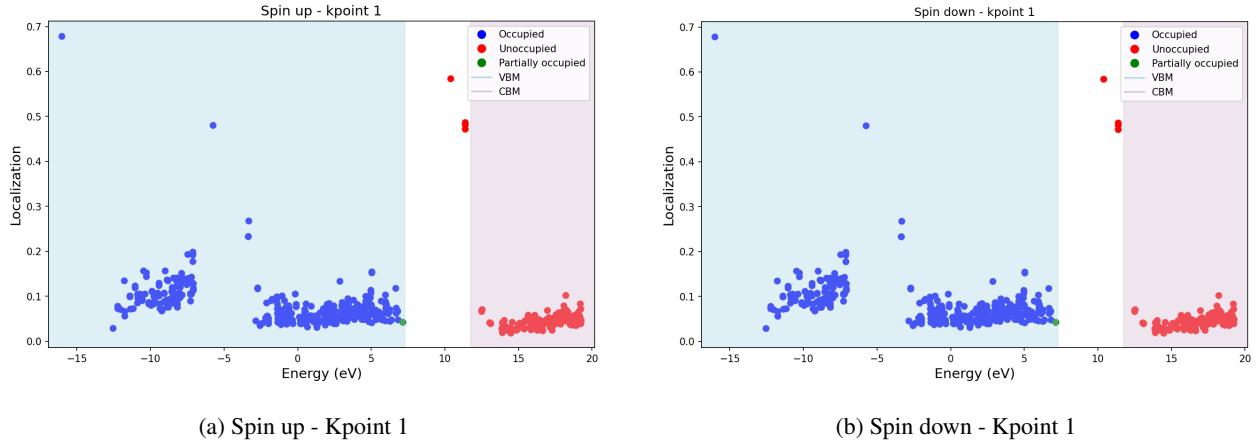


Figure 61: Localization factor using projected orbitals (s, p and d).

6.27 Antisite: N_B^{+4}

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Table 50: N_B^{+4}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	433	108	0.203	*Defect*
		434	108, 150	0.242, 0.176	*Defect*, Y
		435	108, 176, 203	0.241, 0.113, 0.113	*Defect*, Y, Y
		436	108, 123	0.241, 0.150	*Defect*, Y
Down	1	433	108	0.203	*Defect*
		434	108, 150	0.242, 0.176	*Defect*, Y
		435	108, 176, 203	0.241, 0.113, 0.113	*Defect*, Y, Y
		436	108, 123	0.241, 0.150	*Defect*, Y

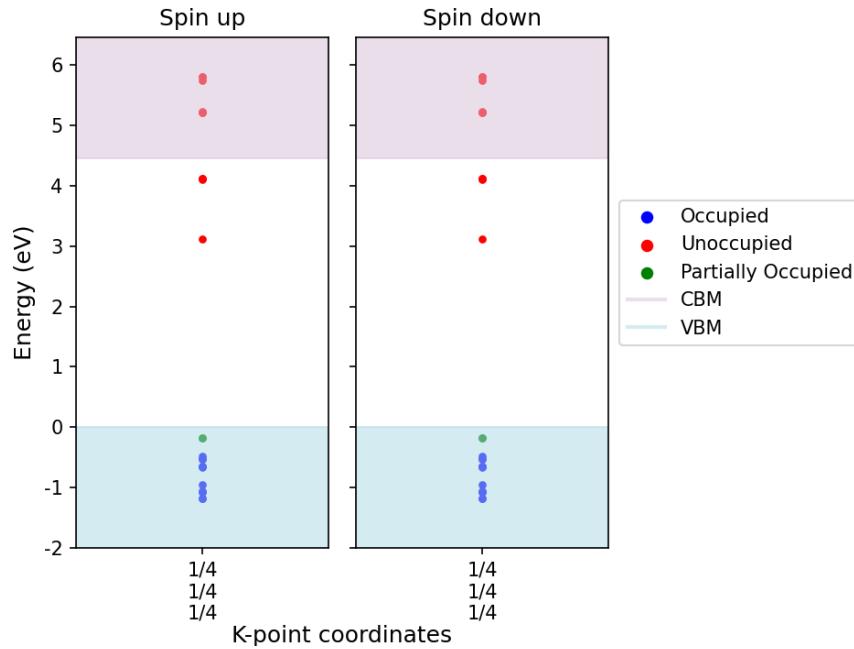


Figure 62: Kohn-Sham states.

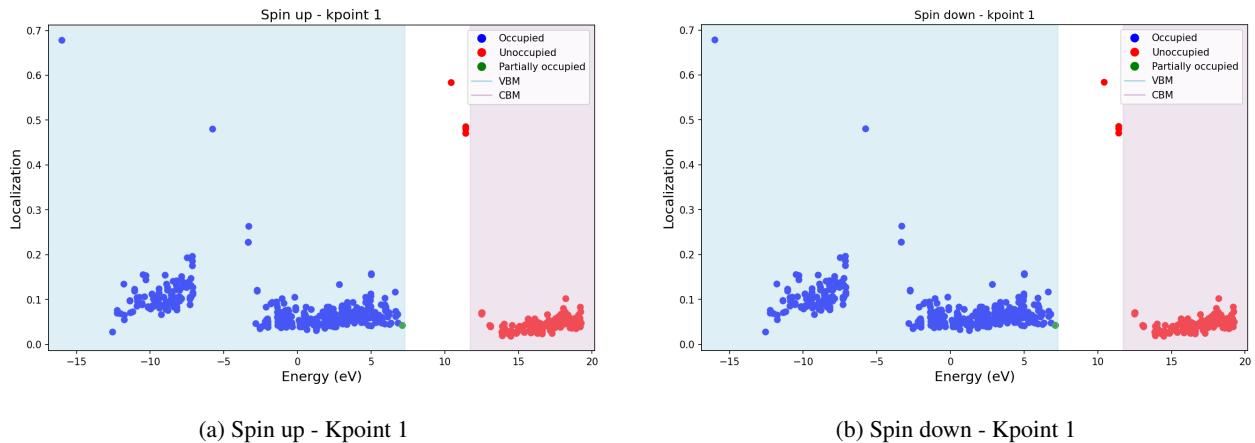


Figure 63: Localization factor using projected orbitals (s, p and d).

6.28 Antisite: N_B^{-1}

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Table 51: N_B^{-1}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
up	1	433	108, 123, 150, 176, 203	0.135, 0.117, 0.115, 0.117, 0.117	*Defect*, Y, Y, Y, Y
		434	108, 150	0.290, 0.184	*Defect*, Y
		435	108, 176, 203	0.289, 0.121, 0.121	*Defect*, Y, Y
		436	108, 123	0.289, 0.160	*Defect*, Y
Down	1	433	108, 123, 150, 176, 203	0.147, 0.115, 0.113, 0.115, 0.115	*Defect*, Y, Y, Y, Y

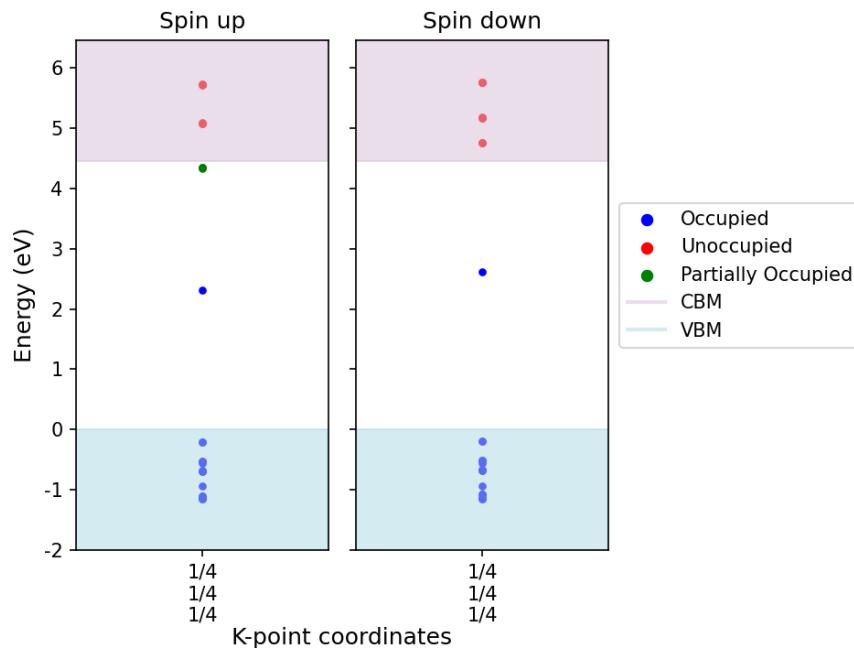


Figure 64: Kohn-Sham states.

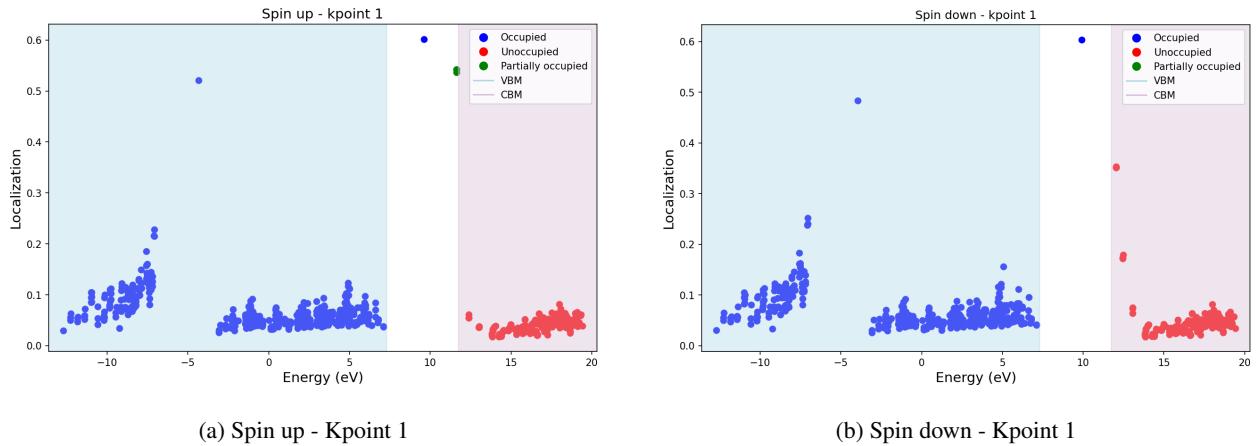


Figure 65: Localization factor using projected orbitals (s, p and d).

6.29 Antisite: N_B^{-2}

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Table 52: N_B^{-2}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
Up	1	433	108, 123, 150, 176, 203	0.138, 0.116, 0.113, 0.116, 0.116	*Defect*, Y, Y, Y, Y
Down	1	433	108, 123, 150, 176, 203	0.138, 0.116, 0.113, 0.116, 0.116	*Defect*, Y, Y, Y, Y

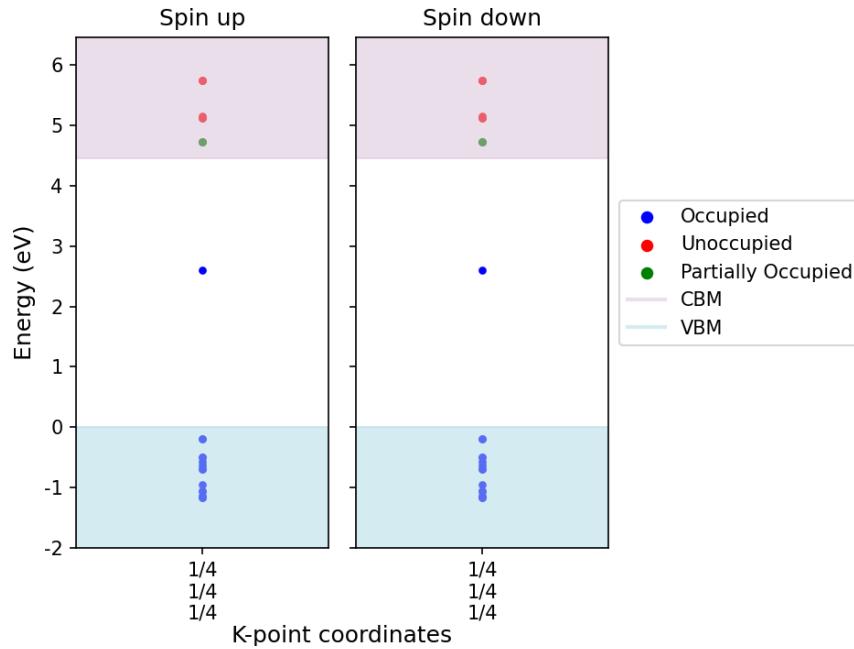


Figure 66: Kohn-Sham states.

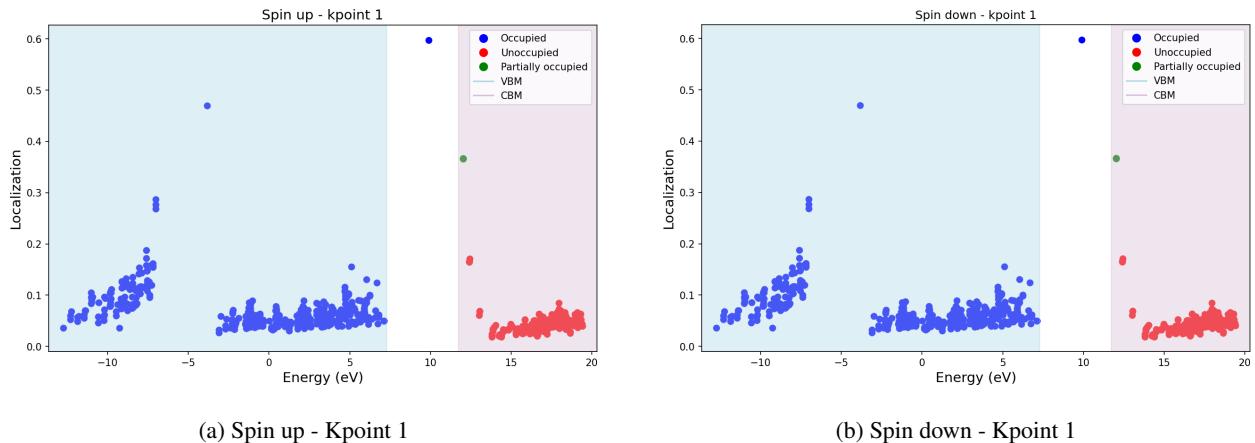


Figure 67: Localization factor using projected orbitals (s, p and d).

6.30 Antisite: N_B^{-3}

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Table 53: N_B^{-3}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
Up	1	433	108, 123, 150, 176, 203	0.137, 0.115, 0.113, 0.115, 0.115	*Defect*, Y, Y, Y, Y
Down	1	433	108, 123, 150, 176, 203	0.137, 0.115, 0.113, 0.115, 0.115	*Defect*, Y, Y, Y, Y

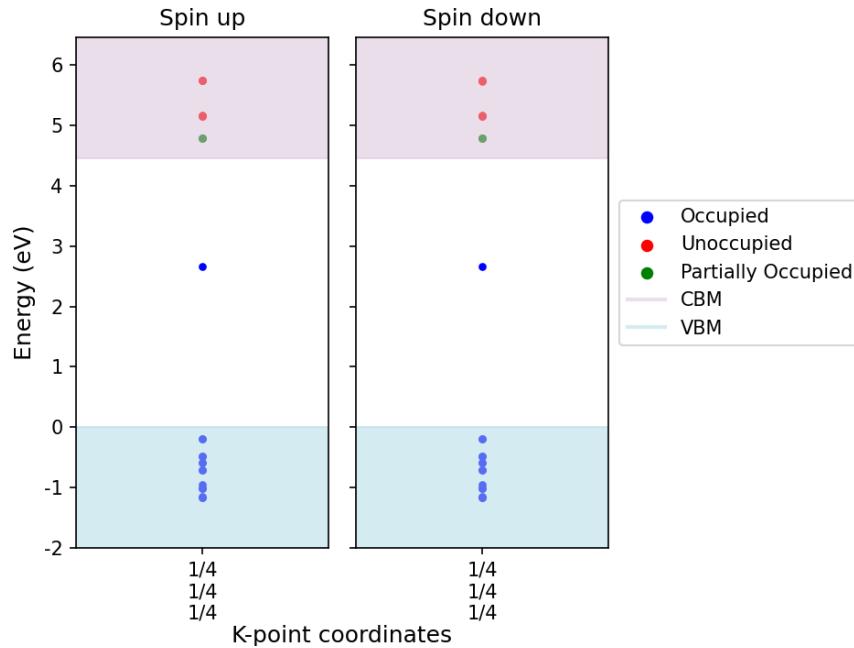


Figure 68: Kohn-Sham states.

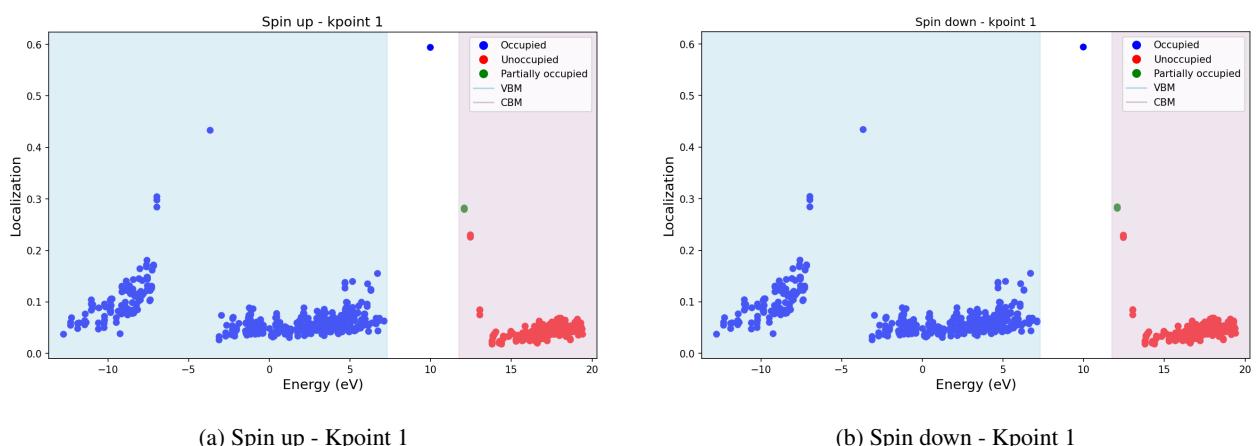


Figure 69: Localization factor using projected orbitals (s, p and d).

6.31 Antisite: N_B^{-4}

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Table 54: N_B^{-4}

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
Up	1	433	108, 123, 150, 176, 203	0.136, 0.115, 0.113, 0.115, 0.115	*Defect*, Y, Y, Y, Y
Down	1	433	108, 123, 150, 176, 203	0.136, 0.115, 0.113, 0.115, 0.115	*Defect*, Y, Y, Y, Y

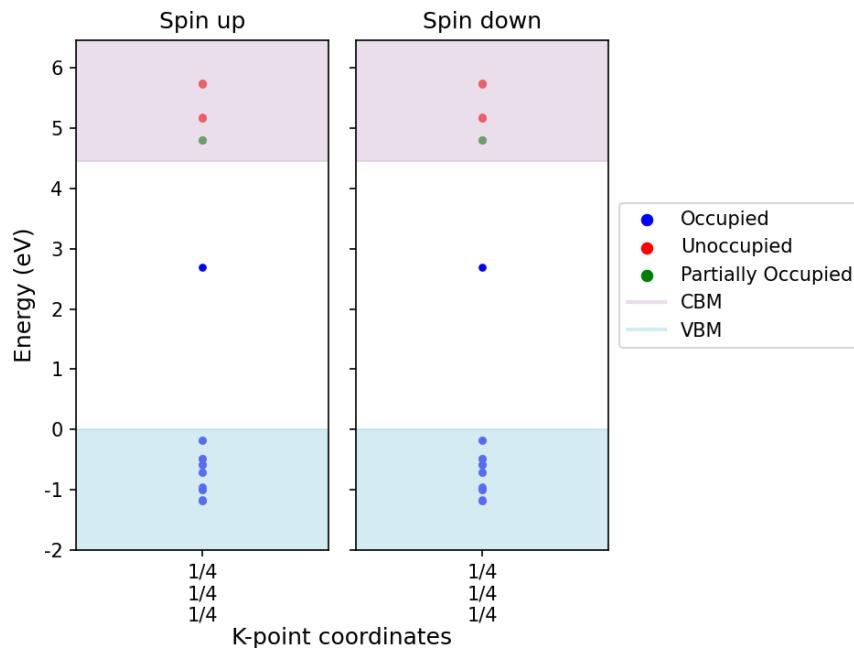


Figure 70: Kohn-Sham states.

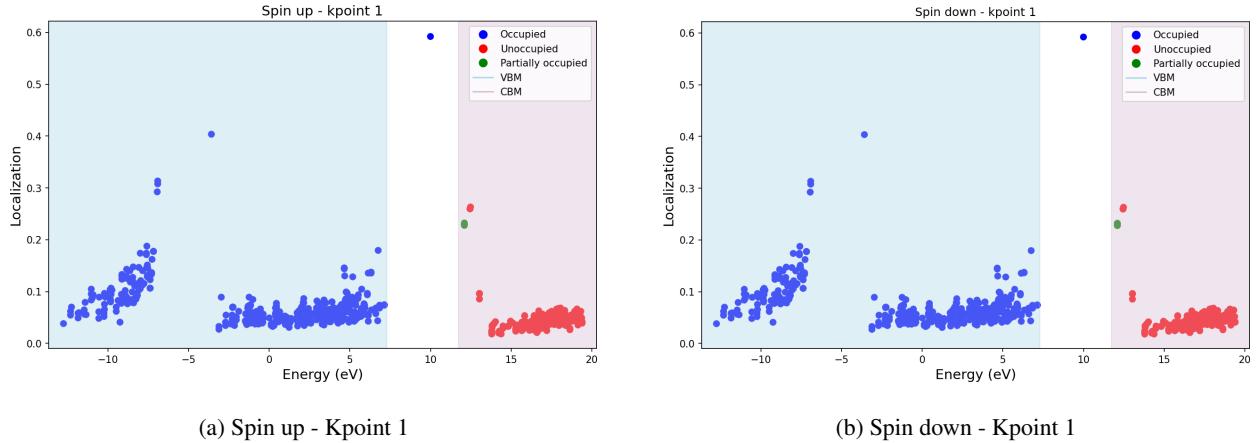


Figure 71: Localization factor using projected orbitals (s, p and d).

6.32 Complex: $(V_B - C_B)^0$

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Table 55: $(V_B - C_B)^0$

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
Up	1	431	121, 174	0.202, 0.111	Y, Y
	1	432	201	0.341	Y
	2	430	148, 174	0.145, 0.145	Y, Y
	2	431	121	0.233	Y
	2	432	201	0.368	Y
	3	431	148, 174	0.145, 0.145	Y, Y
	3	432	201	0.339	Y
Down	1	430	201	0.289	Y
	1	431	148, 174	0.278, 0.157	Y, Y
	1	432	121, 174	0.272, 0.154	Y, Y
	2	430	201	0.308	Y
	2	431	148, 174	0.224, 0.224	Y, Y
	2	432	121	0.290	Y
	3	430	201	0.281	Y
	3	431	148, 174	0.224, 0.224	Y, Y
	3	432	121	0.277	Y

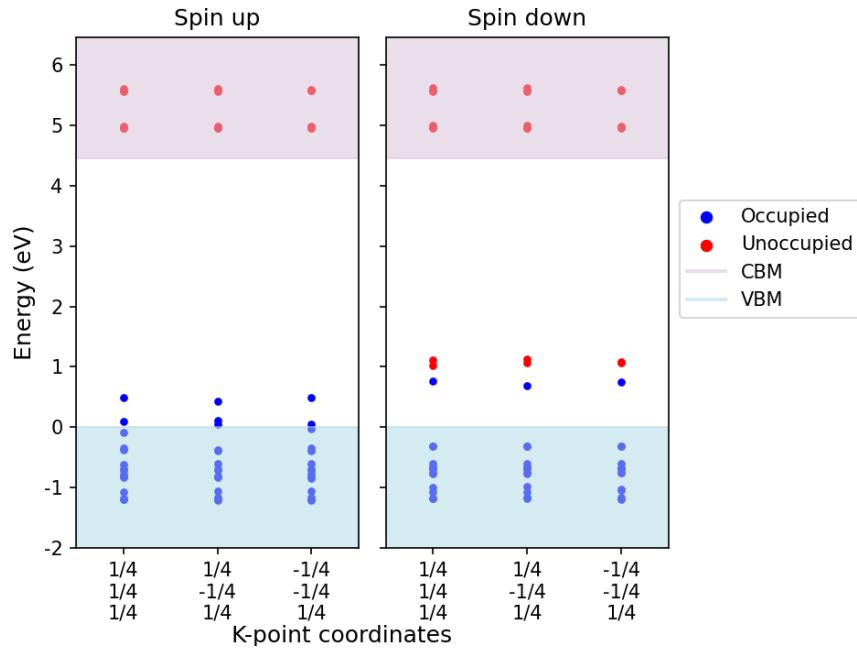


Figure 72: Kohn-Sham states.

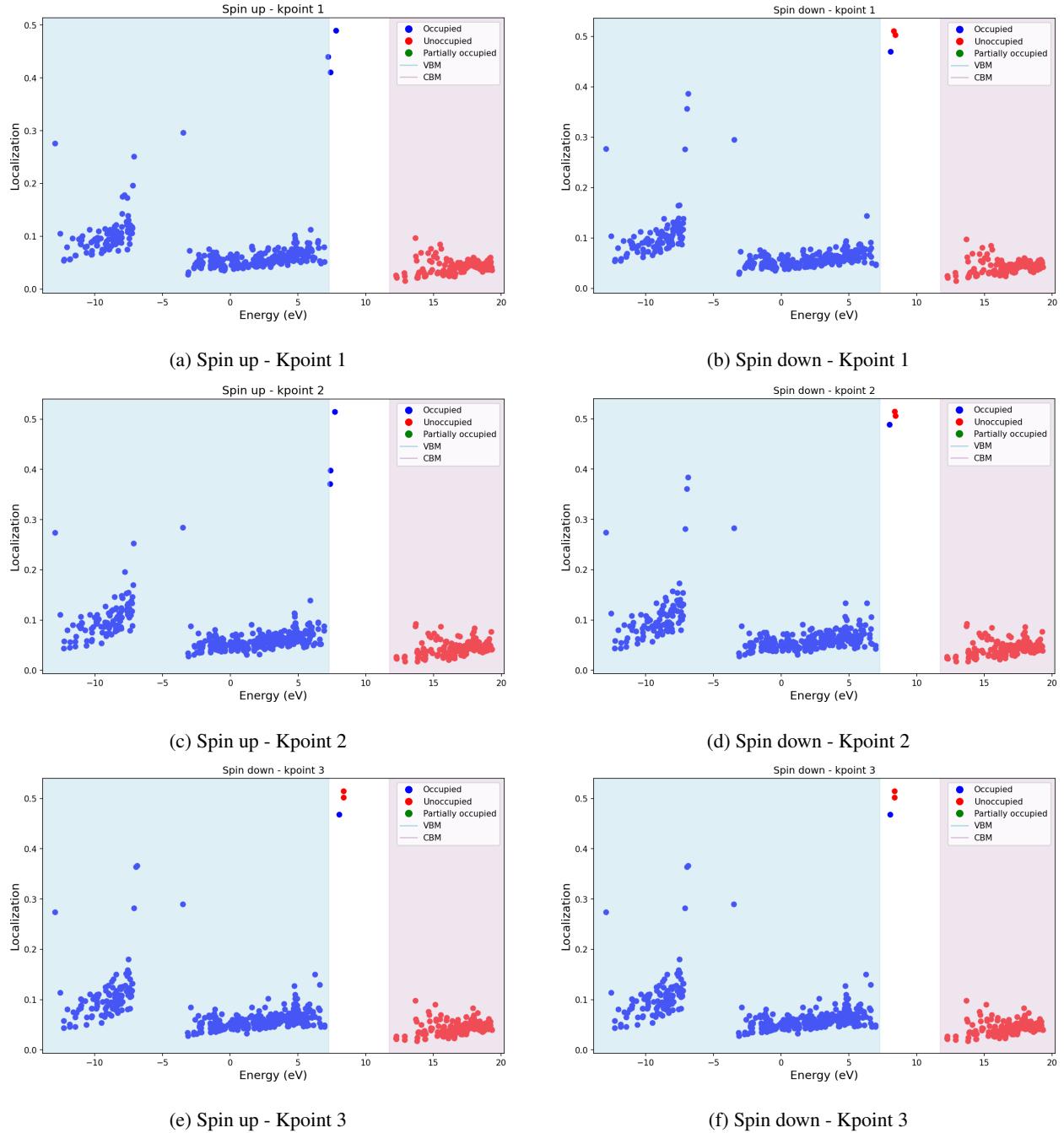


Figure 73: Localization factor using projected orbitals (s, p, and d).

6.33 Complex: $(V_B - C_B)^{+1}$

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Table 56: $(V_B - C_B)^{+1}$

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
	1	430	201	0.243	Y
	1	431	148, 174	0.280, 0.142	Y, Y
	1	432	121, 174	0.268, 0.157	Y, Y
	2	430	201	0.268	Y
Down	2	431	148, 174	0.218, 0.218	Y, Y
	2	432	121	0.292	Y
	3	430	201	0.239	Y
	3	431	121	0.291	Y
	3	432	148, 174	0.219, 0.218	Y, Y

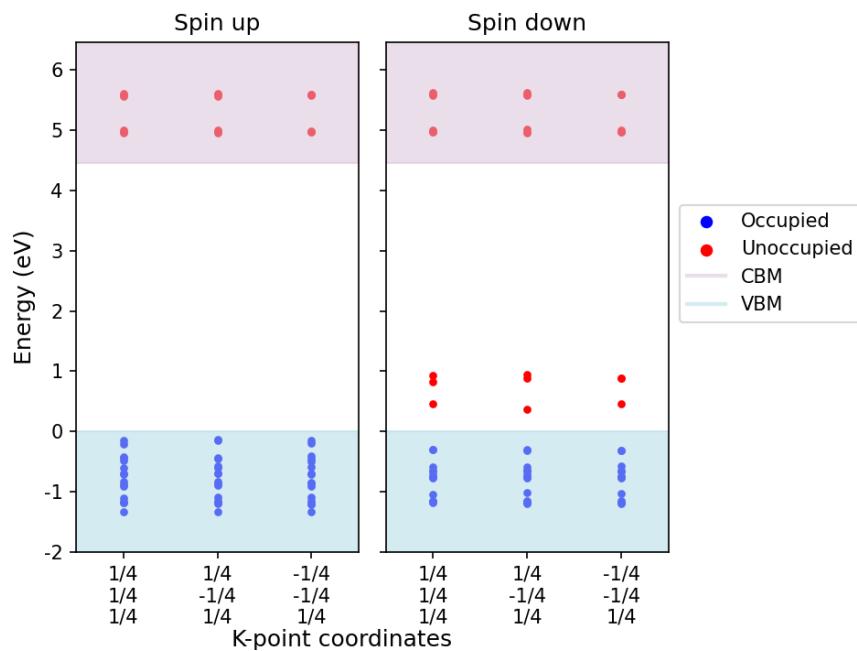


Figure 74: Kohn-Sham states.

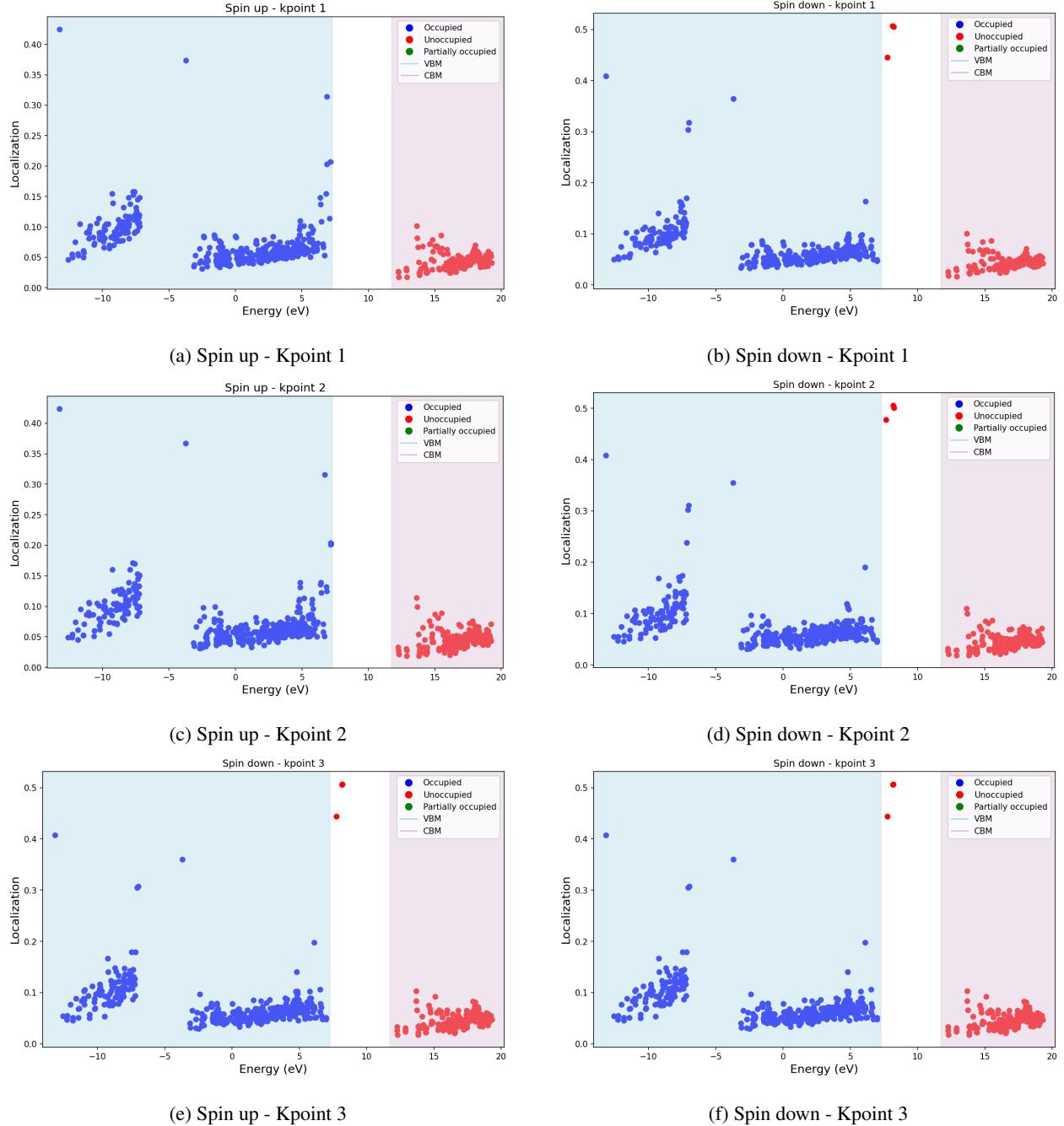


Figure 75: Localization factor using projected orbitals (s, p, and d).

6.34 Complex: $(V_B - C_B)^{+2}$

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Table 57: $(V_B - C_B)^{+2}$

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
	1	430	201	0.242	Y
	1	431	148, 174	0.274, 0.133	Y, Y
	1	432	121, 174	0.252, 0.161	Y, Y
	2	430	201	0.284	Y
Down	2	431	148, 174	0.211, 0.211	Y, Y
	2	432	121	0.280	Y
	3	430	201	0.243	Y
	3	431	121	0.274	Y
	3	432	148, 174	0.211, 0.211	Y, Y

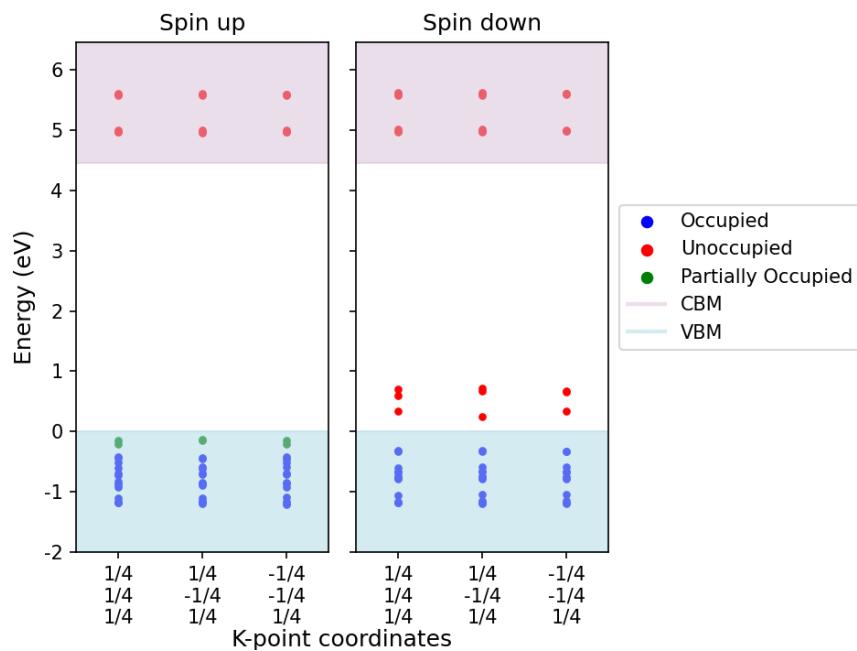


Figure 76: Kohn-Sham states.

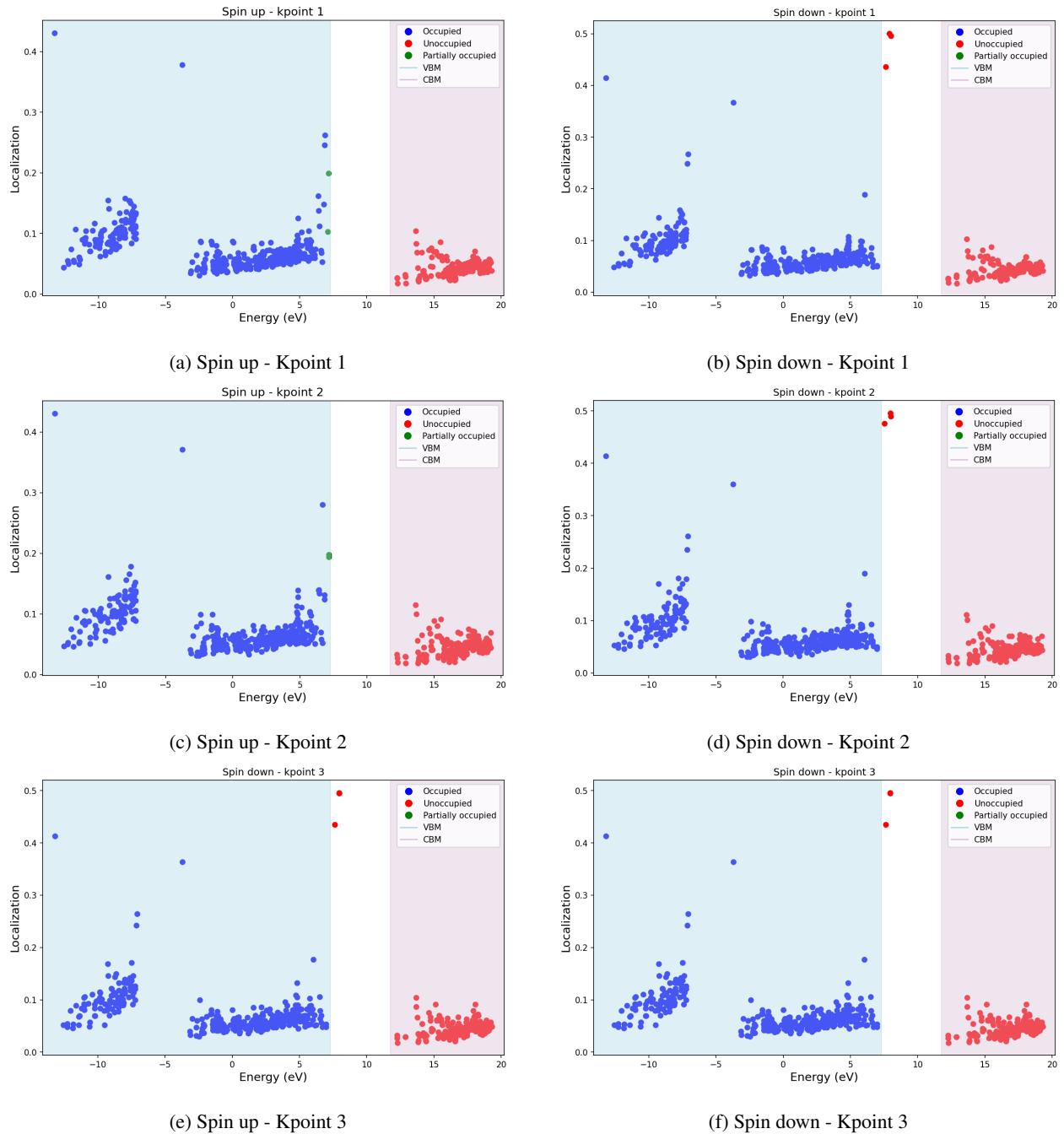


Figure 77: Localization factor using projected orbitals (s, p, and d).

6.35 Complex: $(V_B - C_B)^{-1}$

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Table 58: $(V_B - C_B)^{-1}$

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
Up	1	430	121, 201	0.240, 0.180	Y, Y
	1	431	148	0.342	Y
	1	432	174	0.281	Y
	2	430	121, 148	0.167, 0.267	Y, Y
	2	431	121, 148, 174	0.158, 0.109, 0.109	Y, Y, Y
	2	432	148, 174	0.218, 0.218	Y, Y
	3	430	121, 201	0.295, 0.132	Y, Y
	3	431	148, 174, 201	0.106, 0.107, 0.195	Y, Y, Y
	3	432	148, 174	0.218, 0.217	Y, Y
	1	430	201	0.275	Y
Down	1	431	148, 174	0.297, 0.132	Y, Y
	1	432	121, 174	0.257, 0.183	Y, Y
	2	430	201	0.289	Y
	2	431	148, 174	0.227, 0.227	Y, Y
	2	432	121	0.287	Y
	3	430	201	0.269	Y
	3	431	121	0.279	Y
	3	432	148, 174	0.227, 0.226	Y, Y

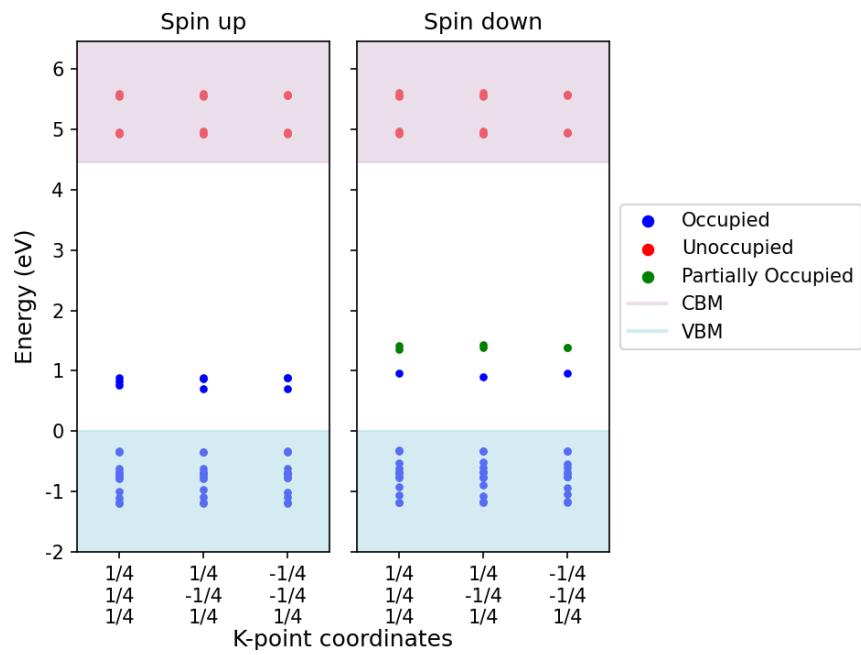


Figure 78: Kohn-Sham states.

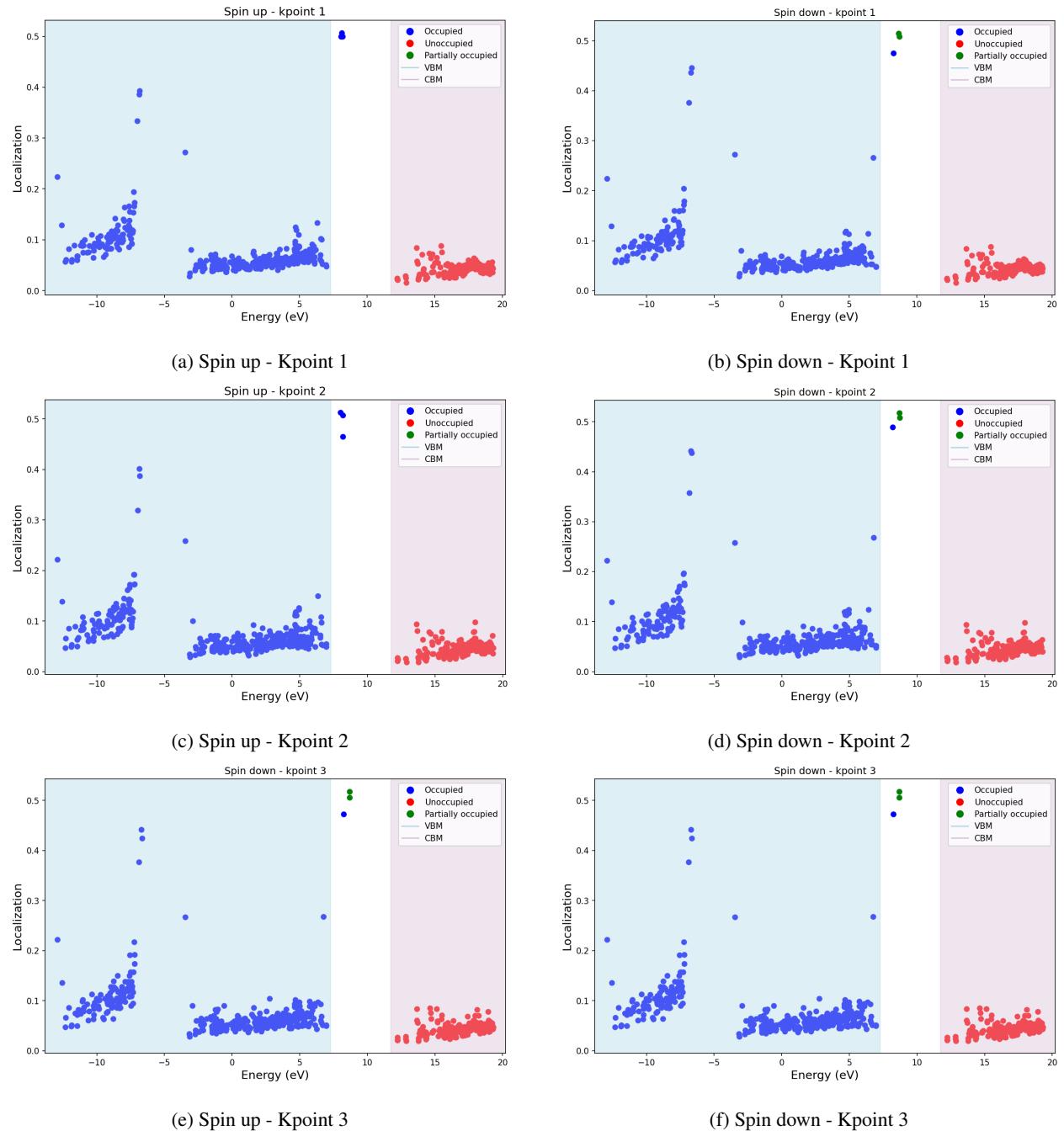


Figure 79: Localization factor using projected orbitals (s, p, and d).

6.36 Complex: $(V_B - C_B)^{-2}$

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Table 59: $(V_B - C_B)^{-2}$

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
Up	1	430	201	0.245	Y
	1	431	148, 174	0.280, 0.158	Y, Y
	1	432	121, 174	0.285, 0.147	Y, Y
	2	430	201	0.256	Y
	2	431	148, 174	0.227, 0.227	Y, Y
	2	432	121	0.301	Y
	3	430	201	0.243	Y
	3	431	148, 174	0.227, 0.227	Y, Y
	3	432	121	0.300	Y
	1	430	201	0.245	Y
Down	1	431	148, 174	0.280, 0.158	Y, Y
	1	432	121, 174	0.285, 0.147	Y, Y
	2	430	201	0.256	Y
	2	431	148, 174	0.227, 0.227	Y, Y
	2	432	121	0.301	Y
	3	430	201	0.243	Y
	3	431	148, 174	0.227, 0.227	Y, Y
	3	432	121	0.300	Y

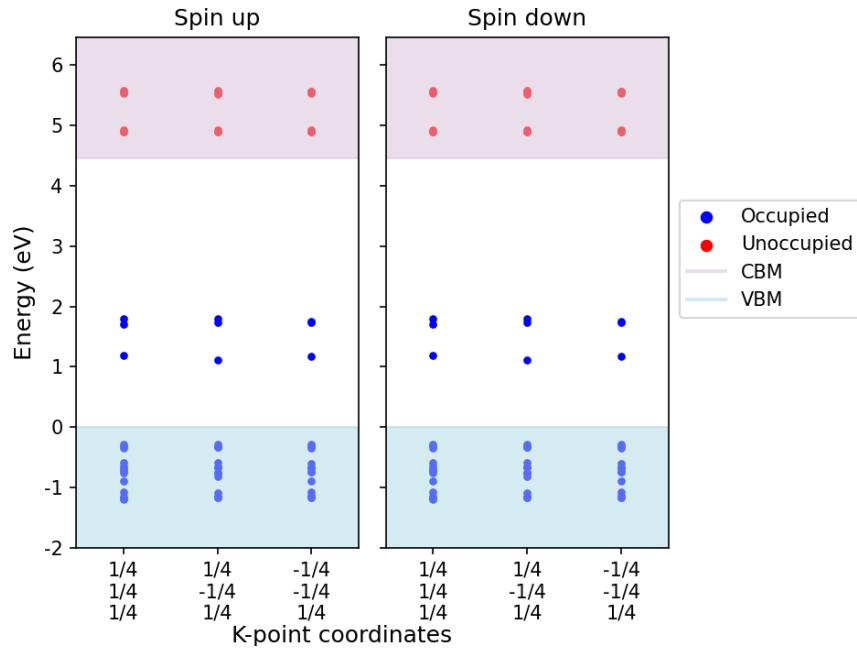


Figure 80: Kohn-Sham states.

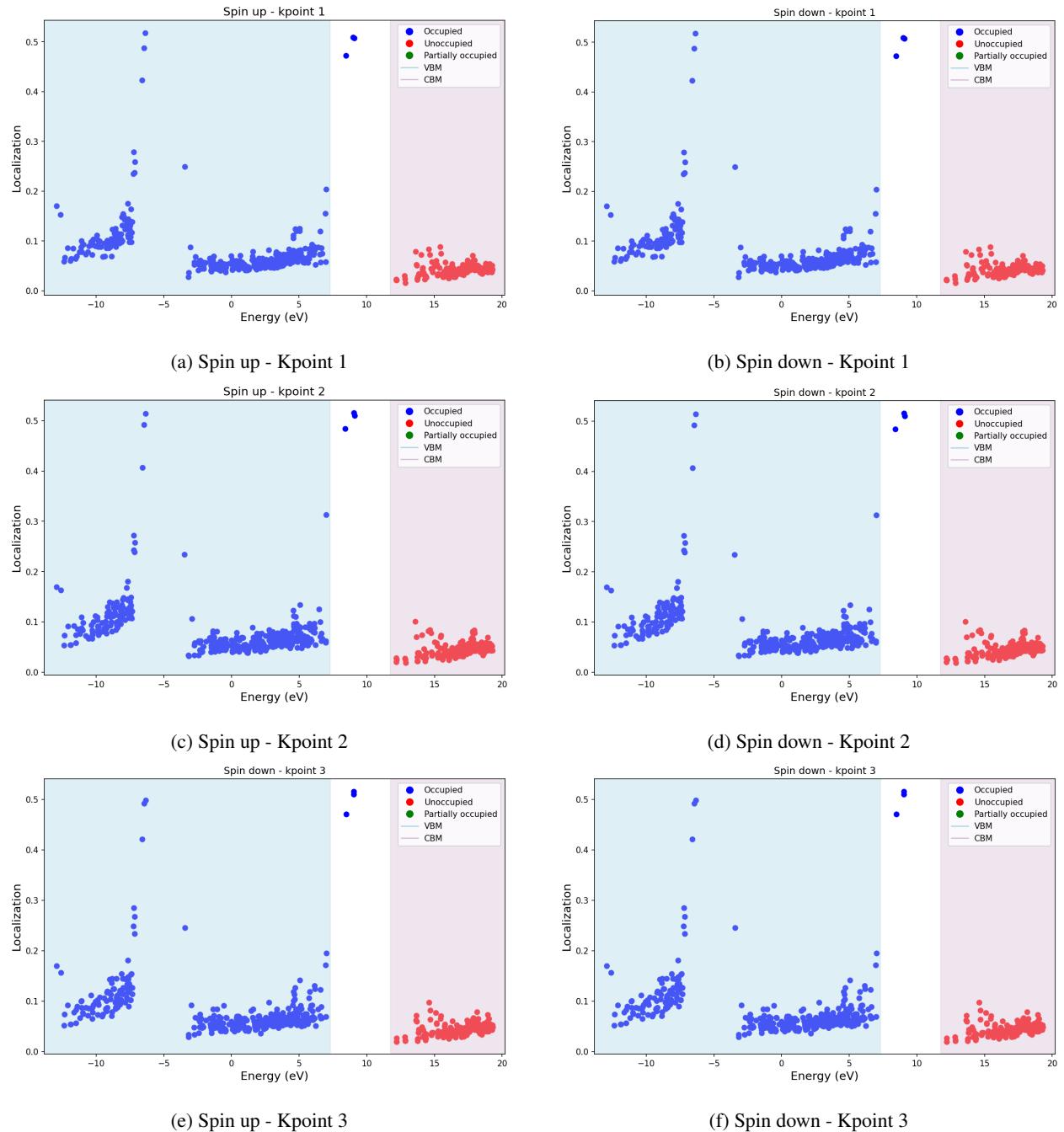


Figure 81: Localization factor using projected orbitals (s, p, and d).

6.37 Complex: $(V_B - C_B)^{-3}$

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Table 60: $(V_B - C_B)^{-3}$

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
Up	1	430	201	0.247	Y
	1	431	148, 174	0.282, 0.155	Y, Y
	1	432	121, 174	0.282, 0.152	Y, Y
	2	430	201	0.258	Y
	2	431	148, 174	0.227, 0.227	Y, Y
	2	432	121	0.300	Y
	3	430	201	0.245	Y
	3	431	148, 174	0.226, 0.227	Y, Y
	3	432	121	0.299	Y
Down	1	430	201	0.247	Y
	1	431	148, 174	0.282, 0.155	Y, Y
	1	432	121, 174	0.282, 0.152	Y, Y
	2	430	201	0.258	Y
	2	431	148, 174	0.227, 0.227	Y, Y
	2	432	121	0.289	Y
	3	430	201	0.245	Y
	3	431	148, 174	0.226, 0.227	Y, Y
	3	432	121	0.299	Y

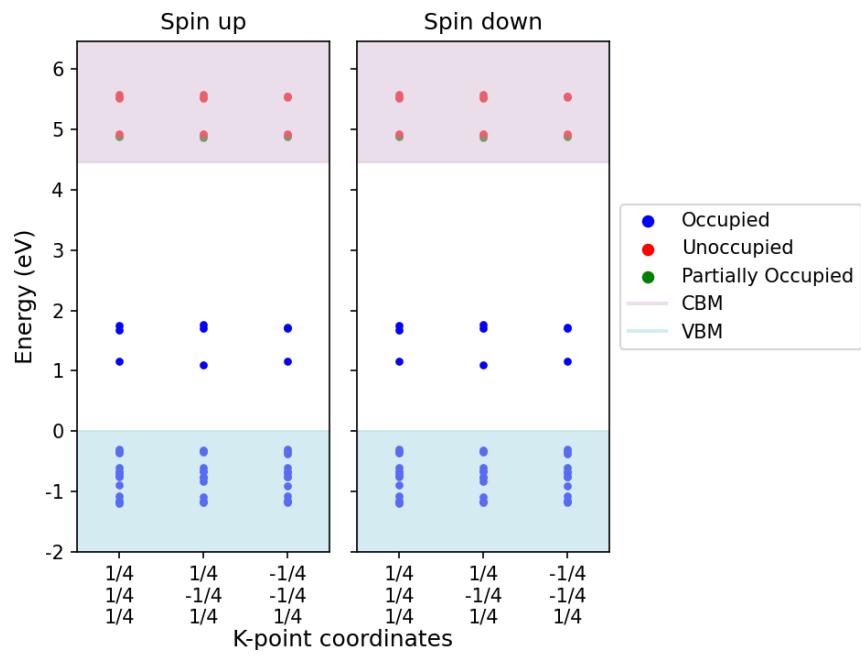


Figure 82: Kohn-Sham states.

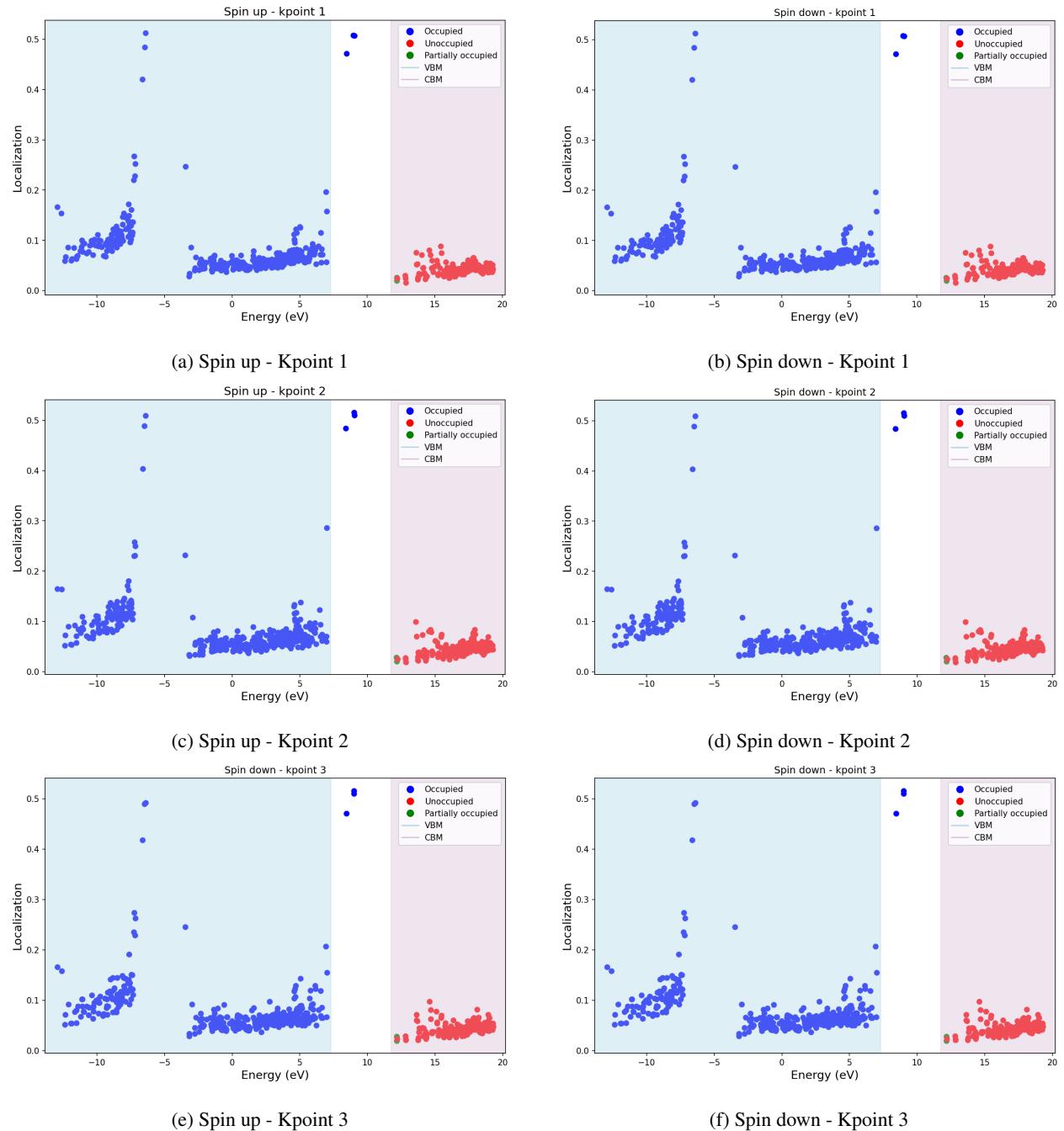


Figure 83: Localization factor using projected orbitals (s, p, and d).

6.38 Complex: $(V_N - C_N)^0$

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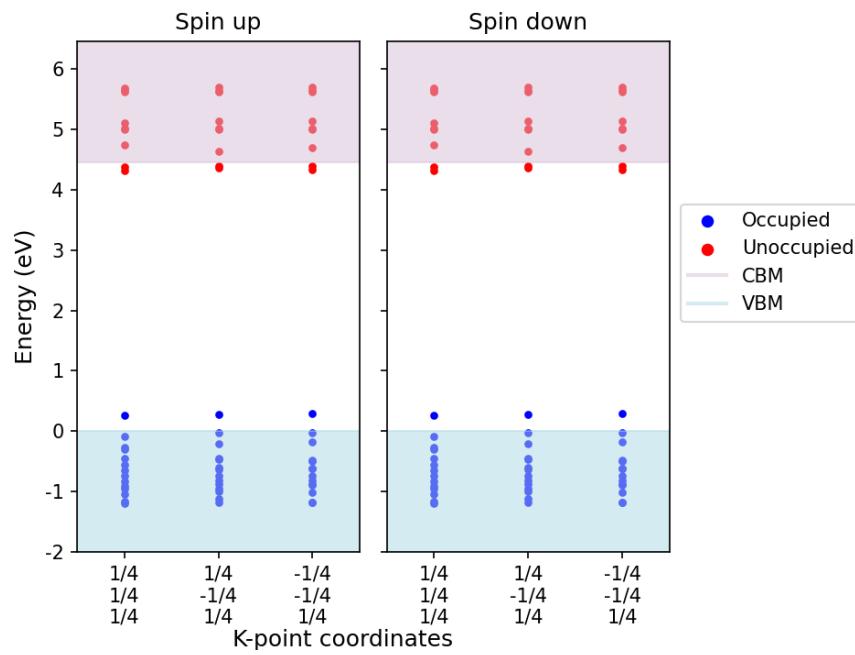


Figure 84: Kohn-Sham states.

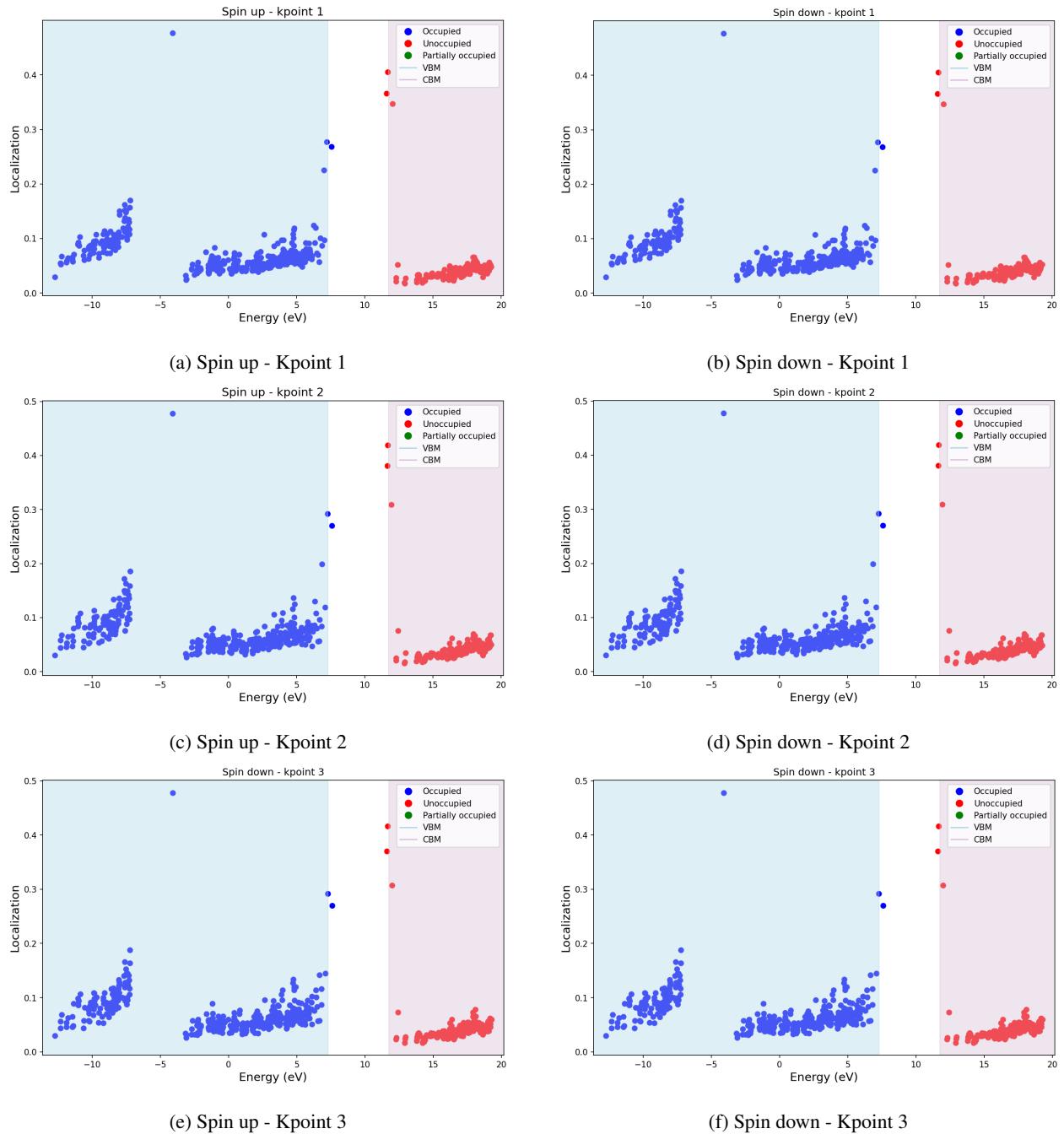


Figure 85: Localization factor using projected orbitals (s, p, and d).

6.39 Complex: $(V_N - C_N)^{+1}$

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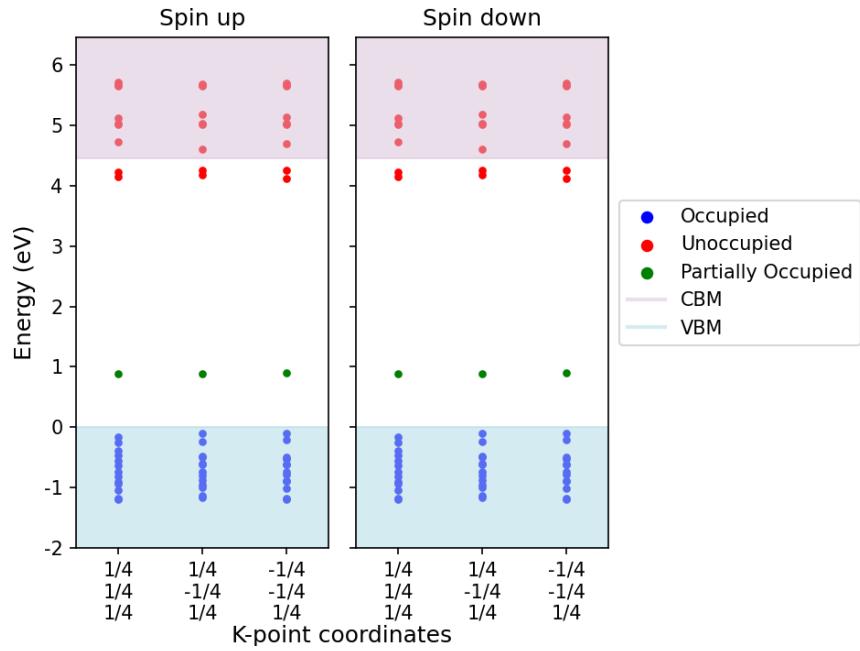


Figure 86: Kohn-Sham states.

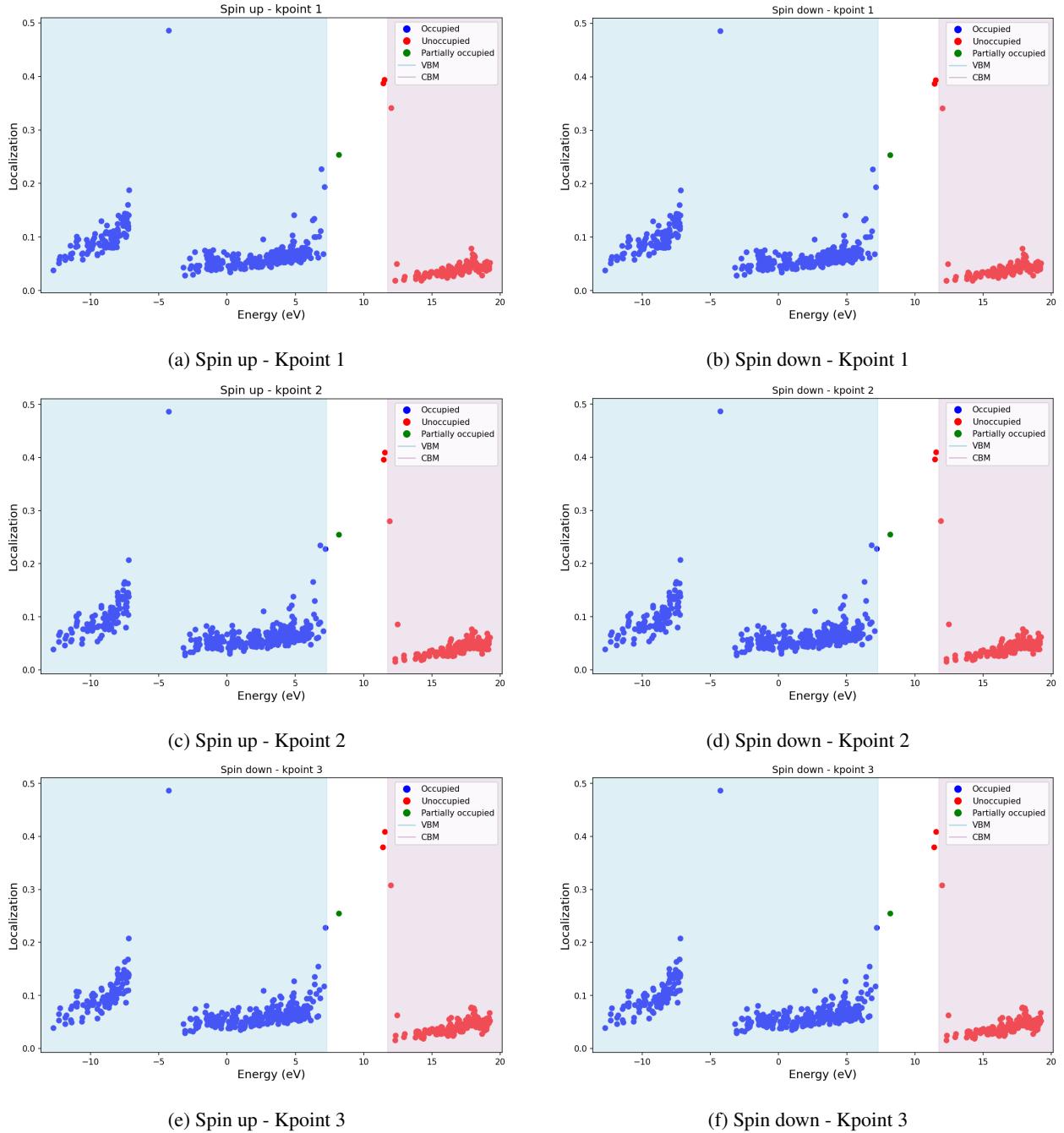


Figure 87: Localization factor using projected orbitals (s, p, and d).

6.40 Complex: $(V_N - C_N)^{+2}$

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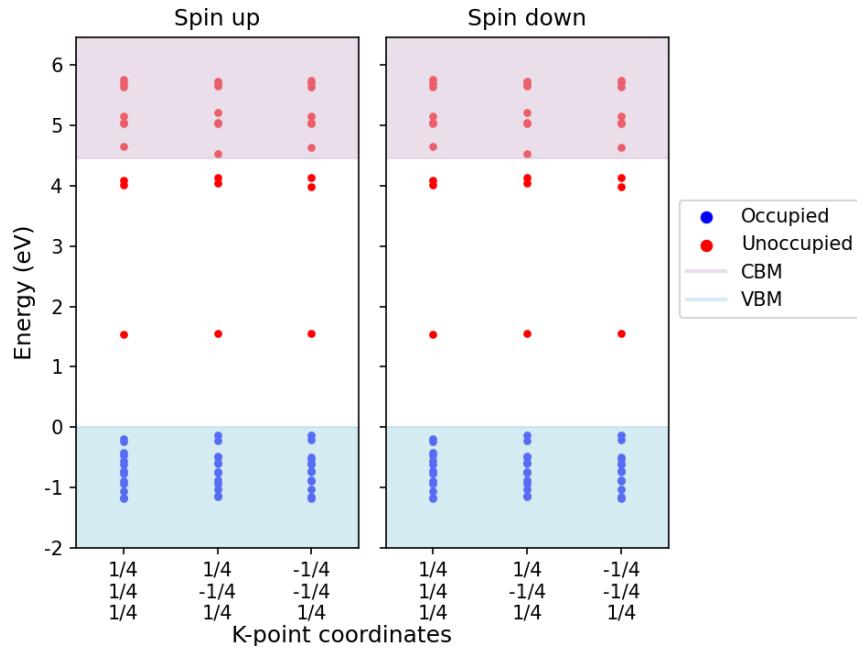


Figure 88: Kohn-Sham states.

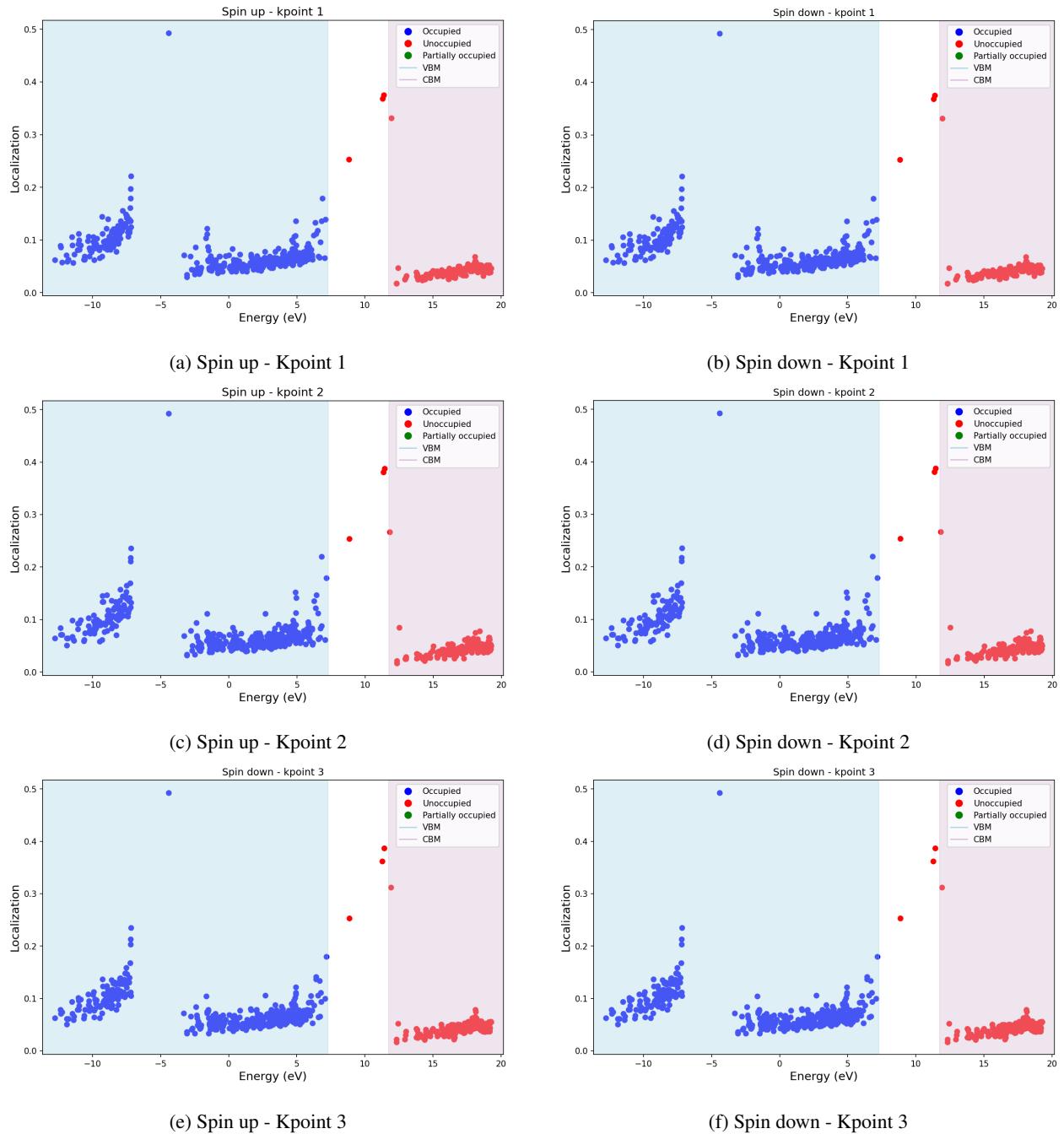


Figure 89: Localization factor using projected orbitals (s, p, and d).

6.41 Complex: $(V_N - C_N)^{+3}$

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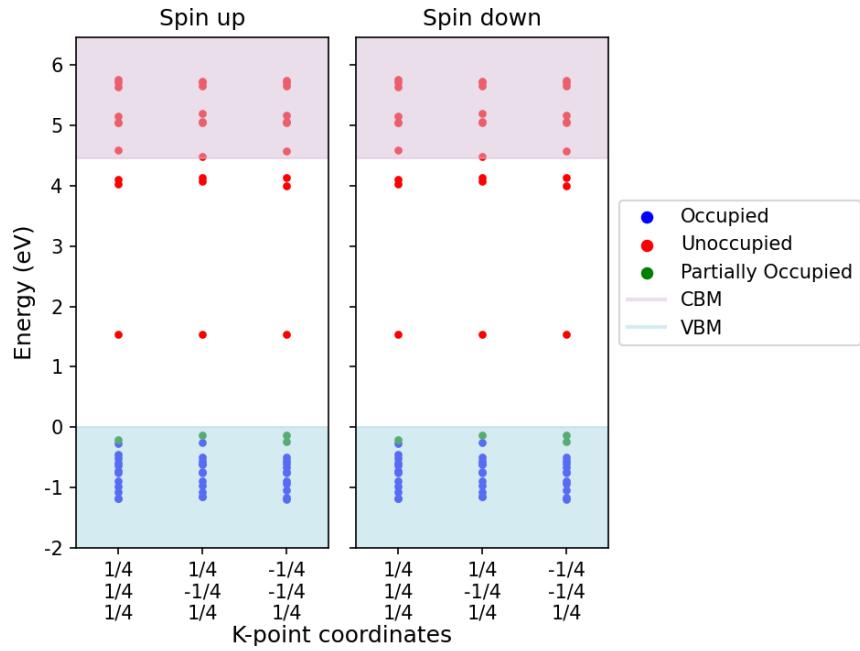


Figure 90: Kohn-Sham states.

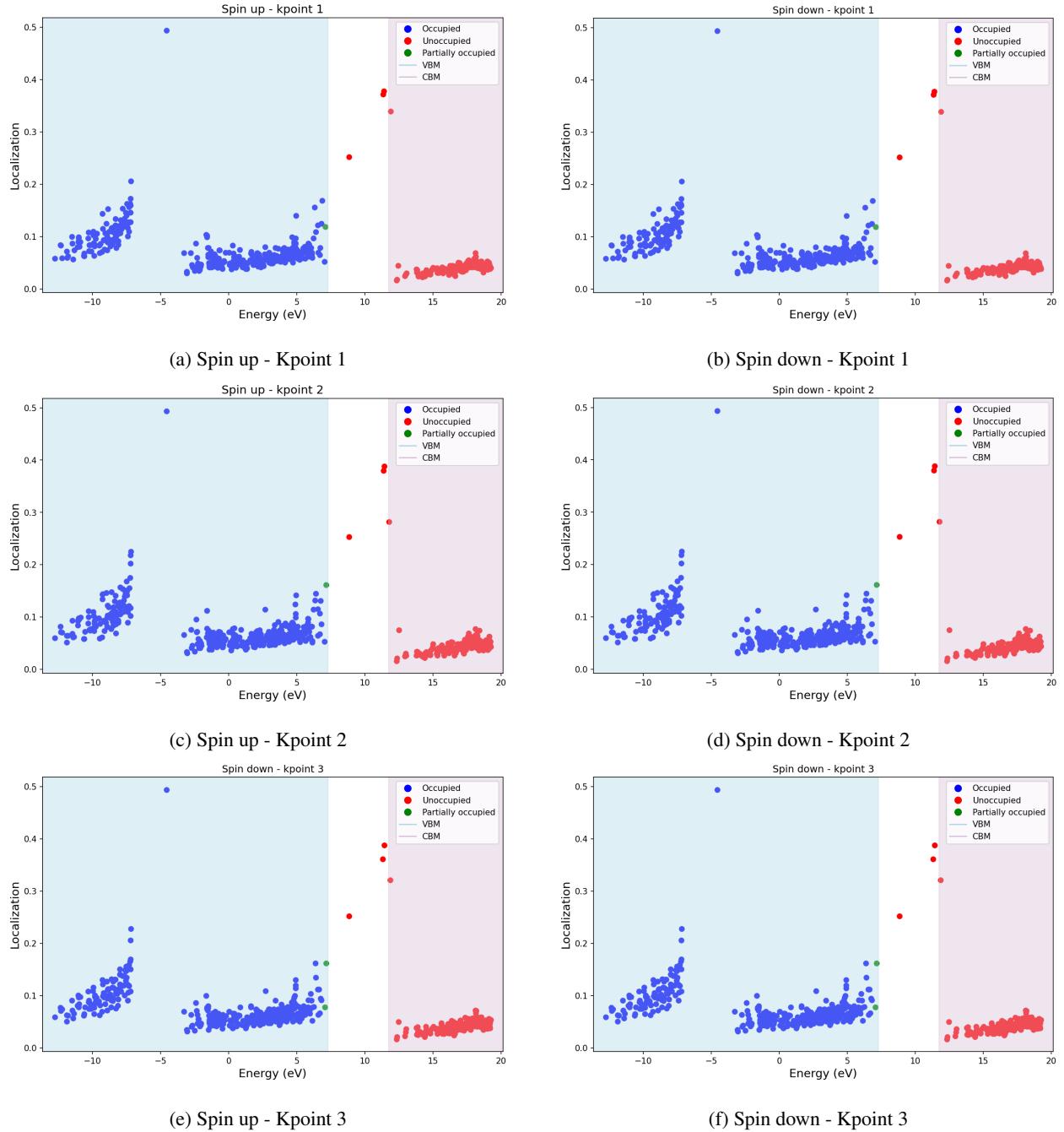


Figure 91: Localization factor using projected orbitals (s, p, and d).

6.42 Complex: $(V_N - C_N)^{+4}$

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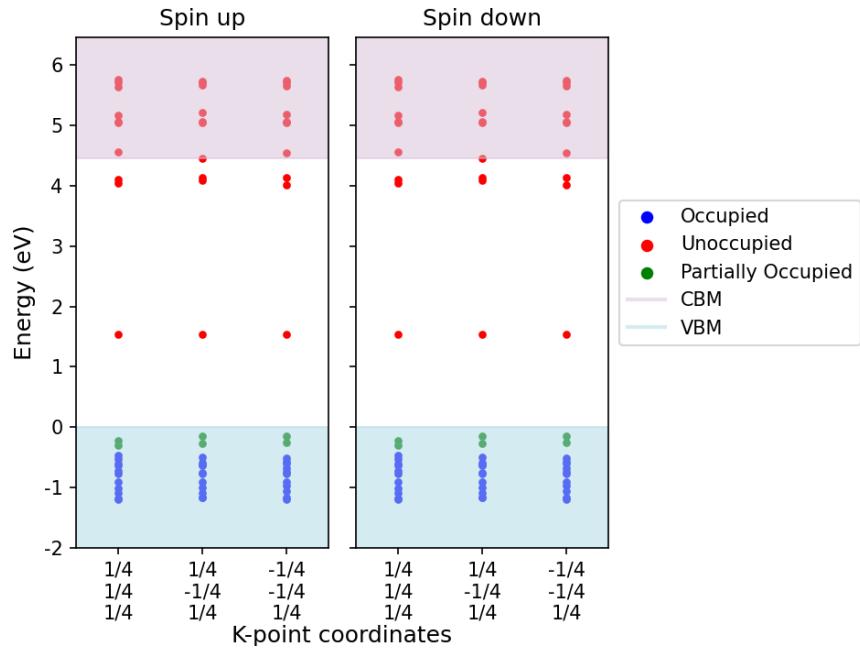


Figure 92: Kohn-Sham states.

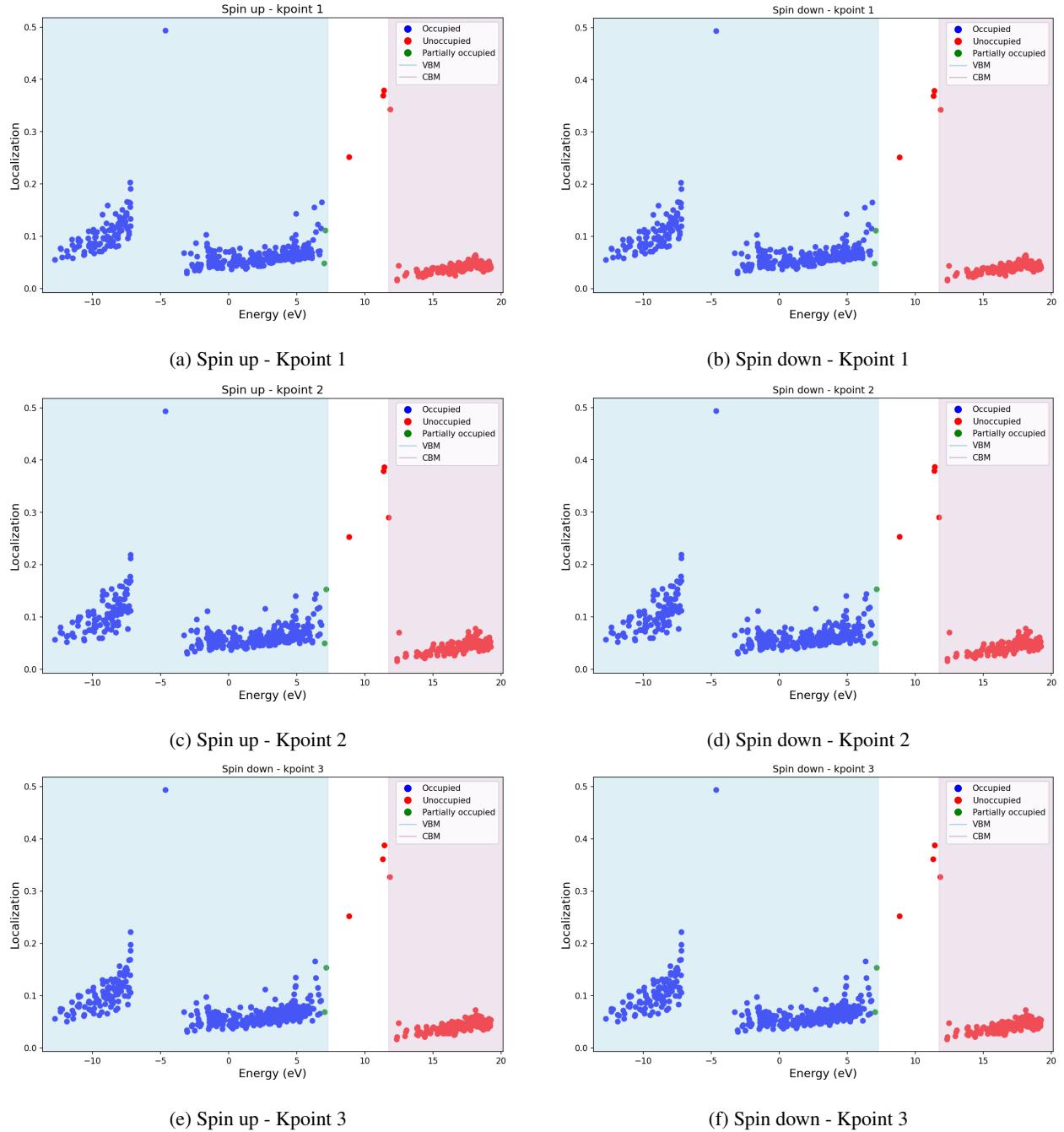


Figure 93: Localization factor using projected orbitals (s, p, and d).

6.43 Complex: $(V_N - C_N)^{-1}$

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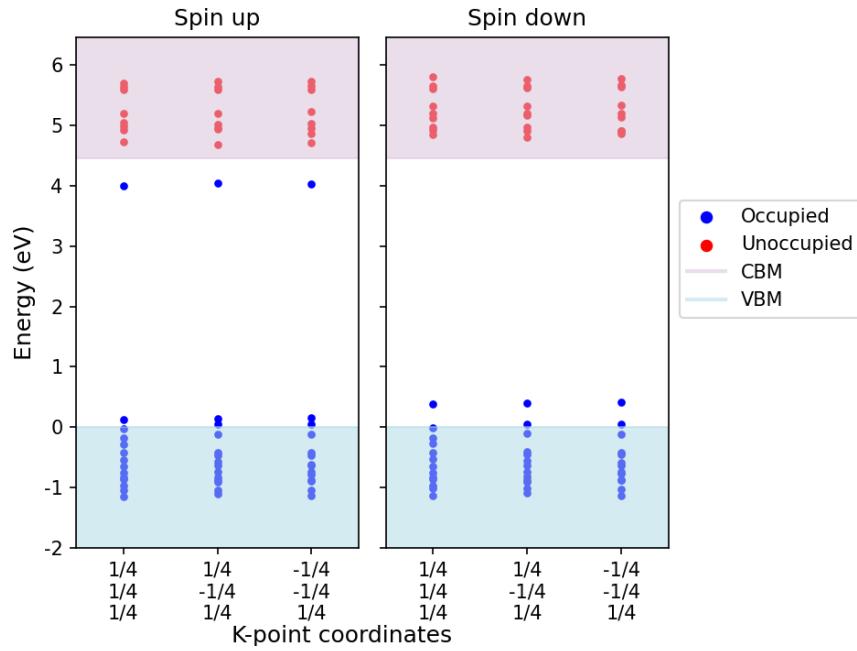


Figure 94: Kohn-Sham states.

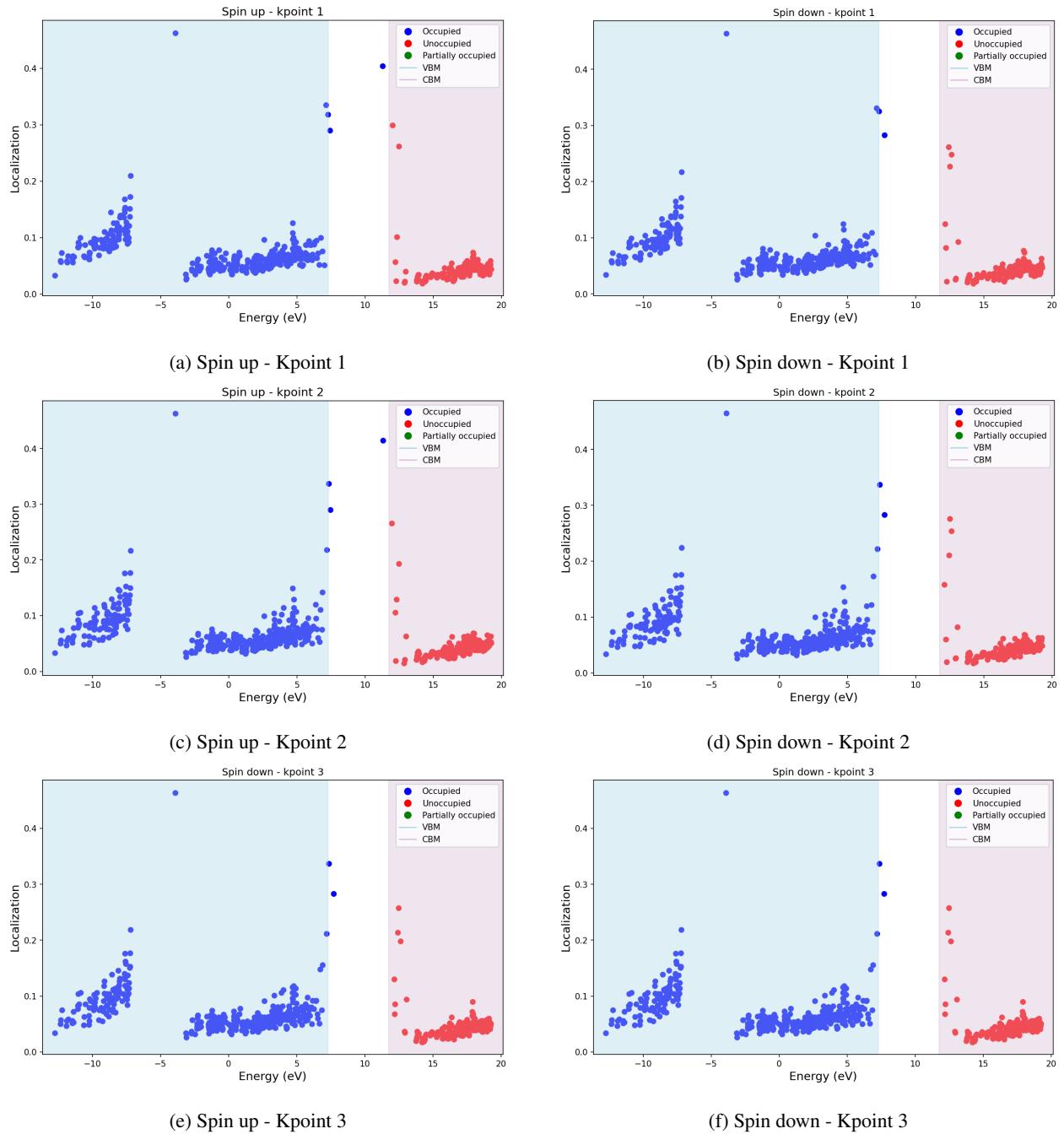


Figure 95: Localization factor using projected orbitals (s, p, and d).

6.44 Complex: $(V_N - C_N)^{-2}$

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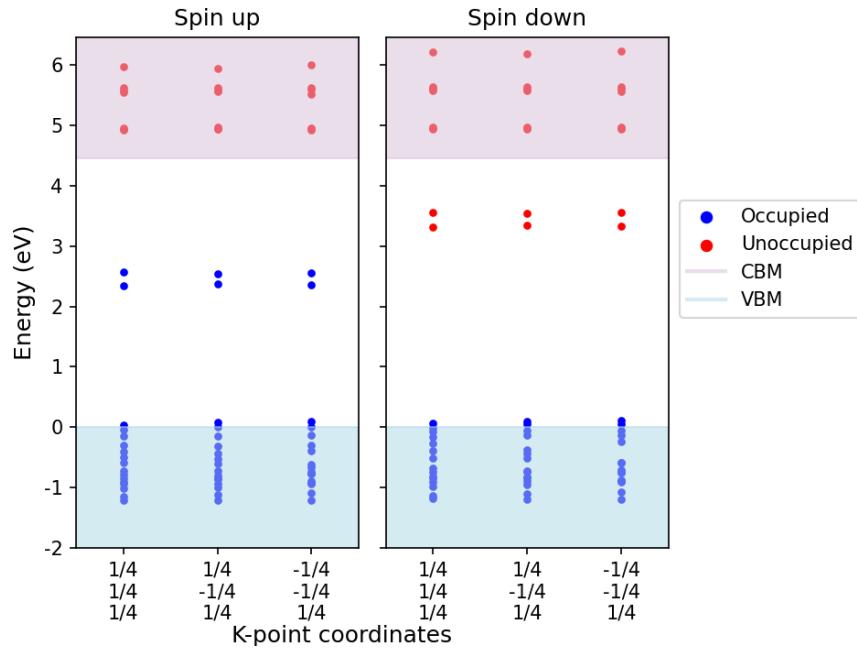


Figure 96: Kohn-Sham states.

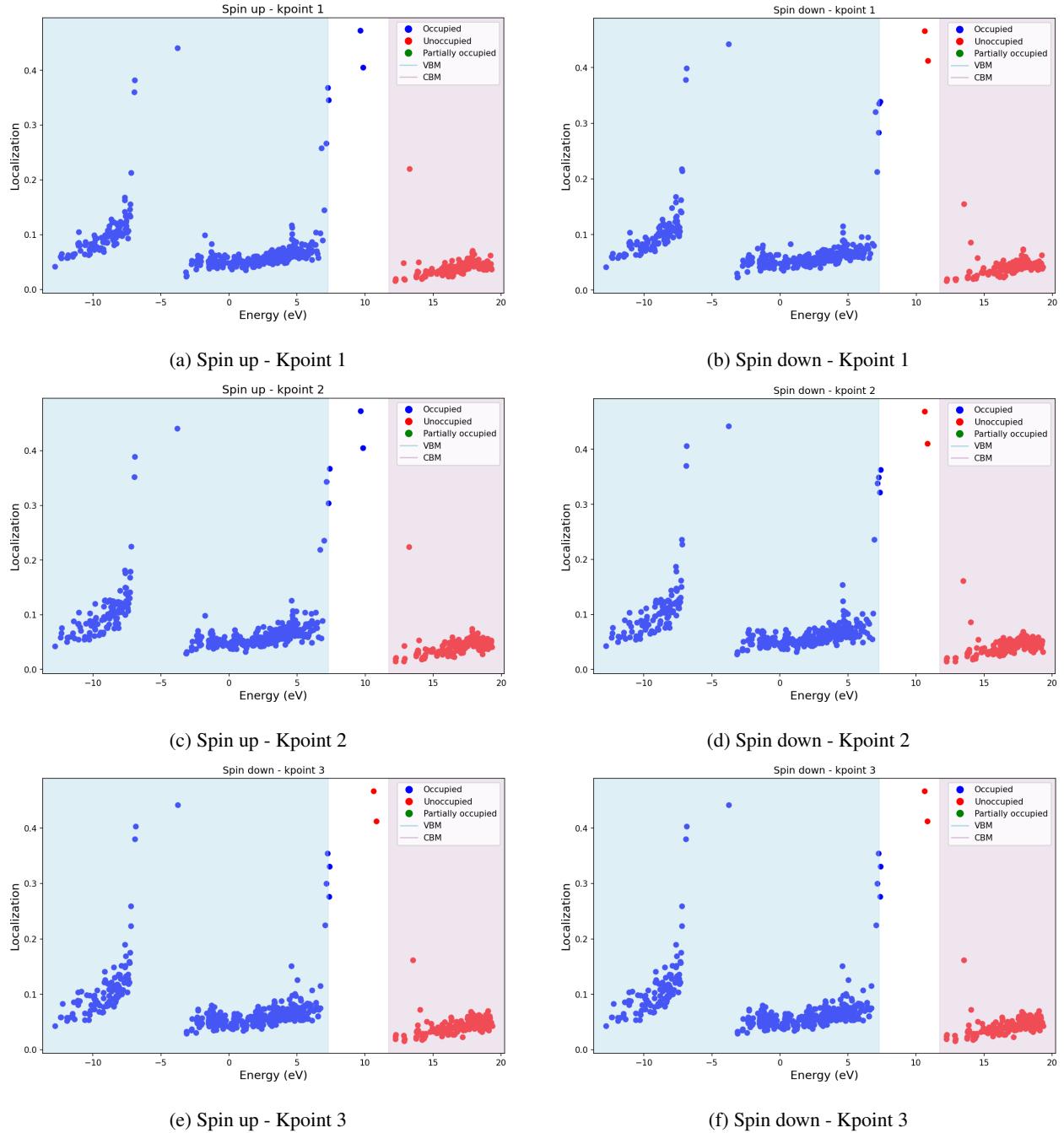


Figure 97: Localization factor using projected orbitals (s, p, and d).

6.45 Complex: $(V_N - C_N)^{-3}$

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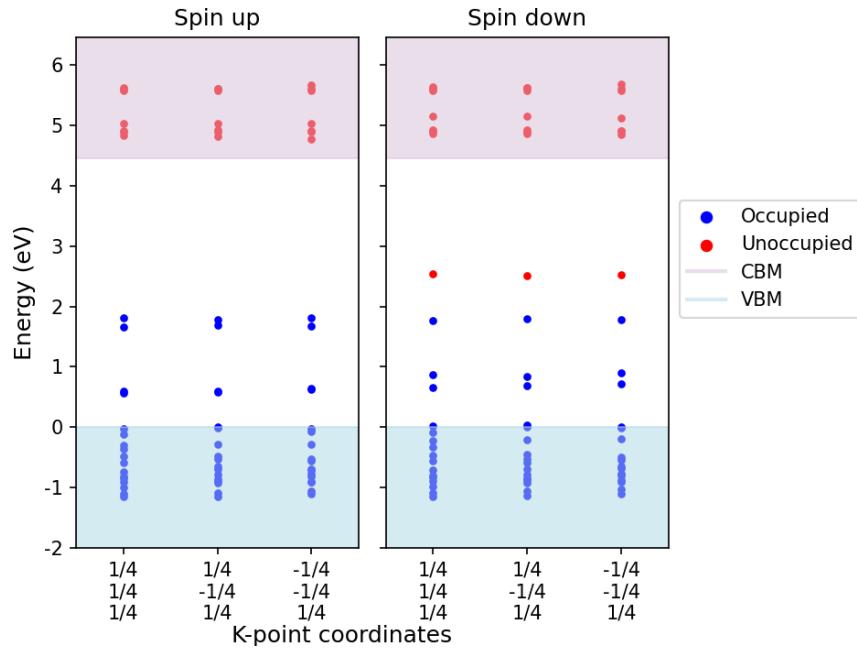


Figure 98: Kohn-Sham states.

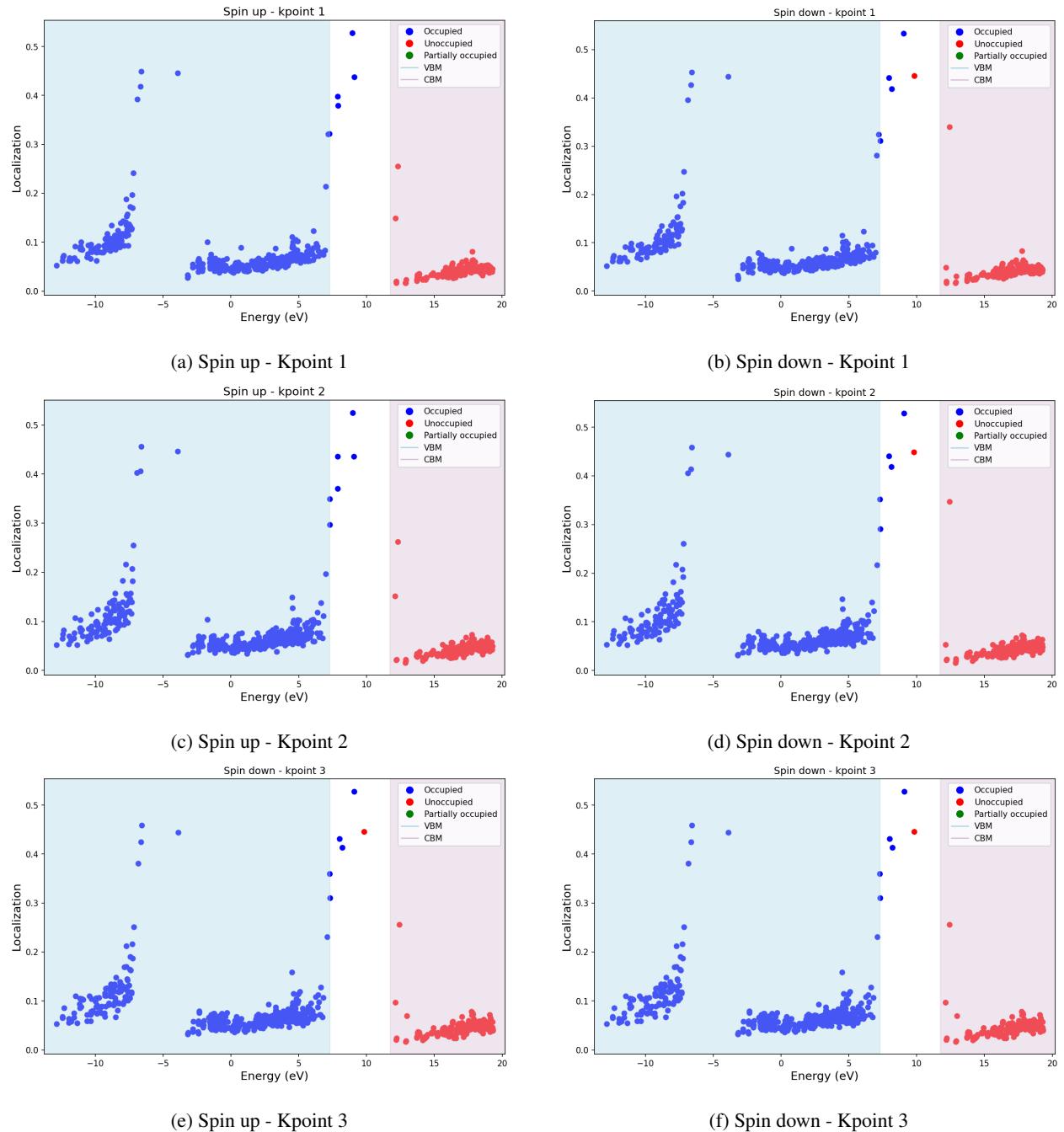


Figure 99: Localization factor using projected orbitals (s, p, and d).

6.46 Complex: $(V_N - C_N)^{-4}$

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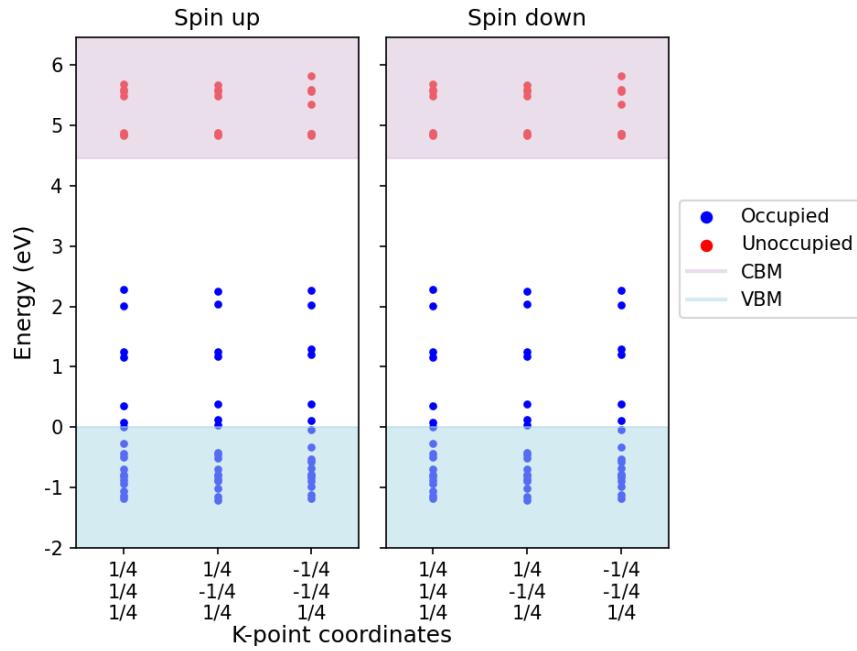


Figure 100: Kohn-Sham states.

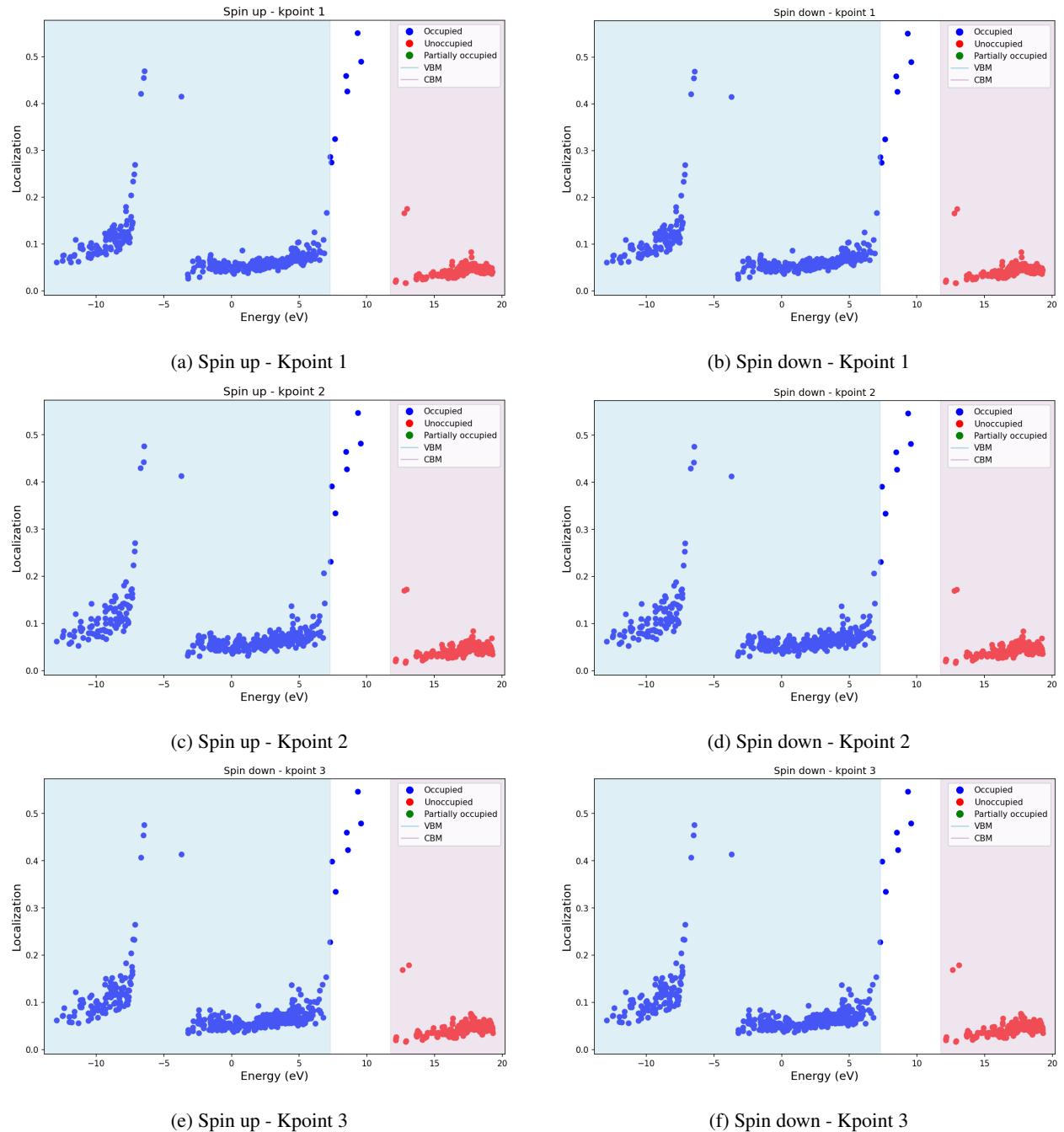


Figure 101: Localization factor using projected orbitals (s, p, and d).

6.47 Complex: $(B_N - V_B)^0$

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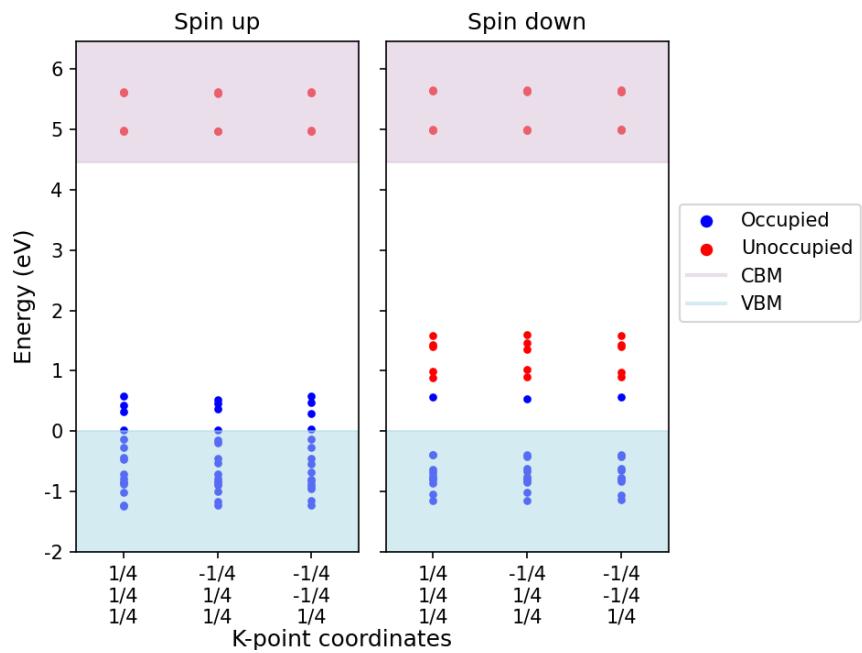


Figure 102: Kohn-Sham states.

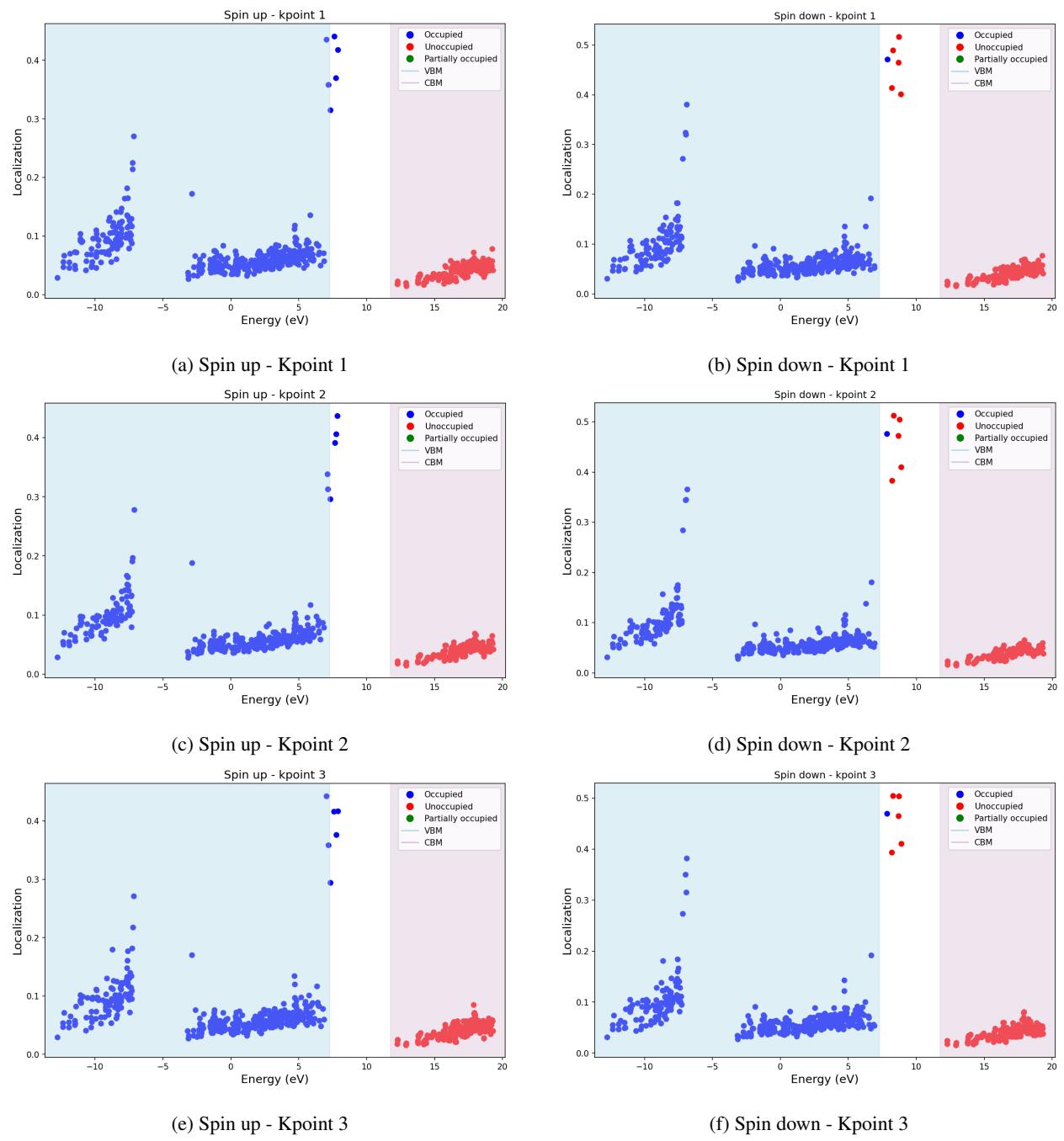


Figure 103: Localization factor using projected orbitals (s, p, and d).

6.48 Complex: $(B_N - V_B)^{+1}$

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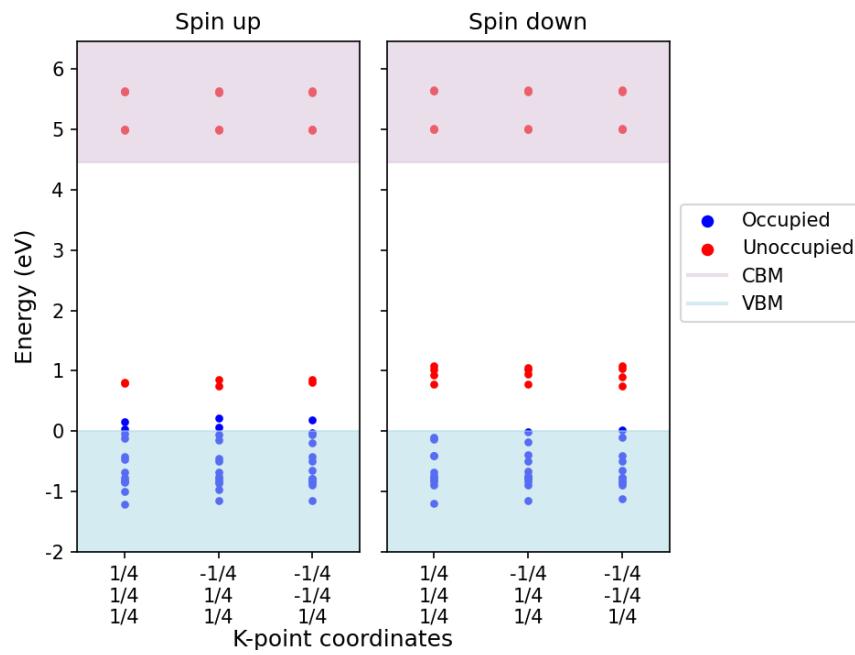


Figure 104: Kohn-Sham states.

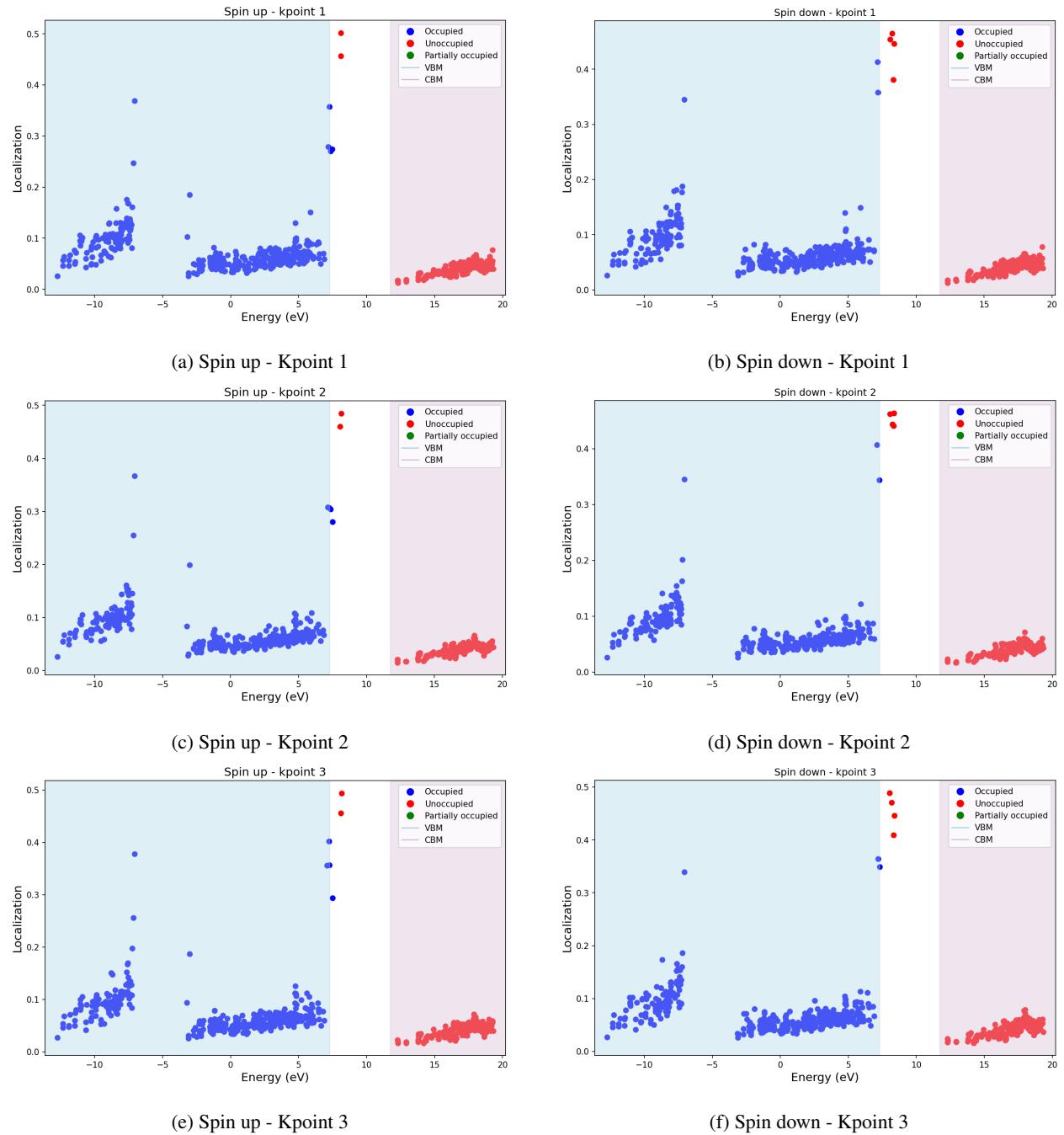


Figure 105: Localization factor using projected orbitals (s, p, and d).

6.49 Complex: $(B_N - V_B)^{+2}$

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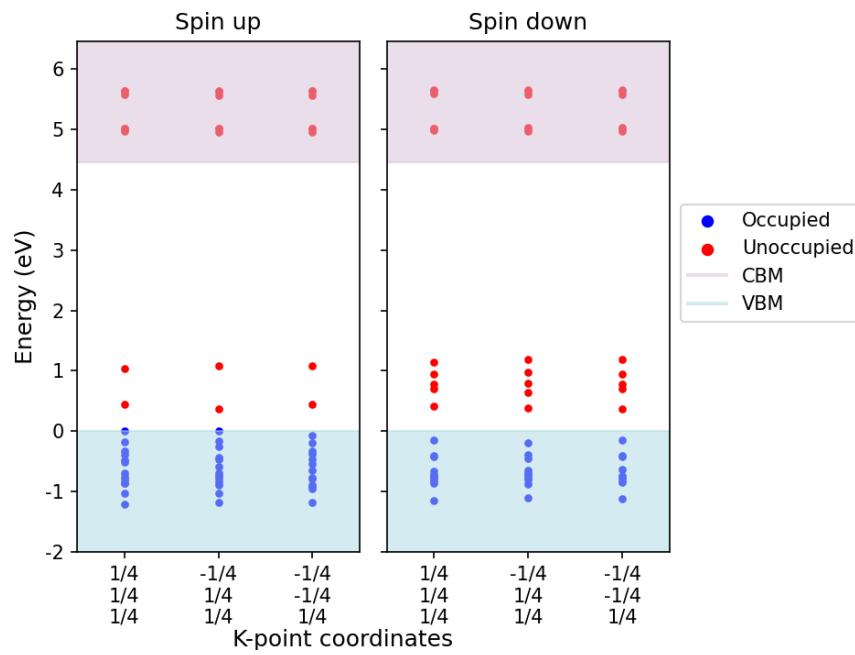


Figure 106: Kohn-Sham states.

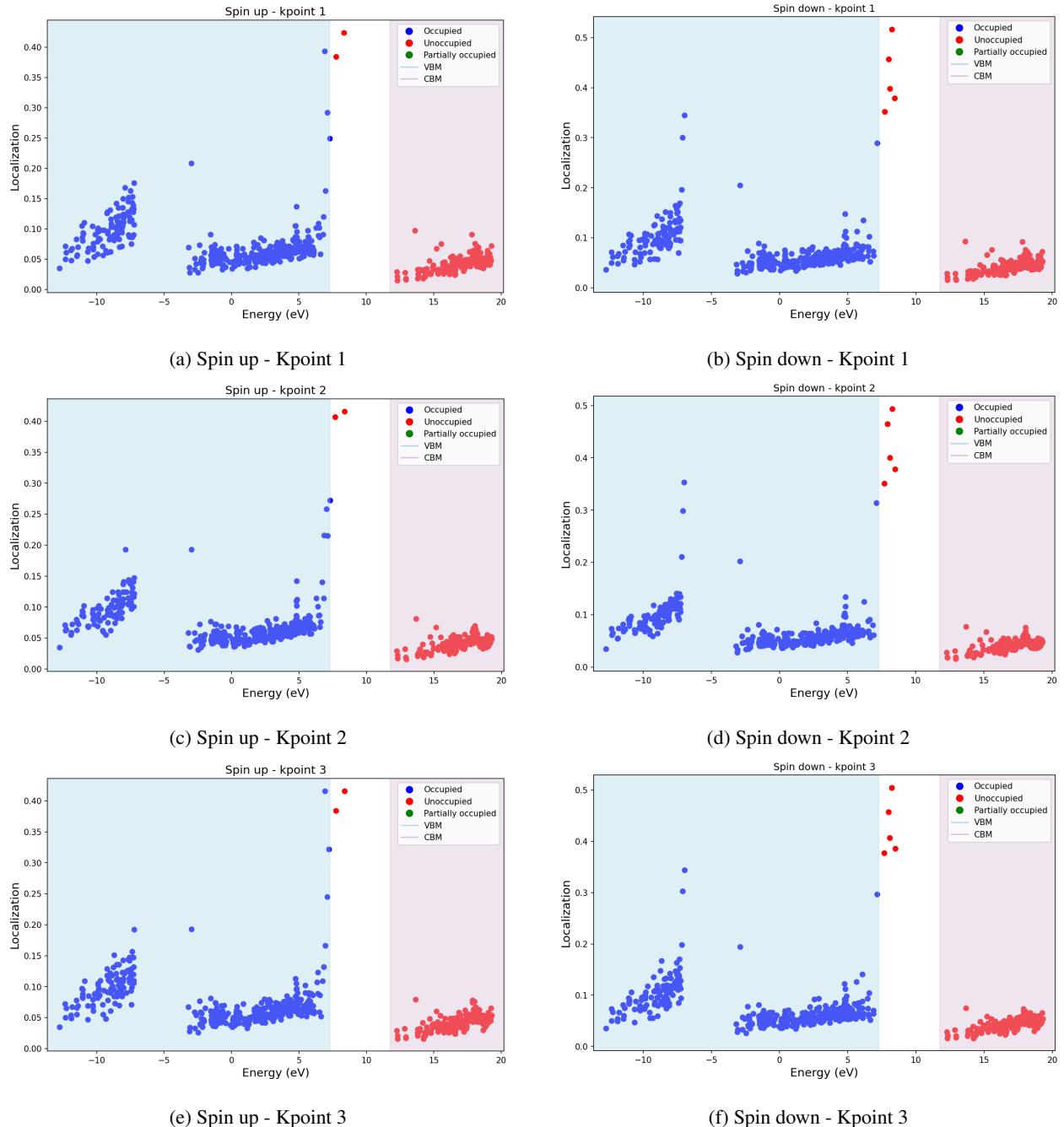


Figure 107: Localization factor using projected orbitals (s, p, and d).

6.50 Complex: $(B_N - V_B)^{+3}$

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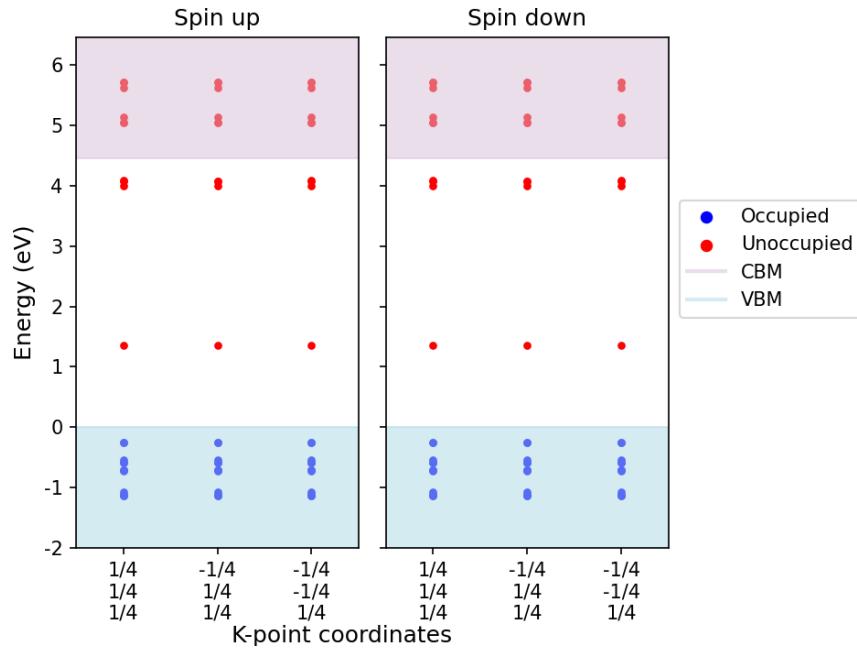


Figure 108: Kohn-Sham states.

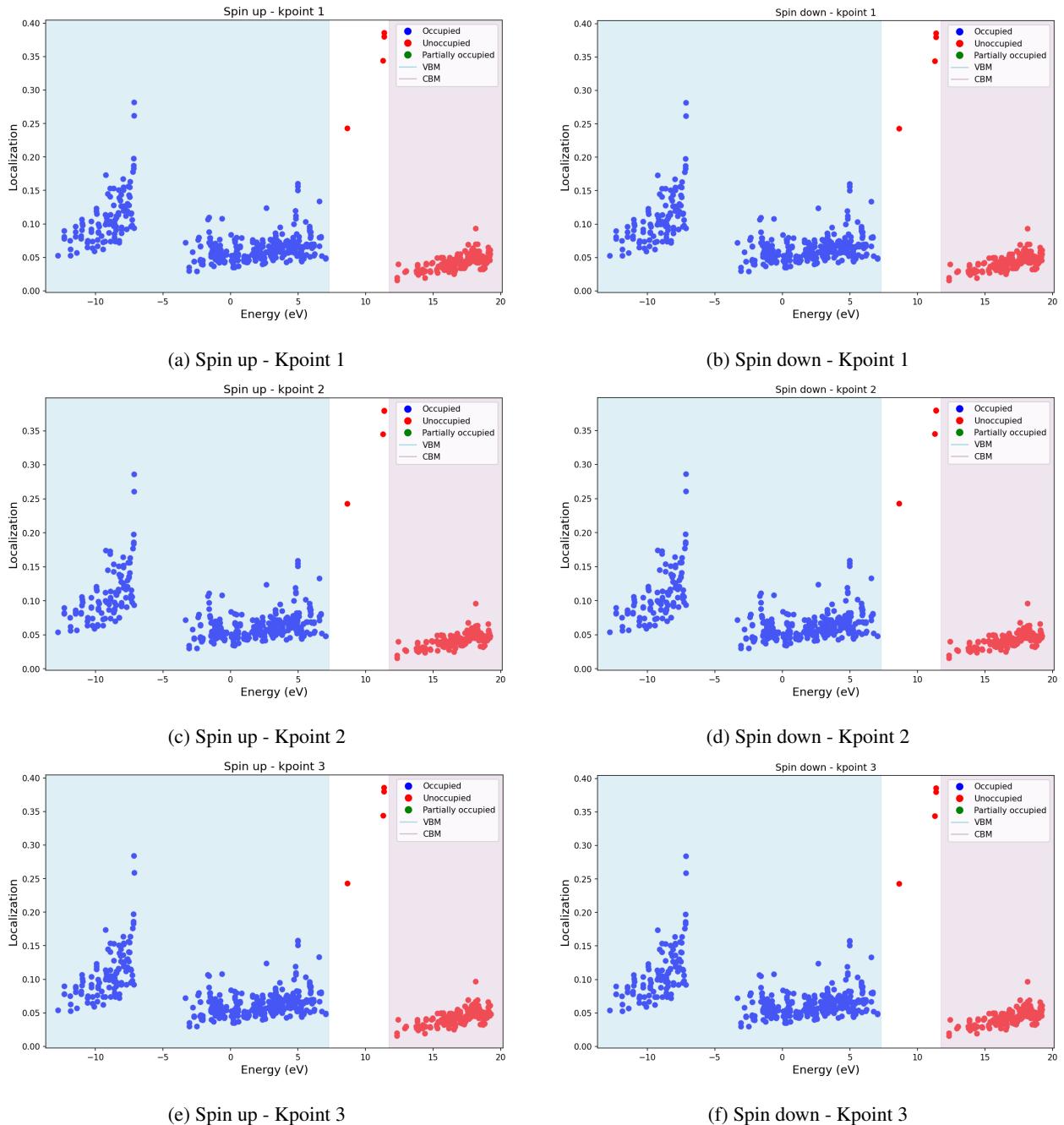


Figure 109: Localization factor using projected orbitals (s, p, and d).

6.51 Complex: $(B_N - V_B)^{+4}$

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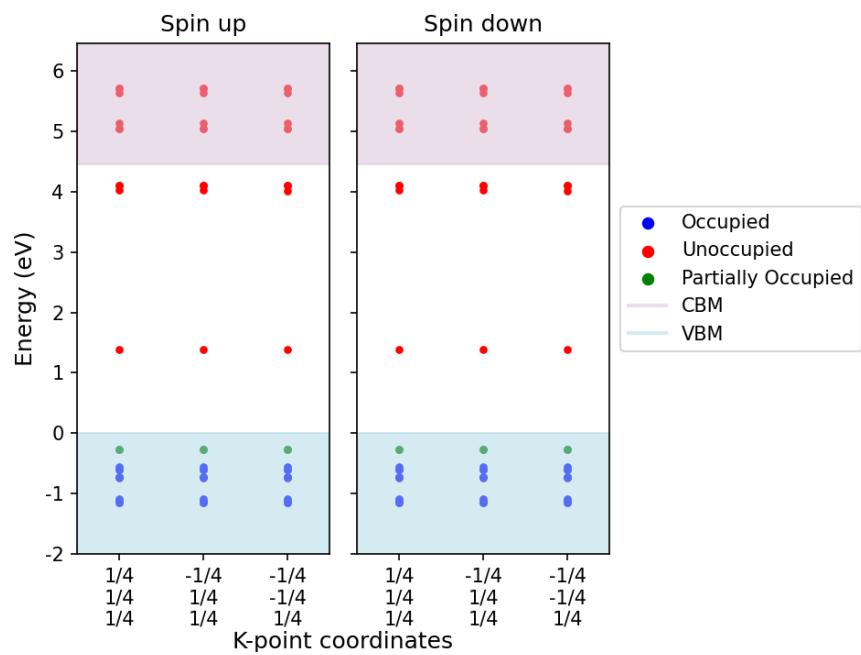


Figure 110: Kohn-Sham states.

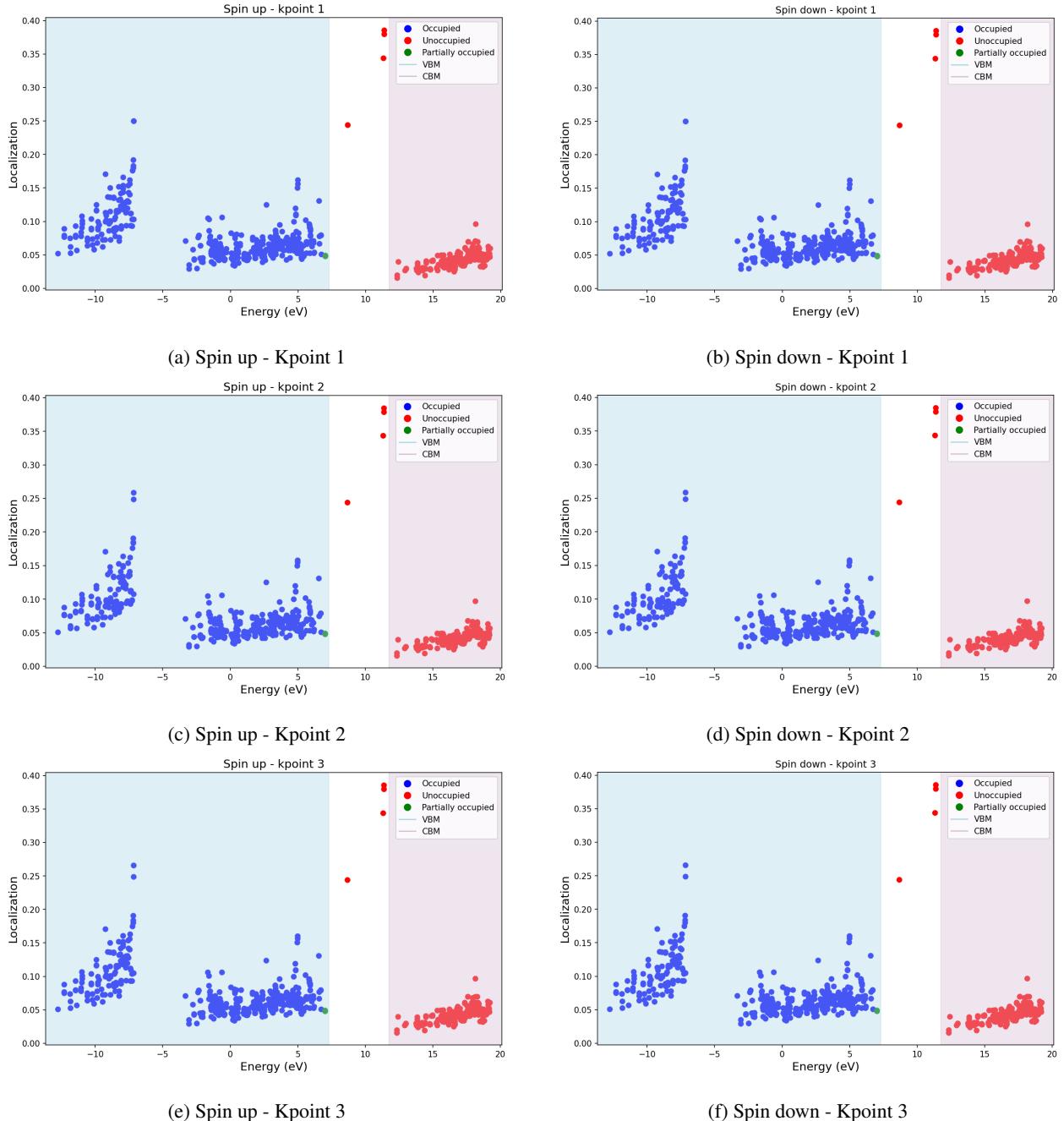


Figure 111: Localization factor using projected orbitals (s, p, and d).

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6.52 Complex: $(B_N - V_B)^{-1}$

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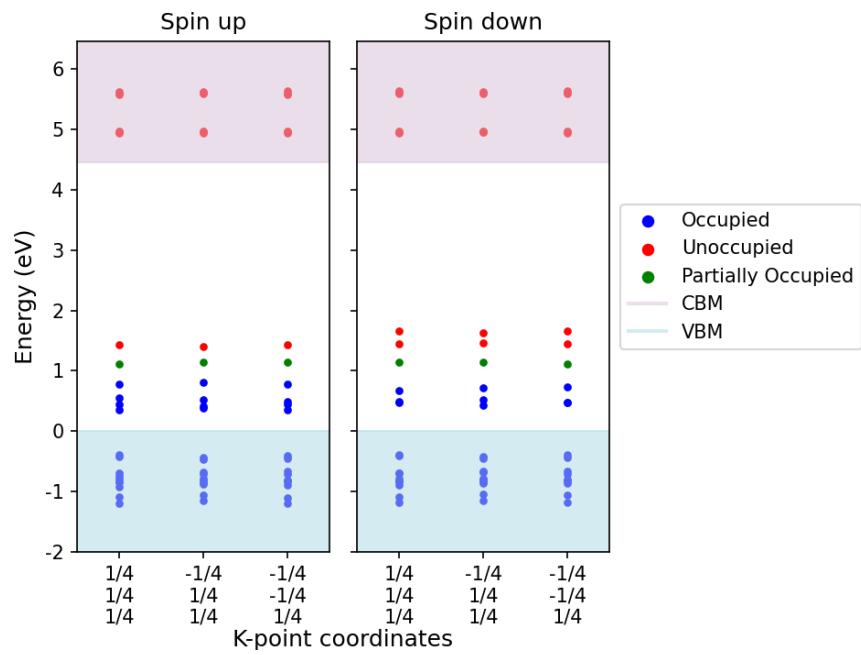


Figure 112: Kohn-Sham states.

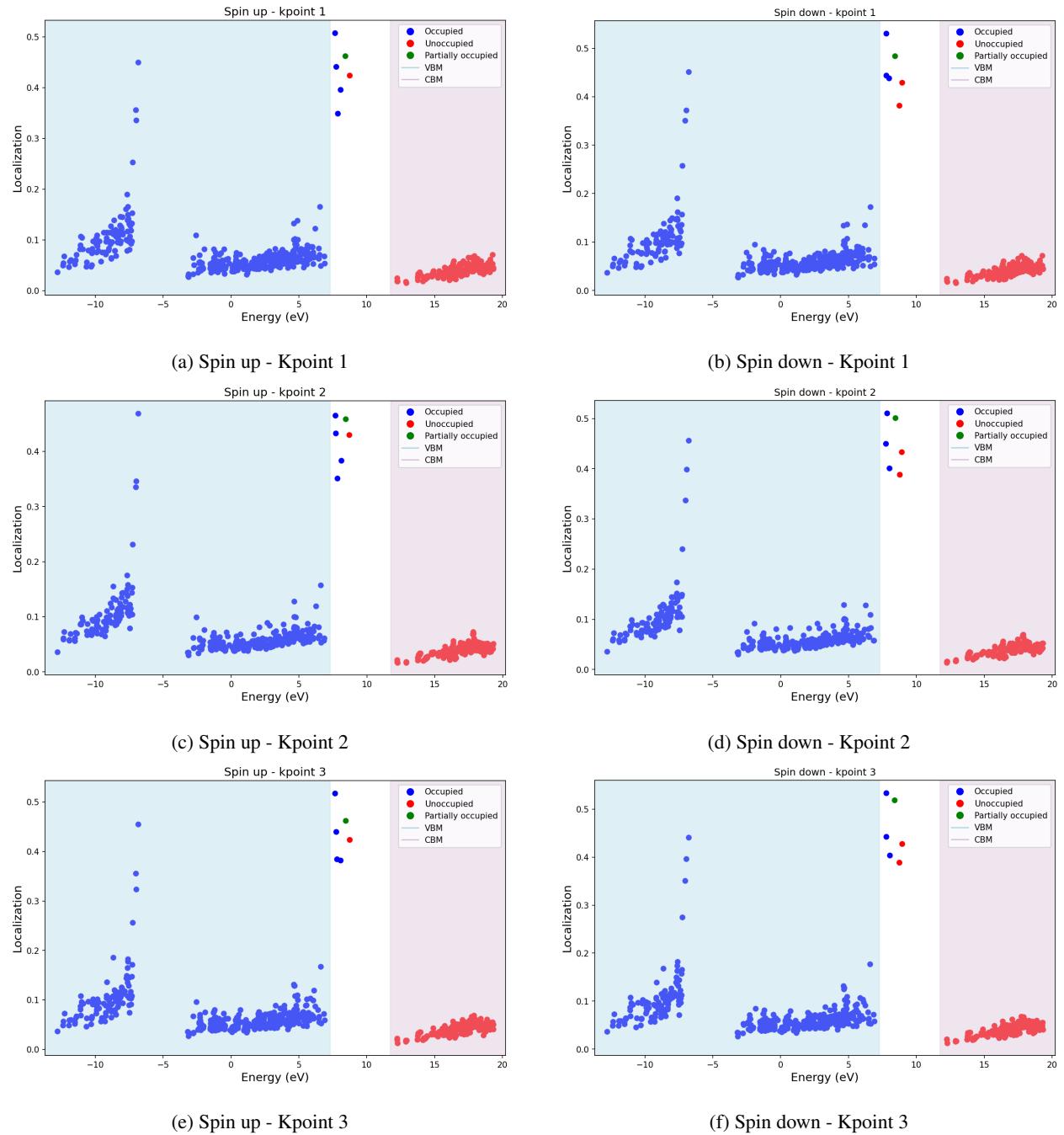


Figure 113: Localization factor using projected orbitals (s, p, and d).

6.53 Complex: $(B_N - V_B)^{-2}$

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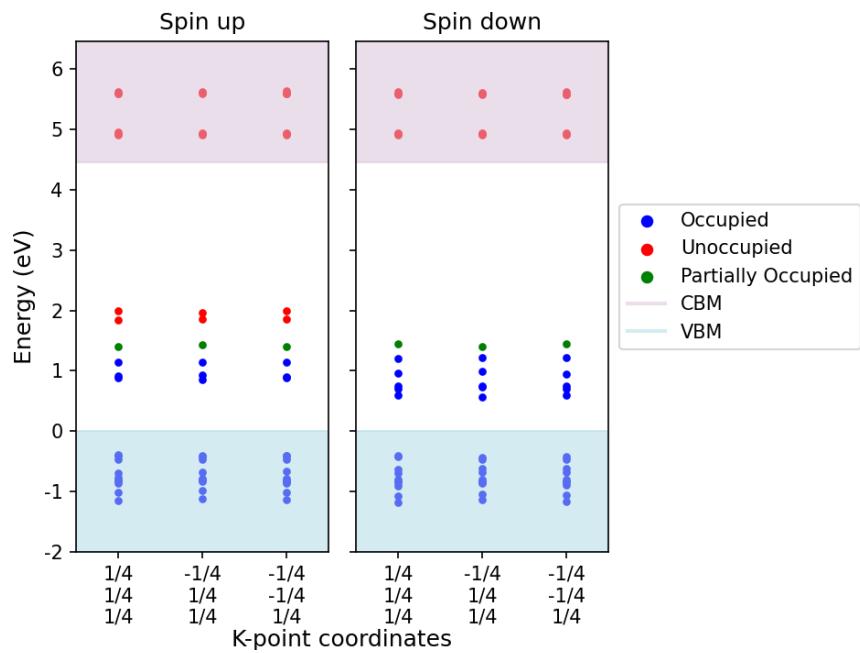


Figure 114: Kohn-Sham states.

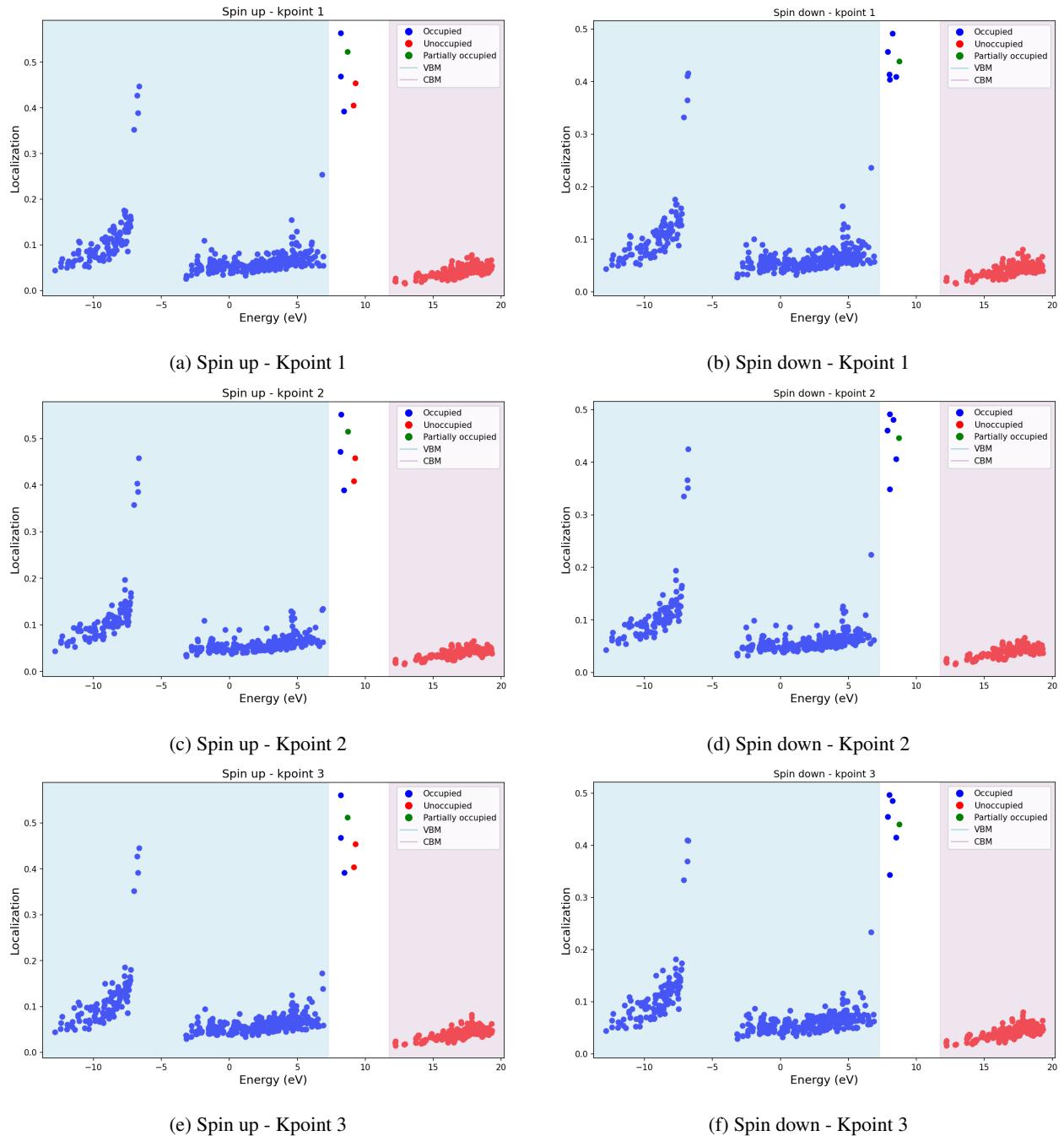


Figure 115: Localization factor using projected orbitals (s, p, and d).

6.54 Complex: $(B_N - V_B)^{-3}$

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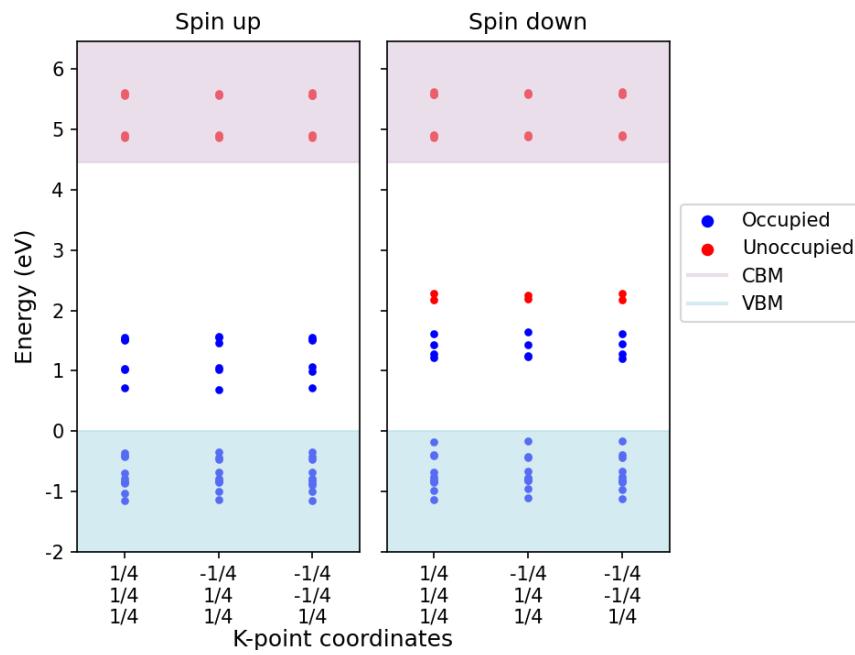


Figure 116: Kohn-Sham states.

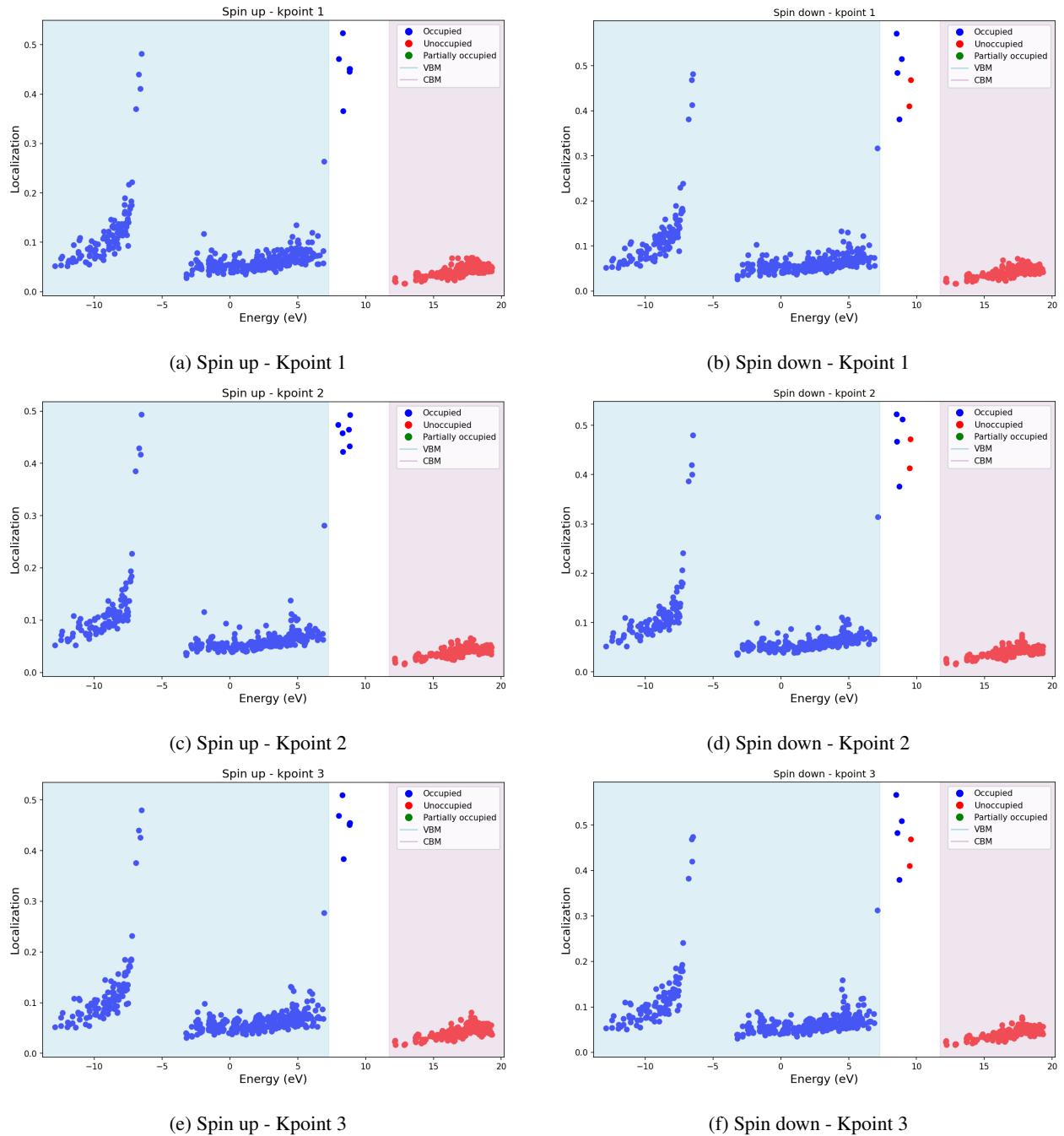


Figure 117: Localization factor using projected orbitals (s, p, and d).

6.55 Complex: $(B_N - V_B)^{-4}$

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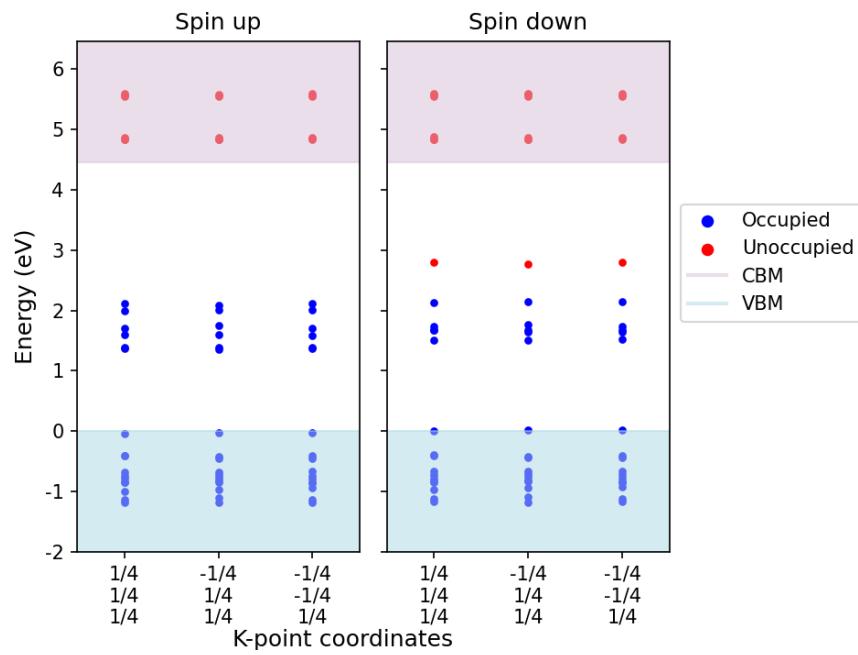


Figure 118: Kohn-Sham states.

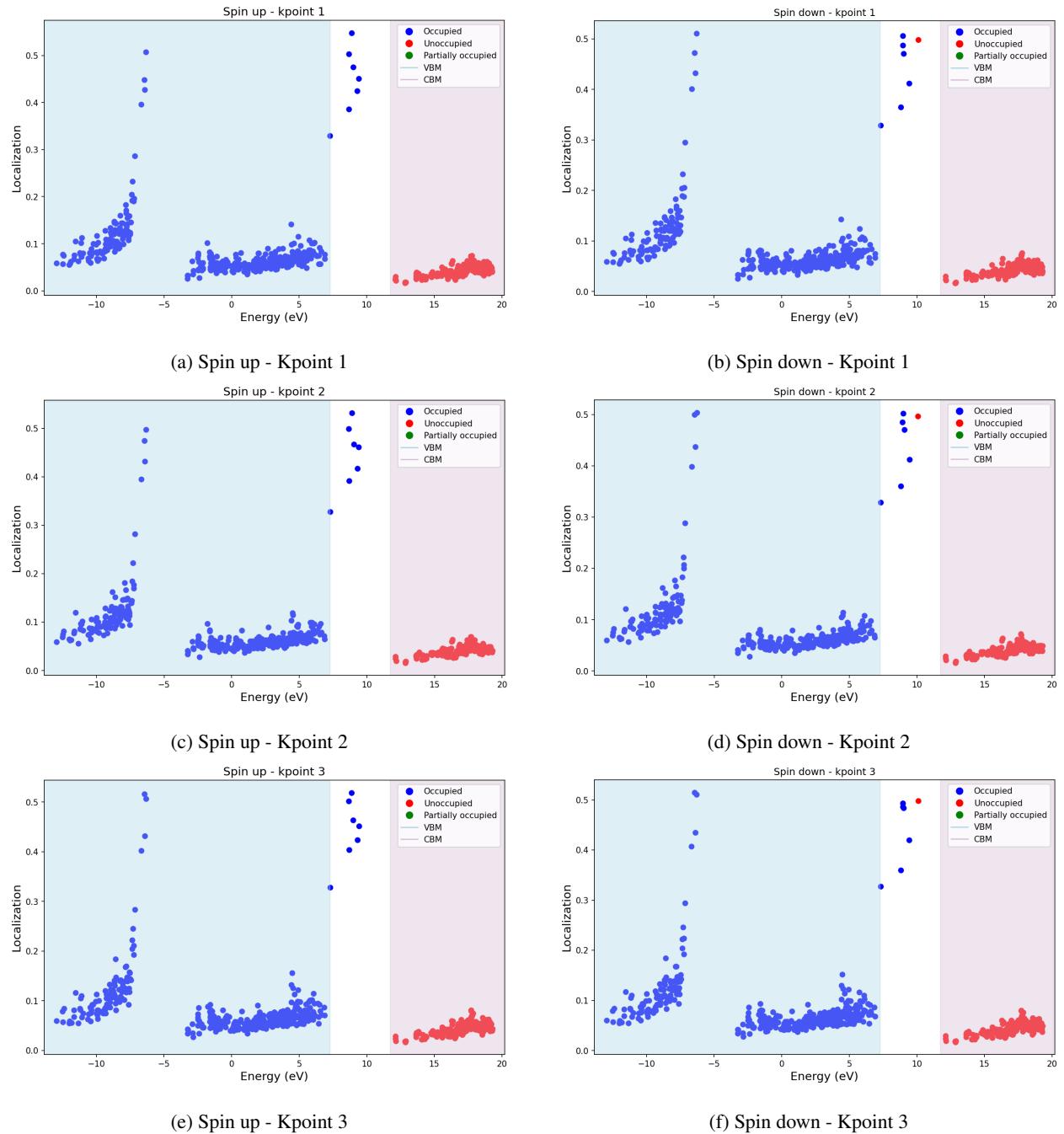


Figure 119: Localization factor using projected orbitals (s, p, and d).

6.56 Complex: $(N_B - V_N)^0$

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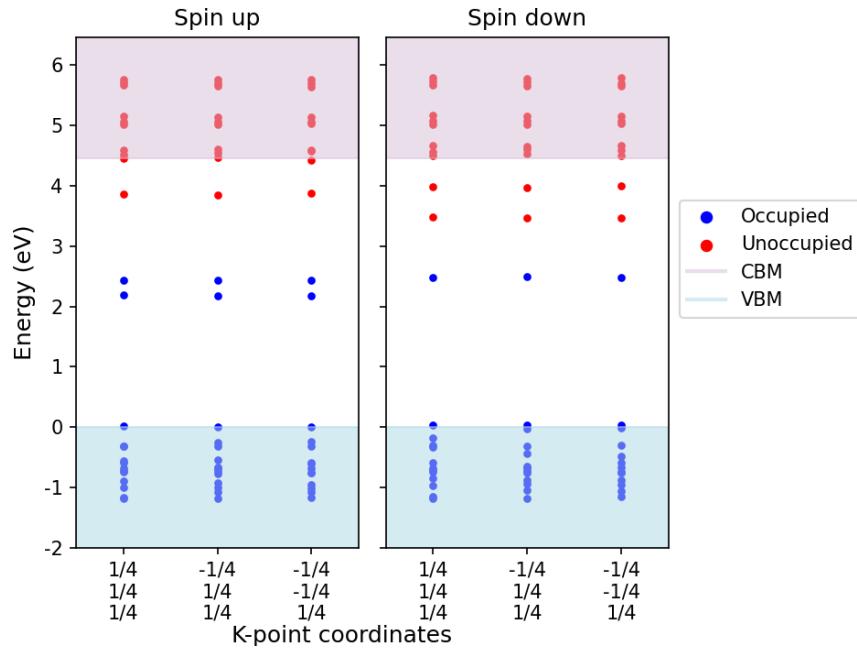


Figure 120: Kohn-Sham states.

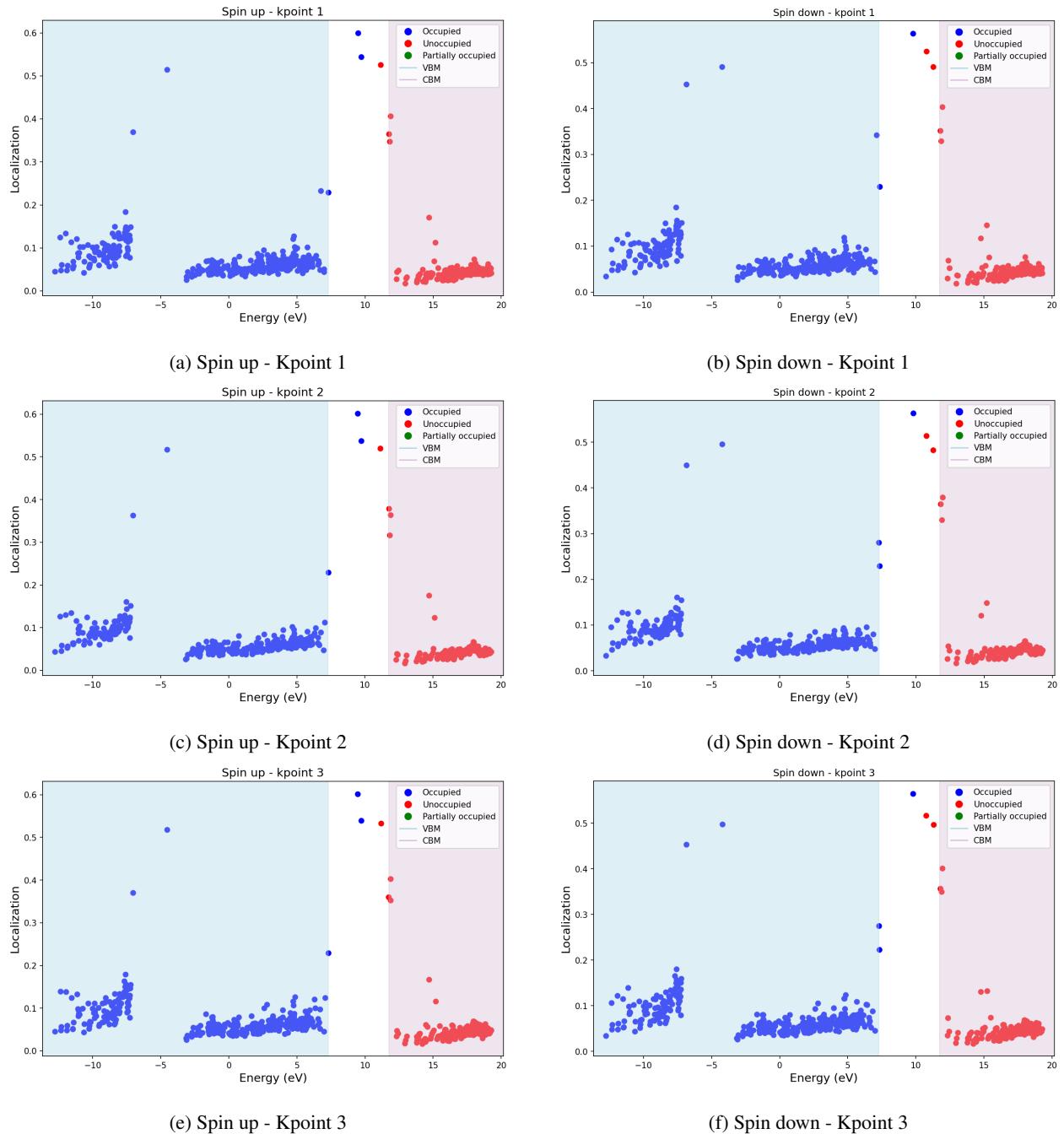


Figure 121: Localization factor using projected orbitals (s, p, and d).

6.57 Complex: $(N_B - V_N)^{+1}$

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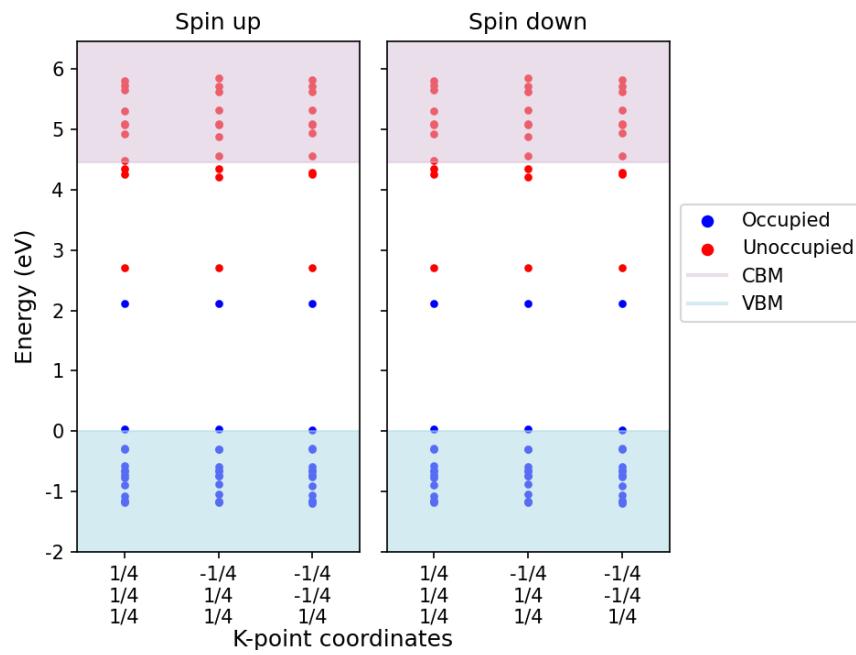


Figure 122: Kohn-Sham states.

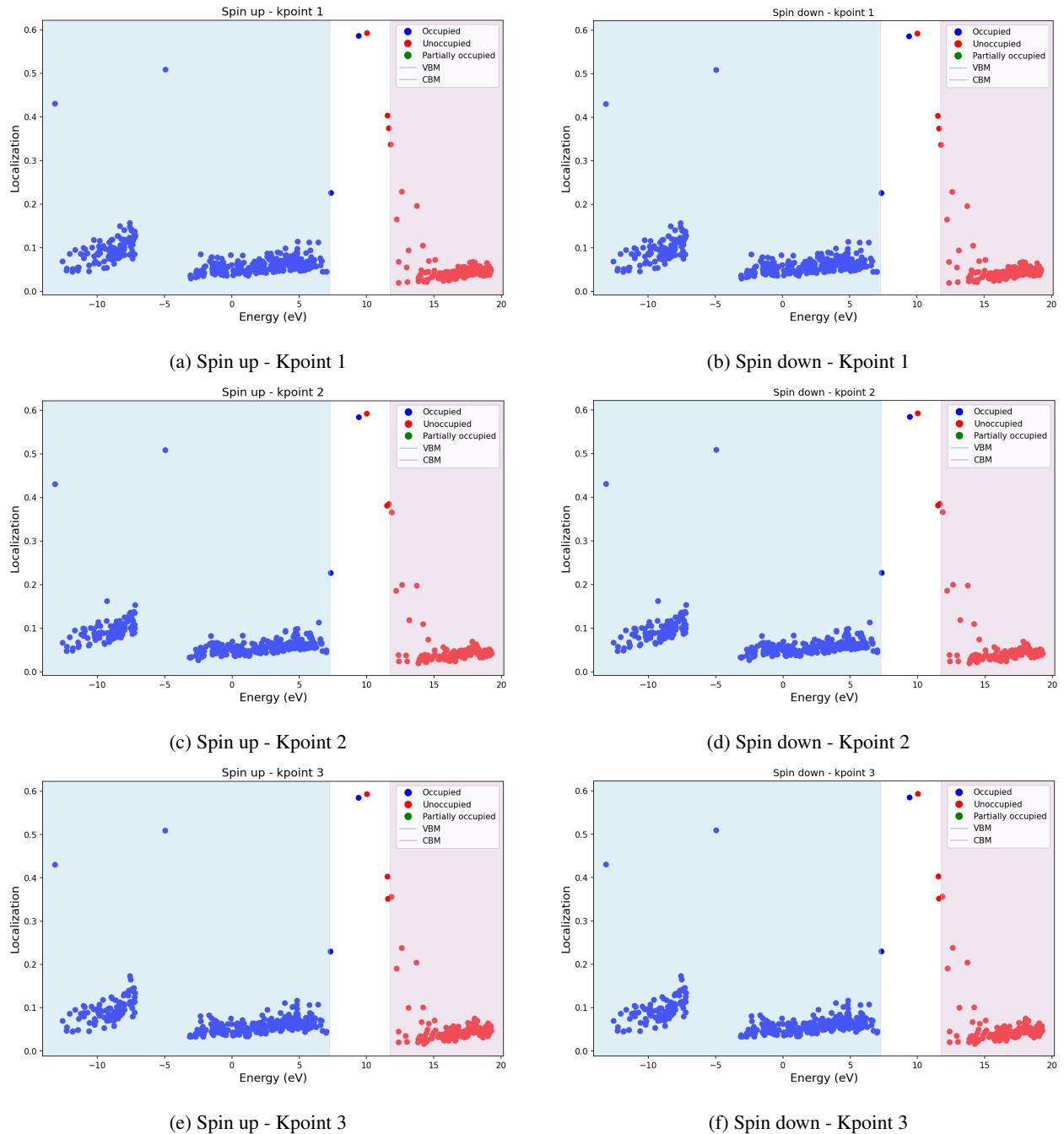


Figure 123: Localization factor using projected orbitals (s, p, and d).

6.58 Complex: $(N_B - V_N)^{+2}$

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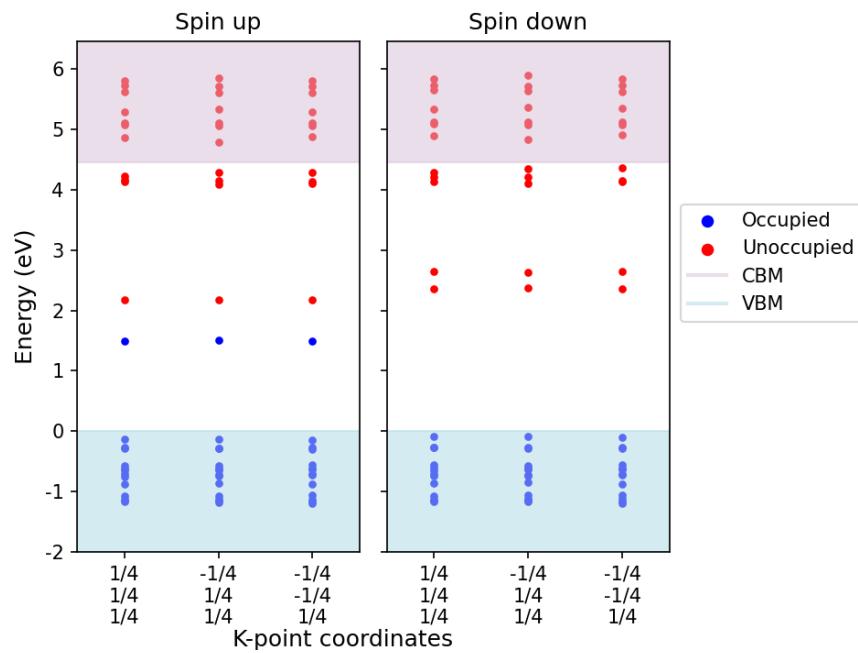


Figure 124: Kohn-Sham states.

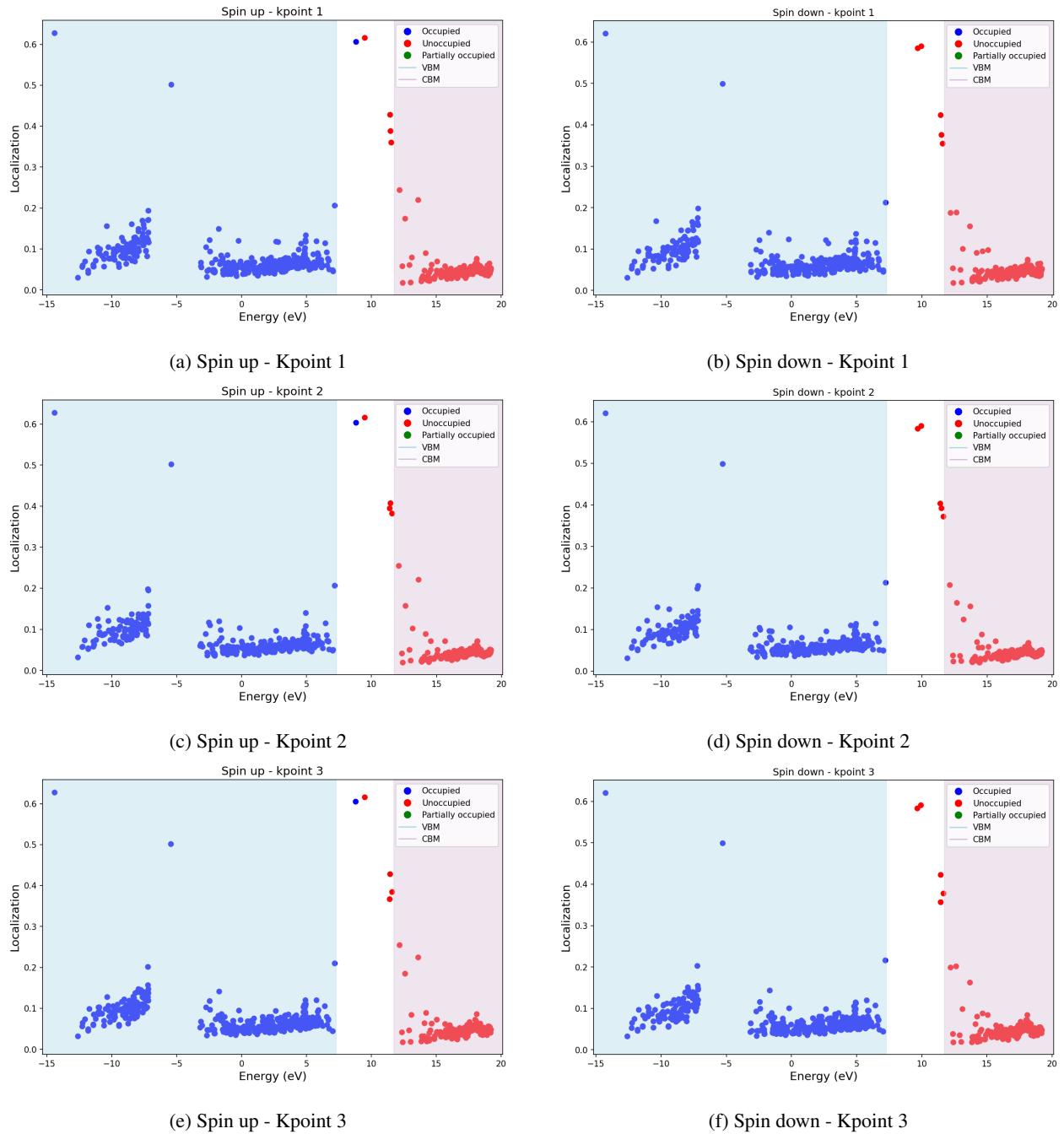


Figure 125: Localization factor using projected orbitals (s, p, and d).

6.59 Complex: $(N_B - V_N)^{+3}$

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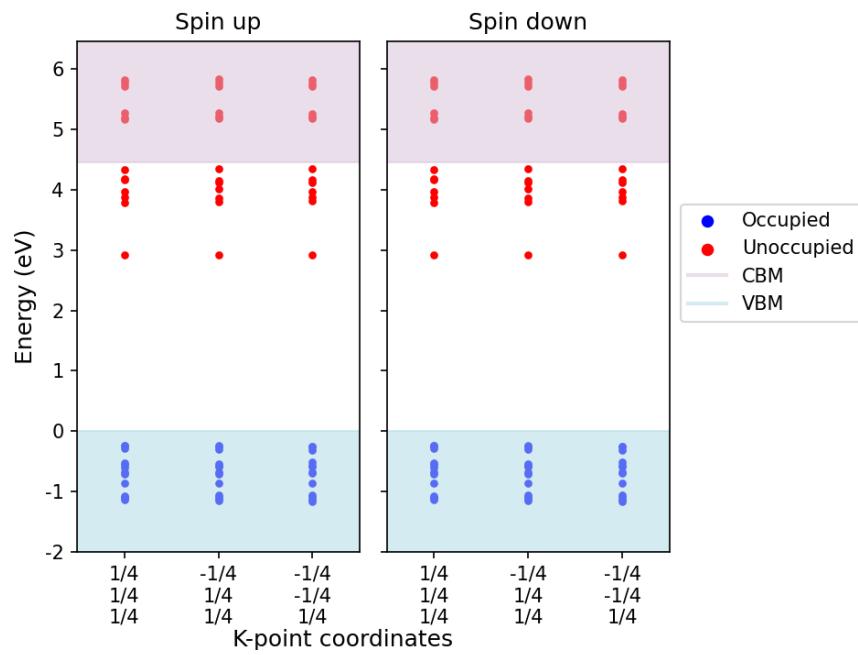


Figure 126: Kohn-Sham states.

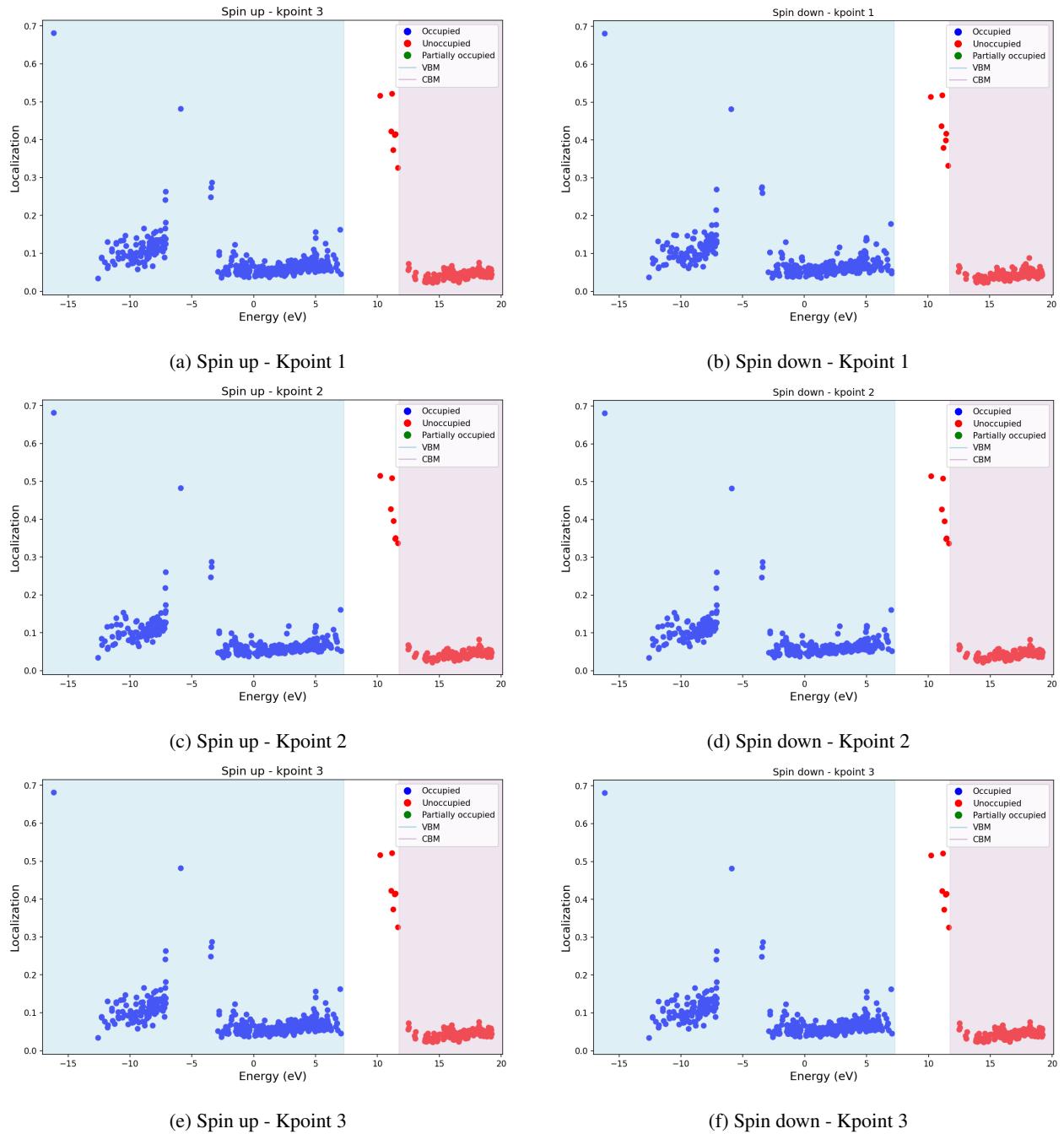


Figure 127: Localization factor using projected orbitals (s, p, and d).

6.60 Complex: $(N_B - V_N)^{+4}$

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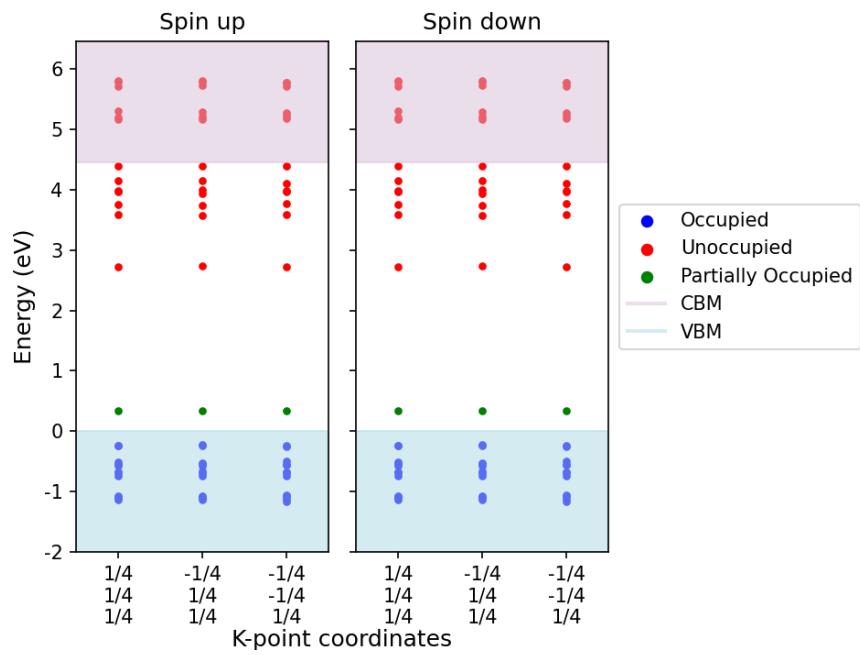


Figure 128: Kohn-Sham states.

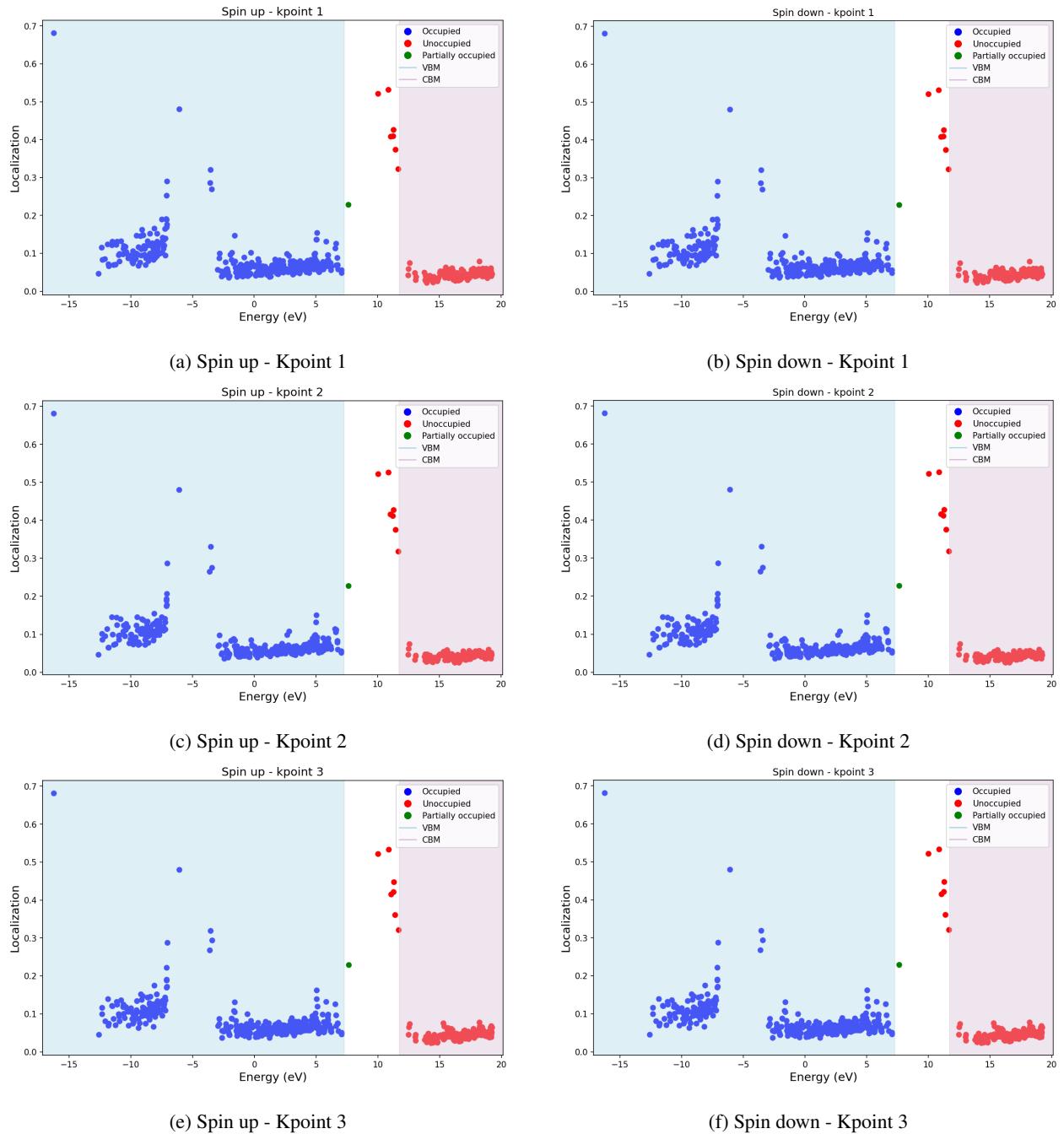


Figure 129: Localization factor using projected orbitals (s, p, and d).

6.61 Complex: $(N_B - V_N)^{-1}$

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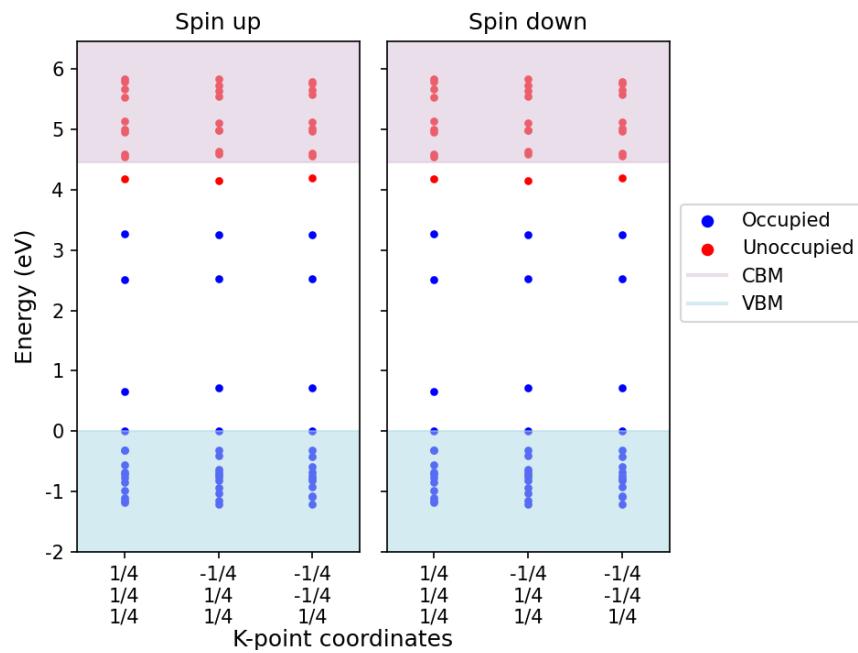


Figure 130: Kohn-Sham states.

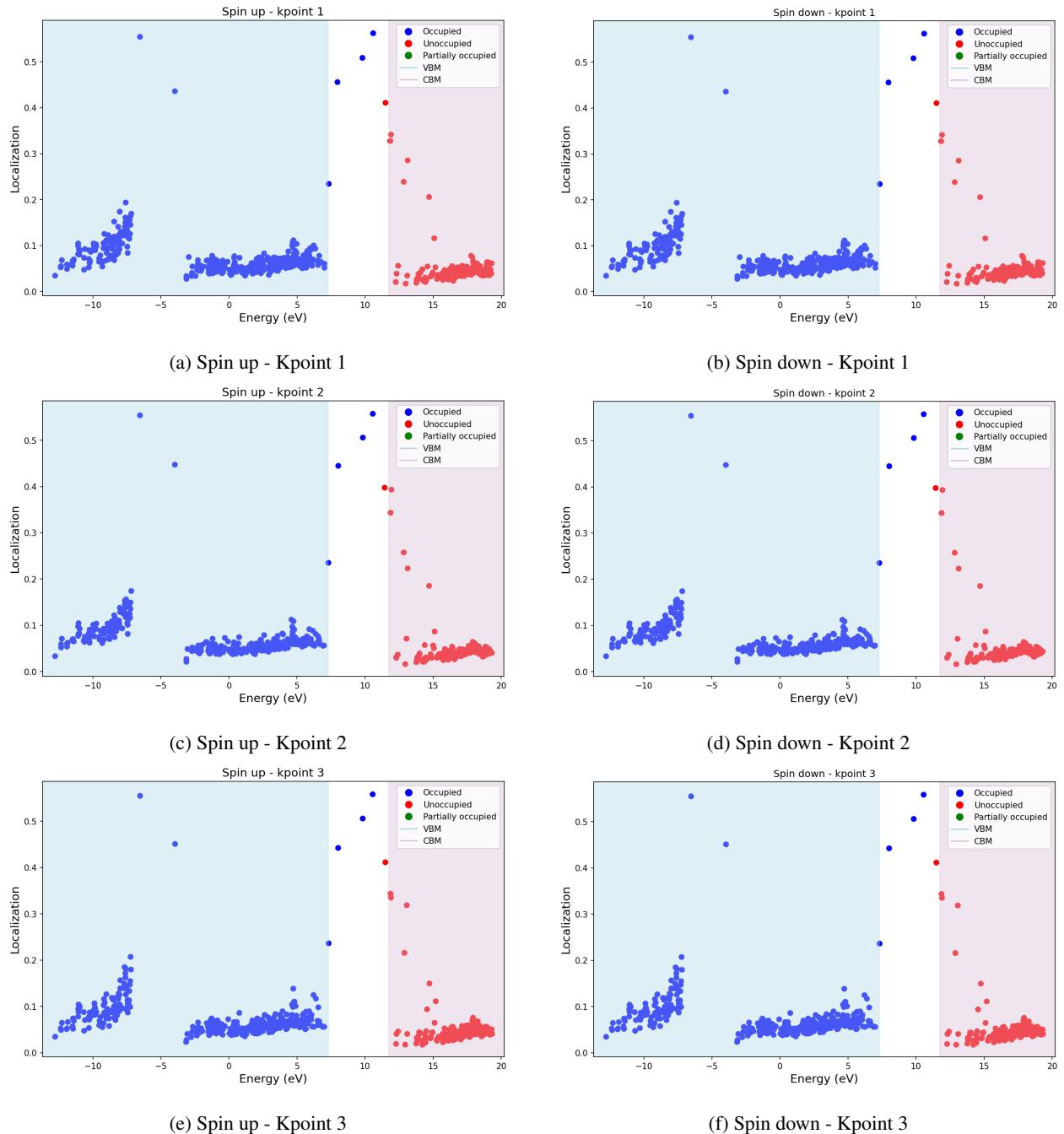


Figure 131: Localization factor using projected orbitals (s, p, and d).

6.62 Complex: $(N_B - V_N)^{-2}$

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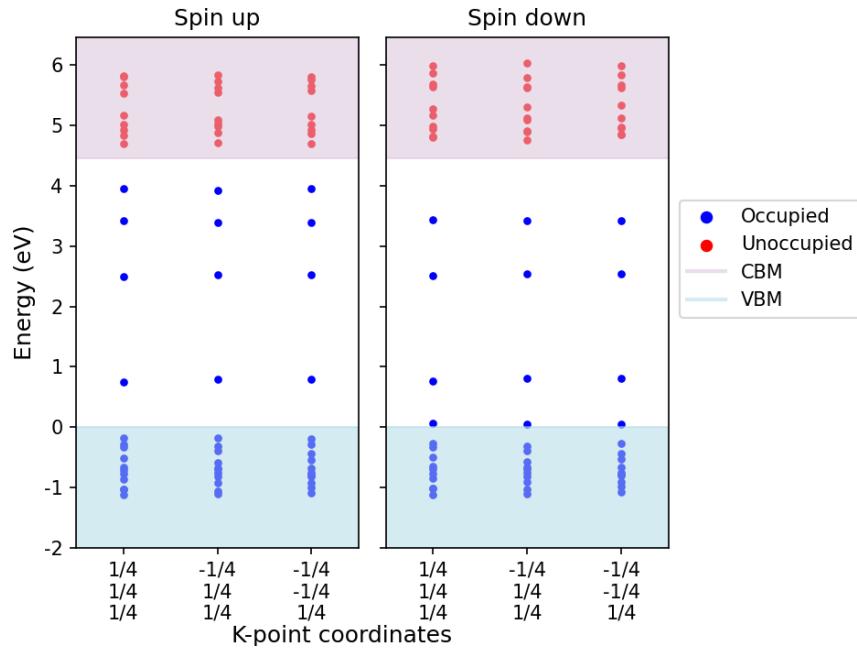


Figure 132: Kohn-Sham states.

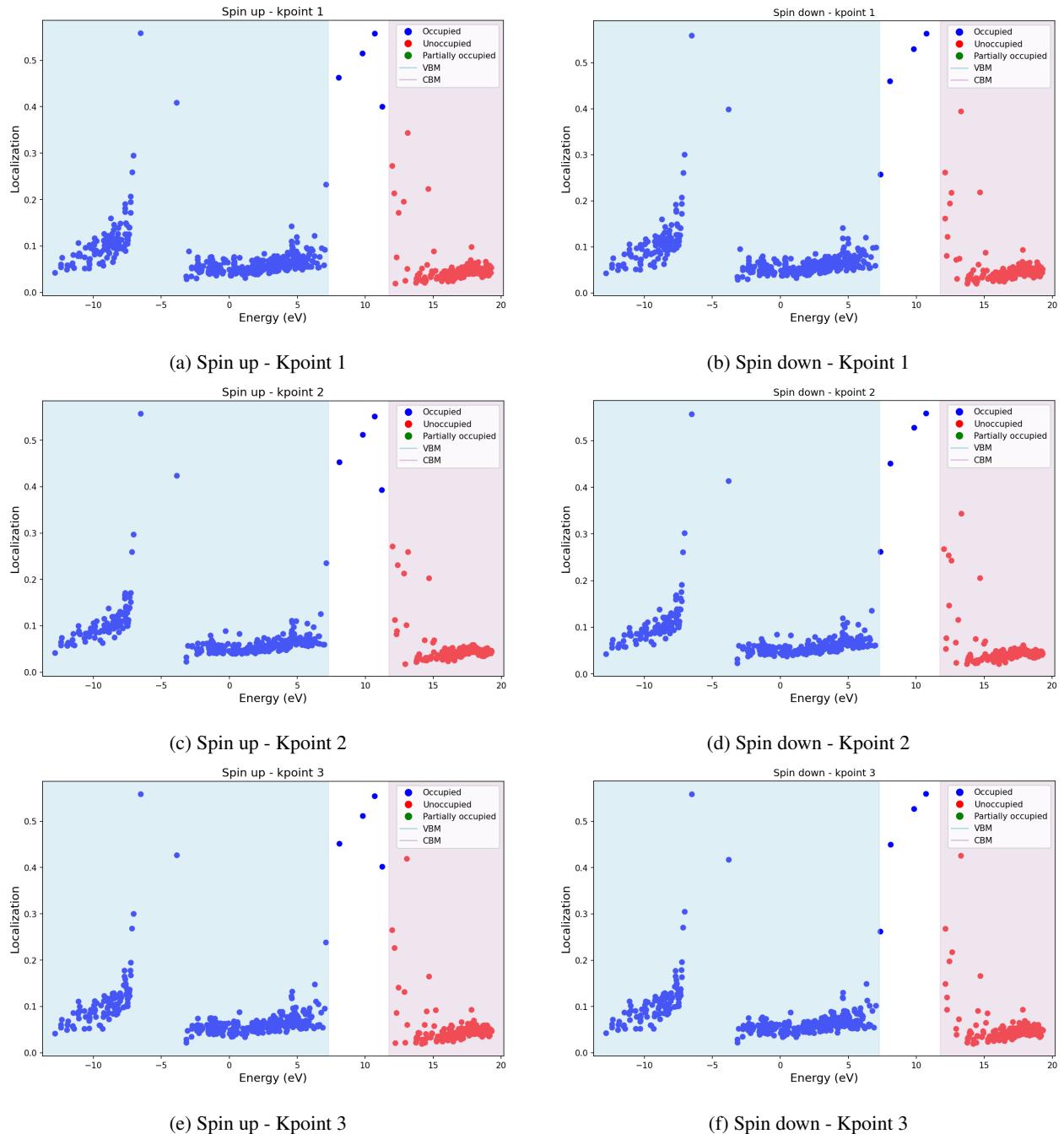


Figure 133: Localization factor using projected orbitals (s, p, and d).

6.63 Complex: $(N_B - V_N)^{-3}$

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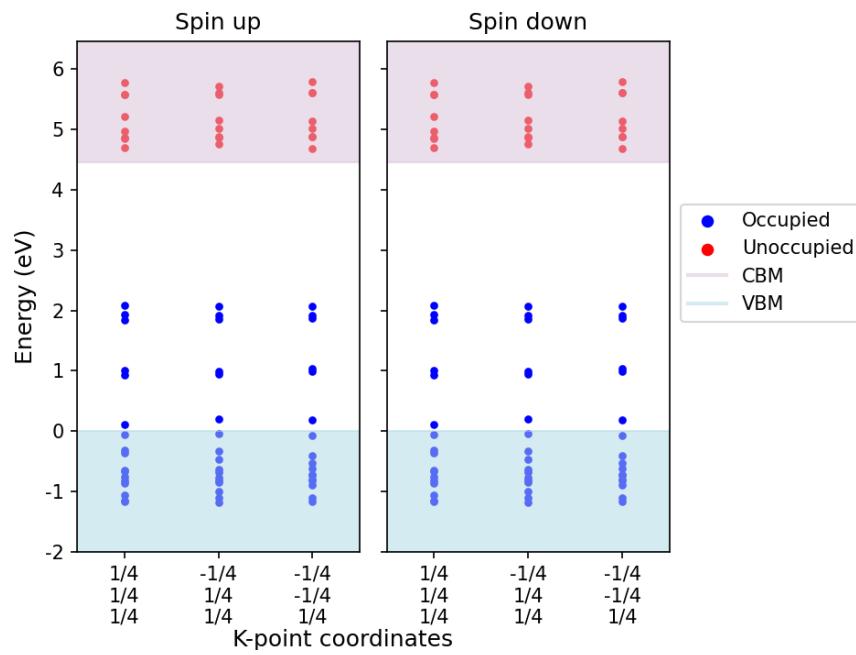


Figure 134: Kohn-Sham states.

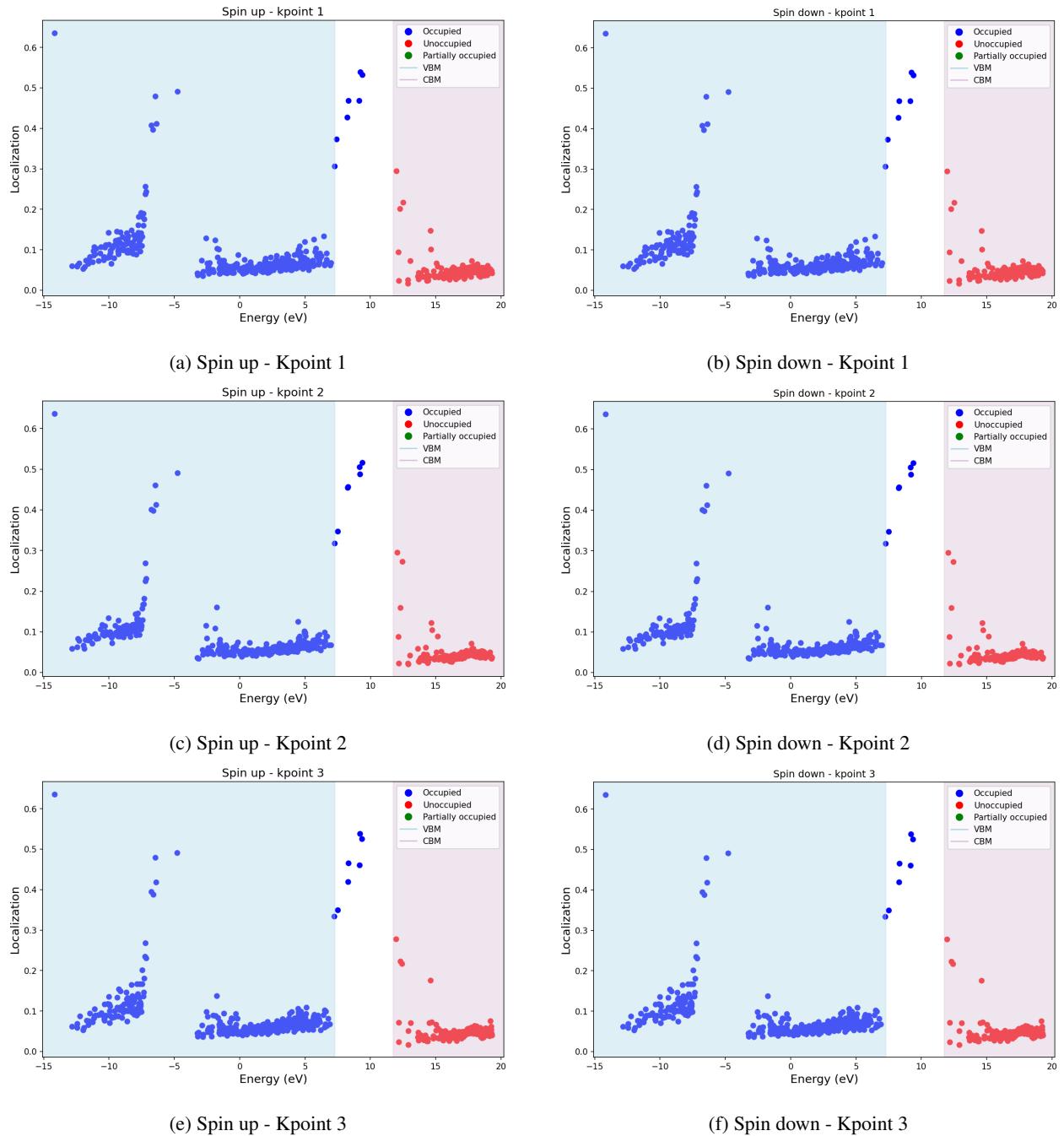


Figure 135: Localization factor using projected orbitals (s, p, and d).

6.64 Complex: $(N_B - V_N)^{-4}$

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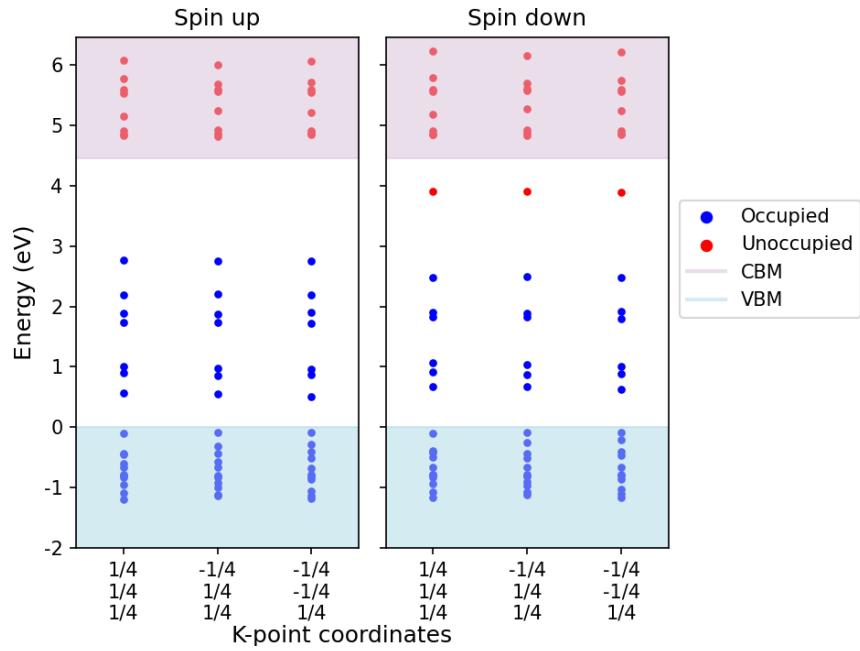


Figure 136: Kohn-Sham states.

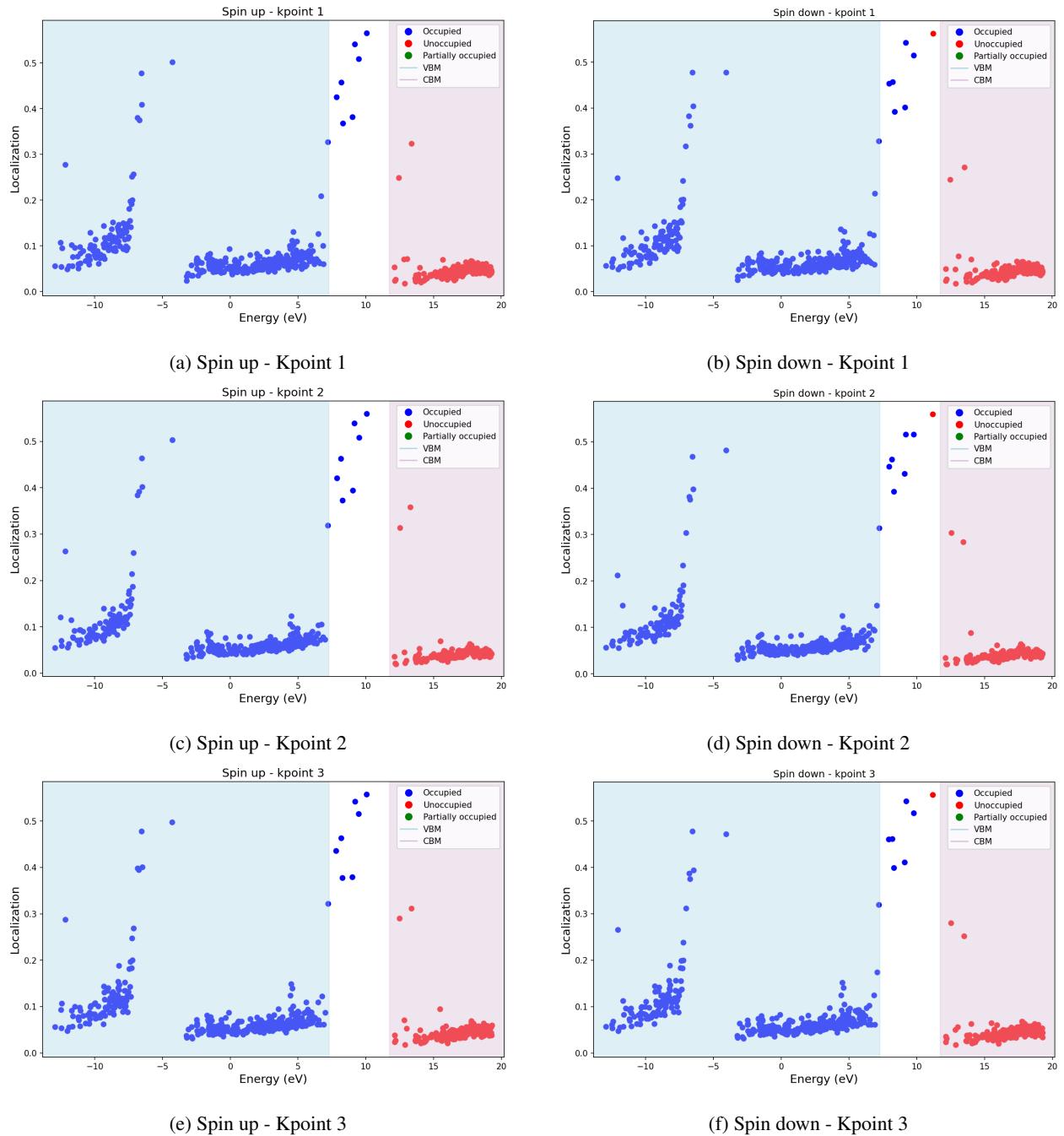


Figure 137: Localization factor using projected orbitals (s, p, and d).

6.65 Complex: $(V_B - V_N)^0$

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Table 61: $(V_B - V_N)^0$

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
Up	1	428	–	< 0.1	–
	1	429	174, 201	0.210, 0.210	Y, Y
	1	430	26, 41	0.224, 0.130	Y, Y
	1	431	41	0.115	Y
	2	428	174	0.269	Y
	2	429	201	0.298	Y
	2	430	26	0.257	Y
	2	431	70	0.187	Y
	3	428	–	< 1	–
	3	429	174, 201	0.210, 0.210	Y, Y
	3	430	26	0.248	Y
Down	1	426	–	< 0.1	–
	1	427	174, 201	0.221, 0.221	Y, Y
	1	428	148	0.296	Y
	1	429	122	0.339	Y
	1	430	26, 41	0.233, 0.112	Y, Y
	2	426	–	< 0.1	–
	2	427	174, 201	0.267, 0.179	Y, Y
	2	428	122, 201	0.159, 0.139	Y, Y
	2	429	122, 148	0.184, 0.259	Y, Y
	2	430	26	0.238	Y
	2	431	70, 103	0.141, 0.115	Y, Y
	3	426	–	< 0.1	–
	3	427	174, 201	0.220, 0.220	Y, Y
	3	428	122	0.324	Y
	3	429	148	0.324	Y
	3	430	26	0.247	Y

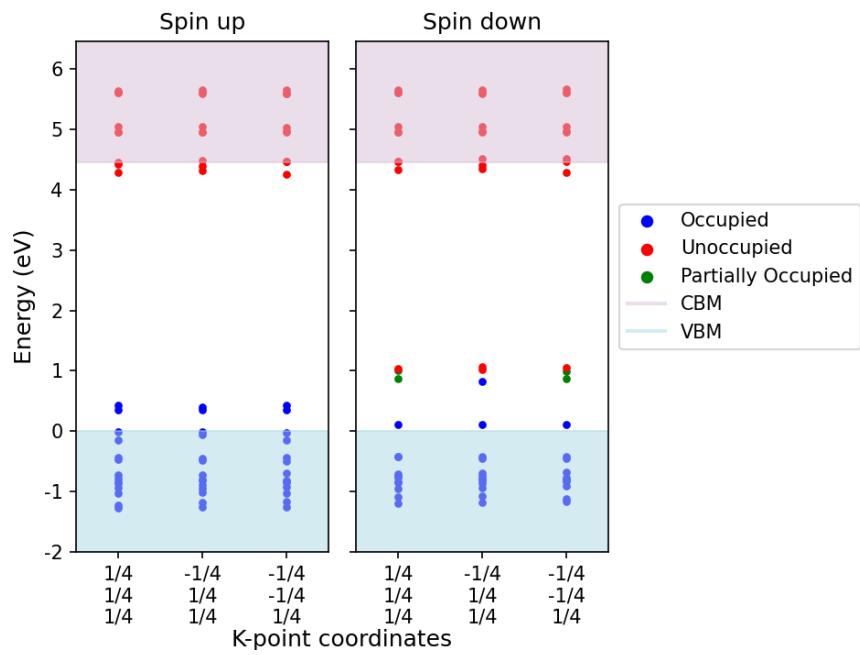


Figure 138: Kohn-Sham states.

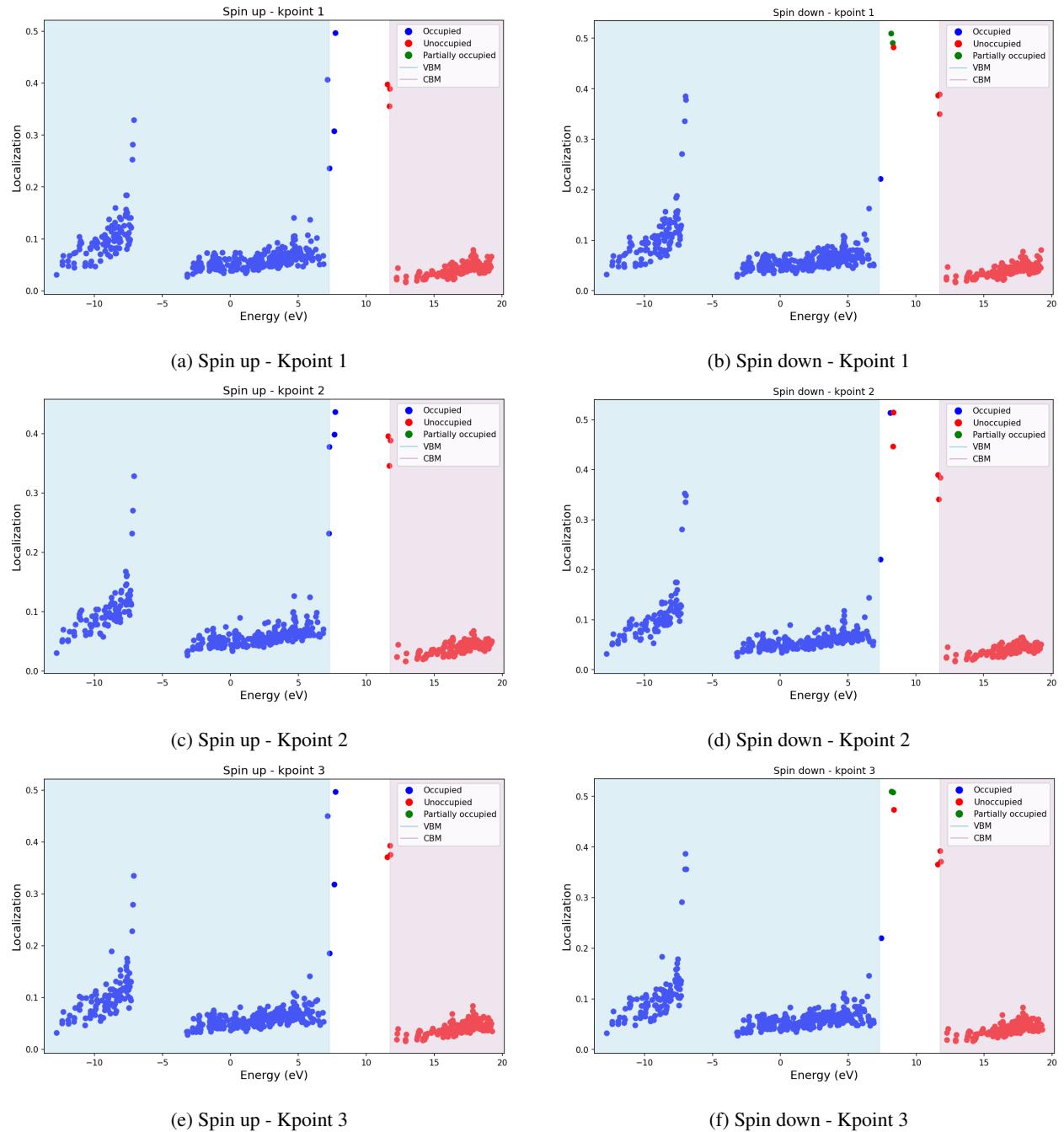


Figure 139: Localization factor using projected orbitals (s, p, and d).

6.66 Complex: $(V_B - V_N)^{+1}$

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Table 62: $(V_B - V_N)^{+1}$

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
Up	1	430	26, 41	0.177, 0.187	Y, Y
	1	431	26	0.102	Y
	1	432	70, 103	0.185, 0.185	Y, Y
	2	430	26	0.255	Y
	2	431	70	0.230	Y
	2	432	41, 103	0.130, 0.217	Y, Y
	3	430	26	0.253	Y
	3	431	70, 103	0.186, 0.186	Y, Y
	3	432	41	0.194	Y
	1	427	174, 201	0.218, 0.218	Y, Y
Down	1	428	148	0.218	Y
	1	429	122, 148	0.308, 0.125	Y, Y
	1	430	26, 41	0.195, 0.168	Y, Y
	1	431	-	< 0.1	-
	1	432	70, 103	0.181, 0.181	Y, Y
	2	427	174, 201	0.265, 0.180	Y, Y
	2	428	122, 148, 201	0.123, 0.105, 0.130	Y, Y, Y
	2	429	122, 148	0.220, 0.222	Y, Y
	2	430	26	0.257	Y
	2	431	70	0.219	Y
	2	432	41, 103	0.149, 0.191	Y, Y
	3	427	174, 201	0.218, 0.218	Y, Y
	3	428	122	0.236	Y
	3	429	122, 148	0.126, 0.296	Y, Y
	3	430	26	0.253	Y
	3	431	70, 103	0.182, 0.182	Y, Y
	3	432	41	0.194	Y

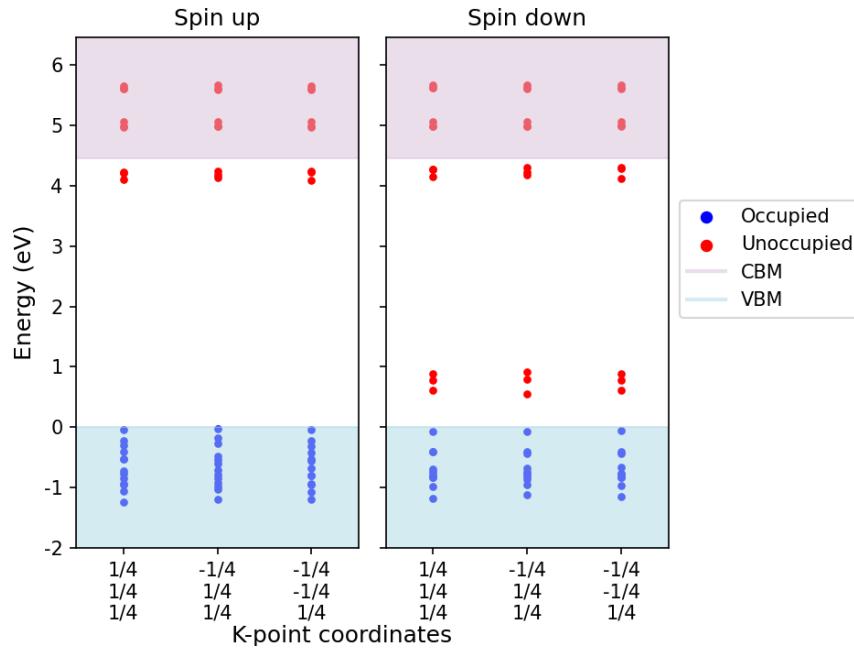


Figure 140: Kohn-Sham states.

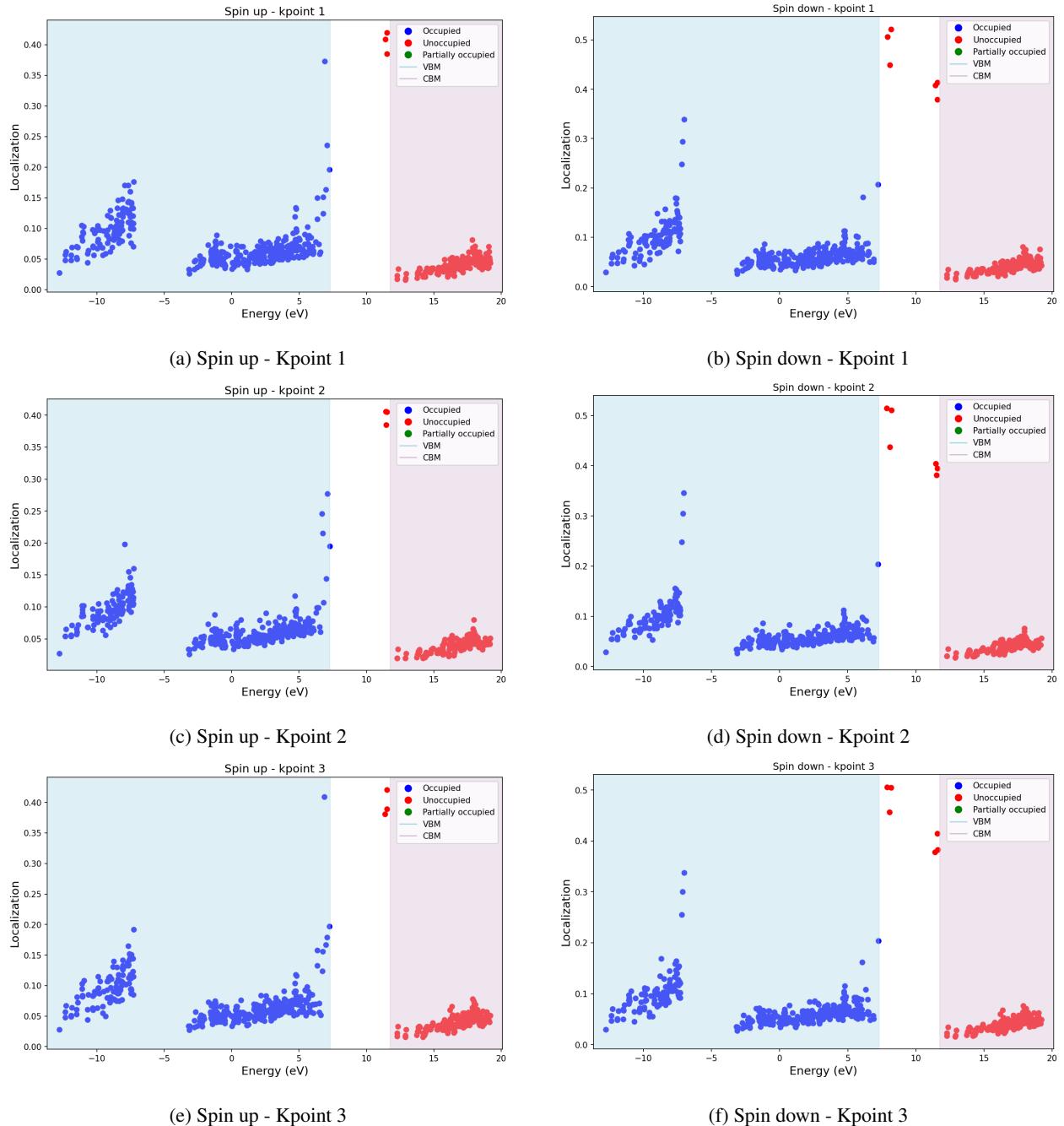


Figure 141: Localization factor using projected orbitals (s, p, and d).

6.67 Complex: $(V_B - V_N)^{+2}$

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Table 63: $(V_B - V_N)^{+2}$

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
	1	427	–	< 0.1	–
	1	428	174, 201	0.200, 0.200	Y, Y
	1	429	–	< 0.1	–
	1	430	26, 41	0.184, 0.150	Y, Y
	1	431	–	< 0.1	–
	1	432	70, 103	0.159, 0.159	Y, Y
	2	427	174	0.192	Y
	2	428	174, 201	0.142, 0.259	Y, Y
	2	429	–	< 0.1	–
	2	430	26, 41	0.216, 0.126	Y, Y
Up	2	431	70	0.193	Y
	2	432	103	0.242	Y
	3	427	148	0.111	Y
	3	428	174, 201	0.200, 0.200	Y, Y
	3	429	–	< 0.1	–
	3	430	26, 41	0.213, 0.106	Y, Y
	3	431	41	0.139	Y
	3	432	70, 103	0.160, 0.160	Y, Y
	1	426	174, 201	0.210, 0.210	Y, Y
	1	427	148	0.237	Y
	1	428	122, 148	0.326, 0.117	Y, Y
	1	429	–	< 0.1	–
	1	430	26, 41	0.185, 0.150	Y, Y
	1	431	–	< 0.1	–
	2	426	174, 201	0.247, 0.186	Y, Y
	2	427	148	0.181	Y
	2	428	122, 148	0.289, 0.157	Y, Y
	2	429	–	< 0.1	–
Down	2	430	26, 41	0.214, 0.127	Y, Y
	2	431	70	0.193	Y
	2	432	103	0.241	Y
	3	426	174, 201	0.210, 0.210	Y, Y
	3	427	122, 148	0.102, 0.162	Y, Y
	3	428	122, 148	0.280, 0.175	Y, Y
	3	429	$\bar{1}41$	< 0.1	–
	3	430	26, 41	0.212, 0.108	Y, Y
	3	431	41	0.137	Y

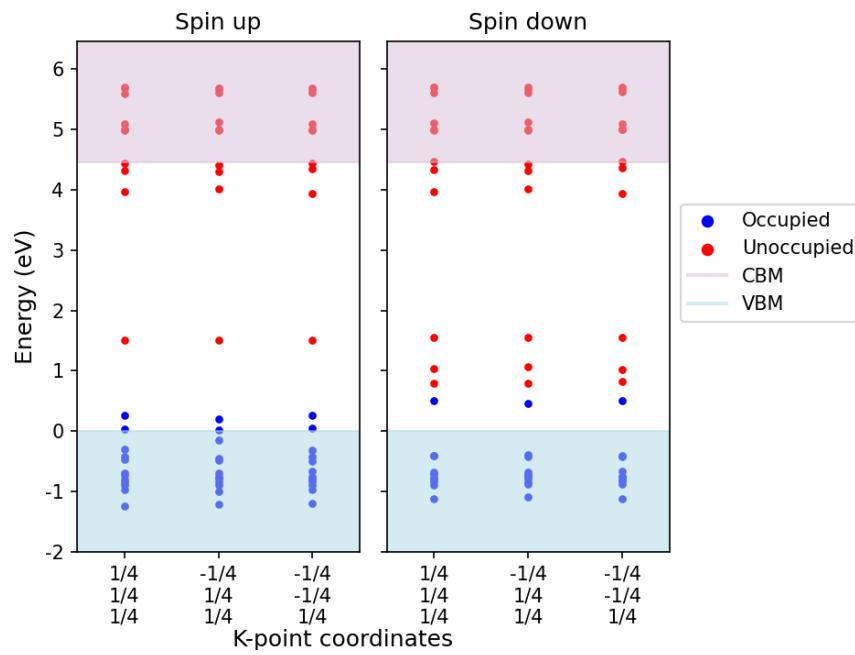


Figure 142: Kohn-Sham states.

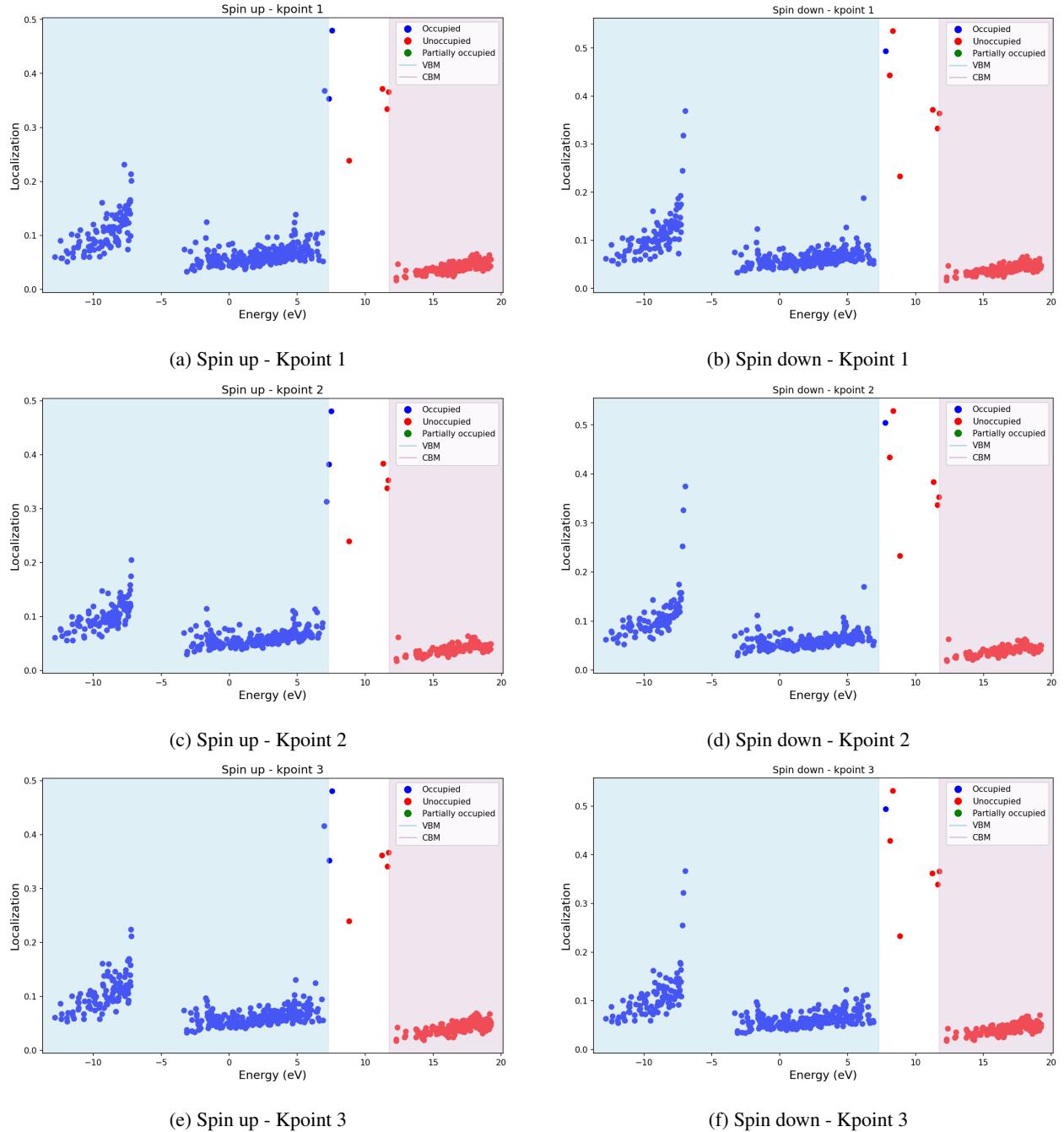


Figure 143: Localization factor using projected orbitals (s, p, and d).

6.68 Complex: $(V_B - V_N)^{+3}$

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Table 64: $(V_B - V_N)^{+3}$

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
Up	1	429	–	< 0.1	–
	1	430	26, 41	0.155, 0.178	Y, Y
	1	431	70, 103	0.171, 0.171	Y, Y
	1	432	26	0.101	Y
	2	429	–	< 0.1	–
	2	430	26, 41	0.214, 0.129	Y, Y
	2	431	70	0.228	Y
	2	432	41, 103	0.101, 0.195	Y, Y
	3	429	–	< 0.1	–
	3	430	26, 41	0.219, 0.102	Y, Y
Down	3	431	70, 103	0.171, 0.171	Y, Y
	3	432	41	0.153	Y
	1	426	174, 201	0.197, 0.197	Y, Y
	1	427	148	0.238	Y
	1	428	122, 148	0.318, 0.121	Y, Y
	1	429	–	< 0.1	–
	1	430	26, 41	0.164, 0.170	Y, Y
	1	431	–	< 0.1	–
	1	432	70, 103	0.167, 0.167	Y, Y
	2	426	174, 201	0.240, 0.179	Y, Y
	2	427	148	0.189	Y
	2	428	122, 148	0.285, 0.151	Y, Y
	2	429	–	< 0.1	–
	2	430	26, 41	0.214, 0.128	Y, Y
	2	431	70	0.228	Y
	2	432	103	0.200	Y
	3	426	174, 201	0.197, 0.197	Y, Y
	3	427	122, 148	0.102, 0.174	Y, Y
	3	428	122, 148	0.283, 0.165	Y, Y
	3	429	–	< 0.1	–
	3	430	26, 41	0.218, 0.103	Y, Y
	3	431	70, 103	0.168, 0.168	Y, Y
	3	432	41	0.150	Y

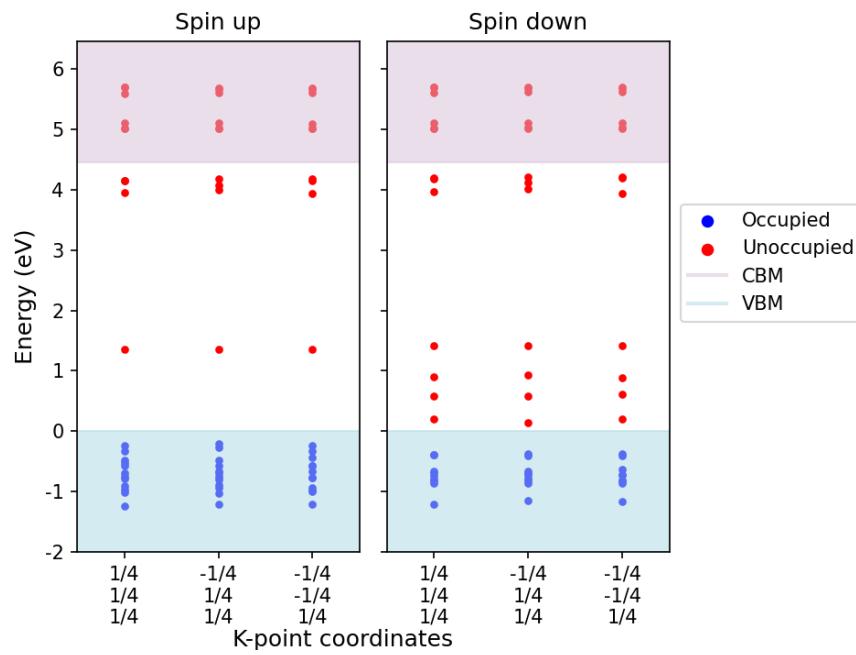


Figure 144: Kohn-Sham states.

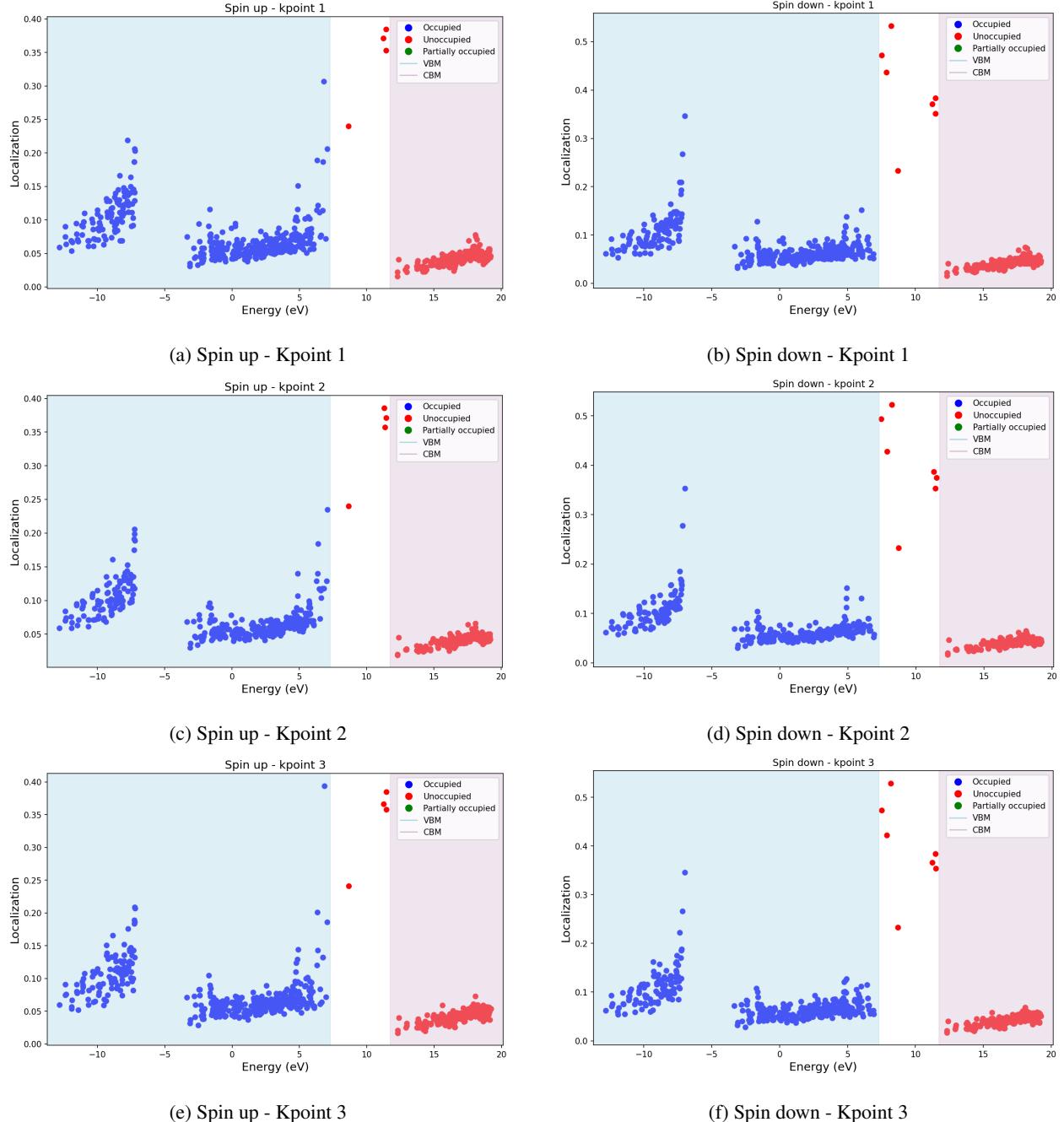


Figure 145: Localization factor using projected orbitals (s, p, and d).

6.69 Complex: $(V_B - V_N)^{+4}$

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Table 65: $(V_B - V_N)^{+4}$

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
Up	1	429	–	< 0.1	–
	1	430	26, 41	0.149, 0.182	Y, Y
	1	431	70, 103	0.172, 0.172	Y, Y
	1	432	26	0.108	Y
	2	429	–	< 0.1	–
	2	430	26, 41	0.216, 0.122	Y, Y
	2	431	70	0.223	Y
	2	432	41, 103	0.105, 0.188	Y, Y
	3	429	–	< 0.1	–
	3	430	26	0.221	Y
Down	3	431	70, 103	0.172, 0.172	Y, Y
	3	432	41	0.158	Y
	1	426	174, 201	0.193, 0.193	Y, Y
	1	427	148	0.238	Y
	1	428	122, 148	0.309, 0.111	Y, Y
	1	429	–	< 0.1	–
	1	430	26, 41	0.160, 0.173	Y, Y
	1	431	70, 103	0.169, 0.169	Y, Y
	1	432	–	< 0.1	–
	2	426	174, 201	0.253, 0.161	Y, Y
	2	427	148, 201	0.158, 0.104	Y, Y
	2	428	122, 148	0.257, 0.163	Y, Y
	2	429	–	< 0.1	–
	2	430	26, 41	0.216, 0.125	Y, Y
	2	431	70	0.225	Y
	2	432	41, 103	0.103, 0.194	Y, Y
	3	426	174, 201	0.193, 0.193	Y, Y
	3	427	122, 148	0.135, 0.123	Y, Y
	3	428	122, 148	0.235, 0.201	Y, Y
	3	429	–	< 0.1	–
	3	430	26	0.220	Y
	3	431	70, 103	0.169, 0.169	Y, Y
	3	432	41	0.154	Y

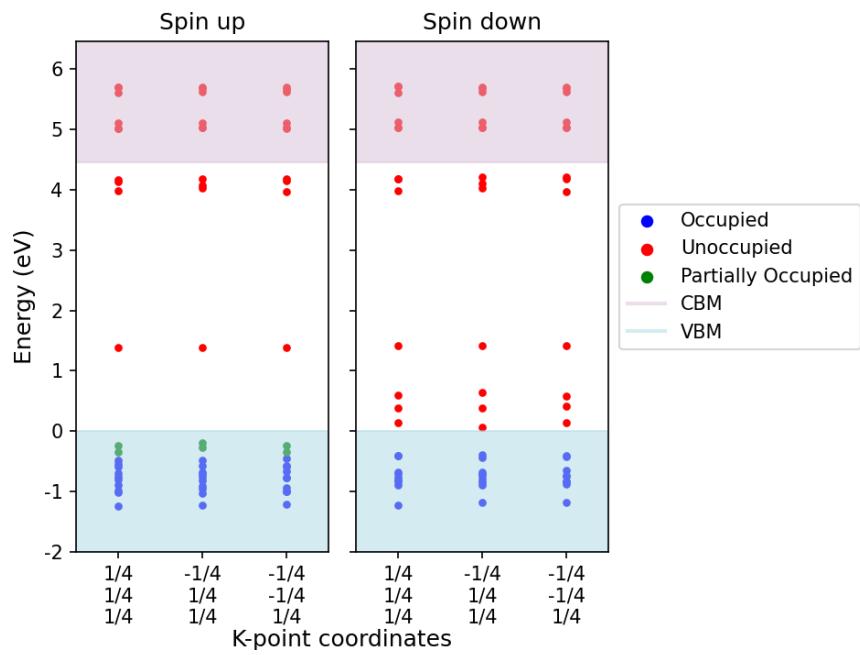


Figure 146: Kohn-Sham states.

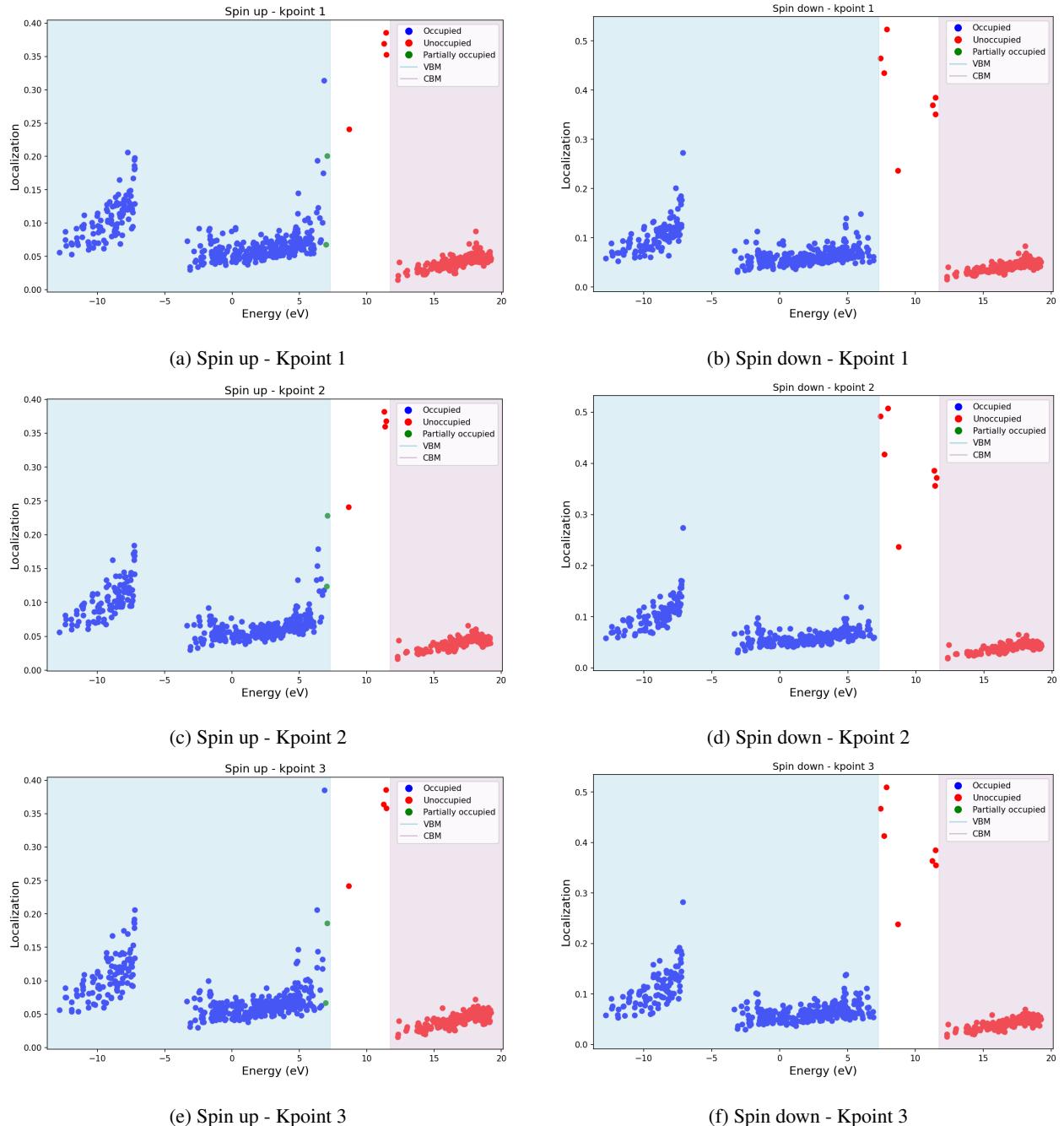


Figure 147: Localization factor using projected orbitals (s, p, and d).

6.70 Complex: $(V_B - V_N)^{-1}$

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Table 66: $(V_B - V_N)^{-1}$

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
Up	1	426	–	< 0.1	–
	1	427	122, 148	0.209, 0.227	Y, Y
	1	428	174, 201	0.122, 0.122	Y, Y
	1	429	174, 201	0.222, 0.222	Y, Y
	1	430	26, 41	0.197, 0.136	Y, Y
	2	426	–	< 0.1	–
	2	427	122, 148	0.241, 0.184	Y, Y
	2	428	174	0.184	Y
	2	429	174, 201	0.171, 0.272	Y, Y
	3	426	–	< 0.1	–
Down	3	427	122, 148	0.282, 0.155	Y, Y
	3	428	148, 174, 201	0.121, 0.121, 0.121	Y, Y, Y
	3	429	174, 201	0.222, 0.222	Y, Y
	3	430	26	0.226	Y
	1	426	–	< 0.1	–
	1	427	174, 201	0.222, 0.222	Y, Y
	1	428	148	0.202	Y
	1	429	122, 148	0.306, 0.142	Y, Y
	1	430	26, 41	0.198, 0.133	Y, Y
	2	426	–	< 0.1	–

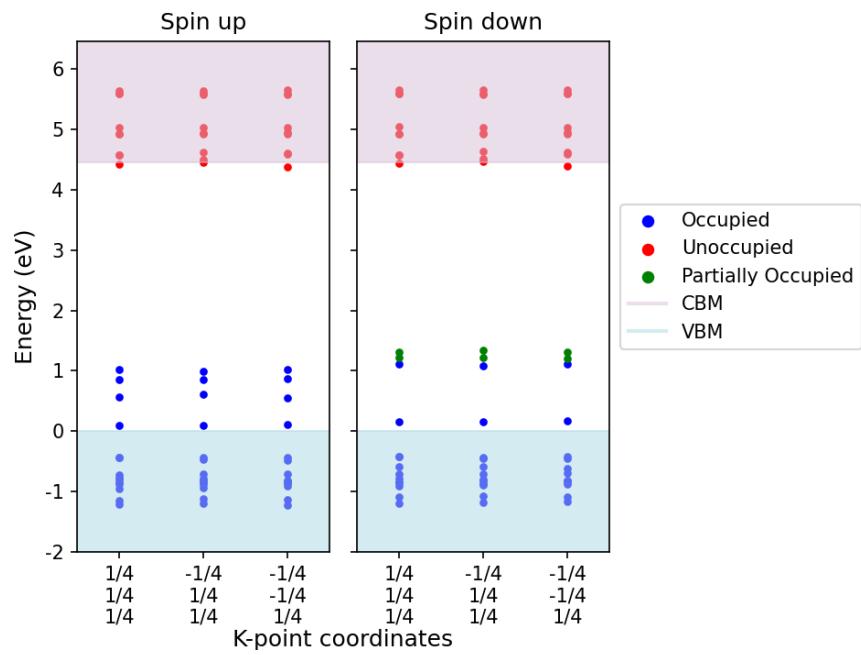


Figure 148: Kohn-Sham states.

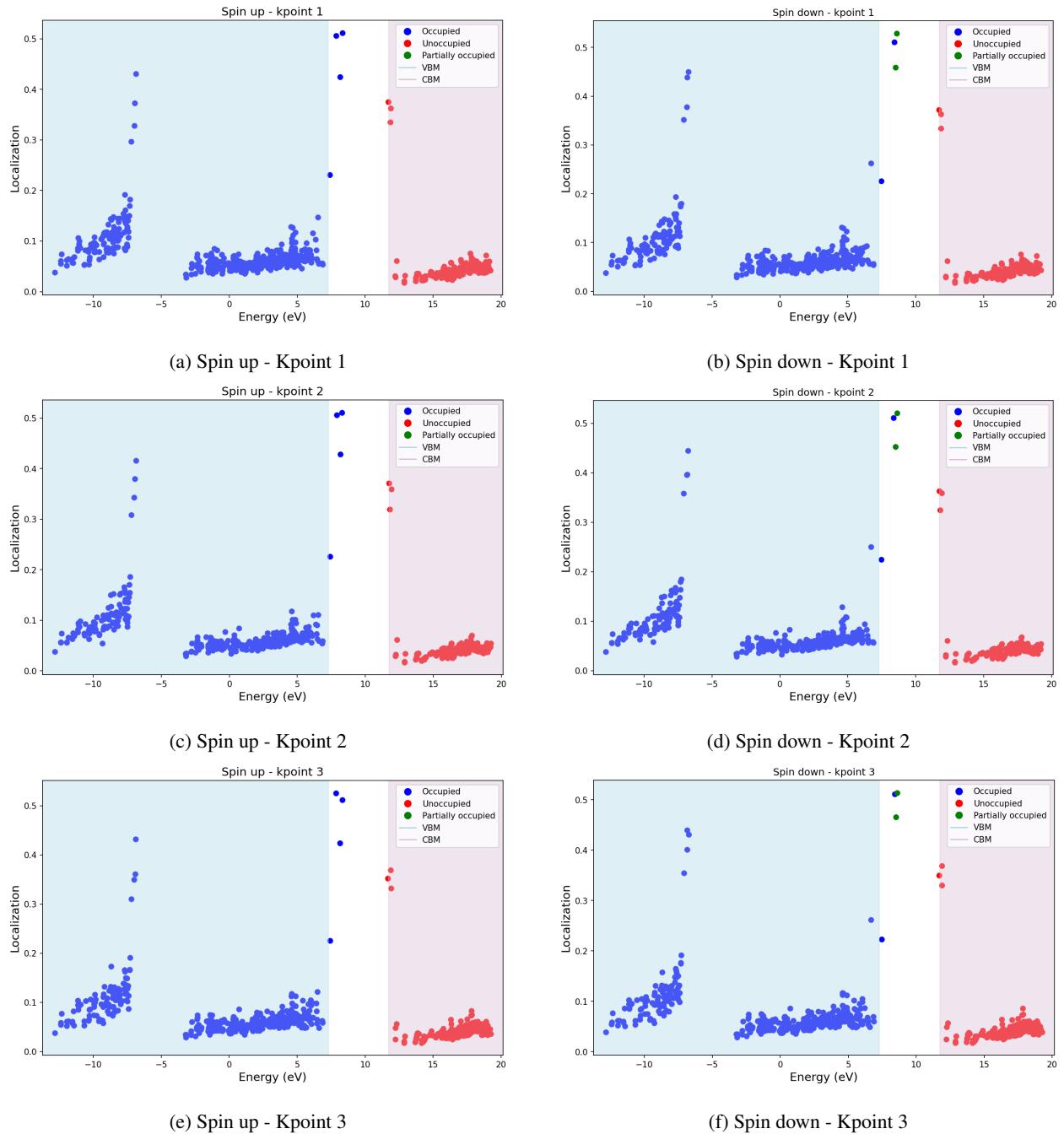


Figure 149: Localization factor using projected orbitals (s, p, and d).

6.71 Complex: $(V_B - V_N)^{-2}$

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Table 67: $(V_B - V_N)^{-2}$

Spin	Kpoint	Band	Index	tot (s+p+d)	Neighbor
Up	1	426	–	< 0.1	–
	1	427	174, 201	0.223, 0.223	Y, Y
	1	428	148	0.174	Y
	1	429	122, 148	0.271, 0.186	Y, Y
	1	430	26, 41	0.174, 0.146	Y, Y
	2	426	–	< 0.1	–
	2	427	174, 201	0.252, 0.197	Y, Y
	2	428	122, 148, 201	0.128, 0.131, 0.114	Y, Y, Y
	2	429	122, 148	0.235, 0.221	Y, Y
	3	426	–	< 0.1	–
Down	3	427	174, 201	0.223, 0.223	Y, Y
	3	428	122	0.170	Y
	3	429	122, 148	0.201, 0.254	Y, Y
	3	430	26	0.211	Y
	1	426	–	< 0.1	–
	1	427	174, 201	0.223, 0.223	Y, Y
	1	428	148	0.174	Y
	1	429	122, 148	0.271, 0.186	Y, Y
	1	430	26, 41	0.174, 0.146	Y, Y
	2	426	–	< 0.1	–
	2	427	174, 201	0.252, 0.197	Y, Y
	2	428	122, 148, 201	0.128, 0.131, 0.114	Y, Y, Y
	2	429	122, 148	0.235, 0.221	Y, Y
	3	426	–	< 0.1	–
	3	427	174, 201	0.223, 0.223	Y, Y
	3	428	122	0.170	Y
	3	429	122, 148	0.201, 0.254	Y, Y
	3	430	26	0.211	Y

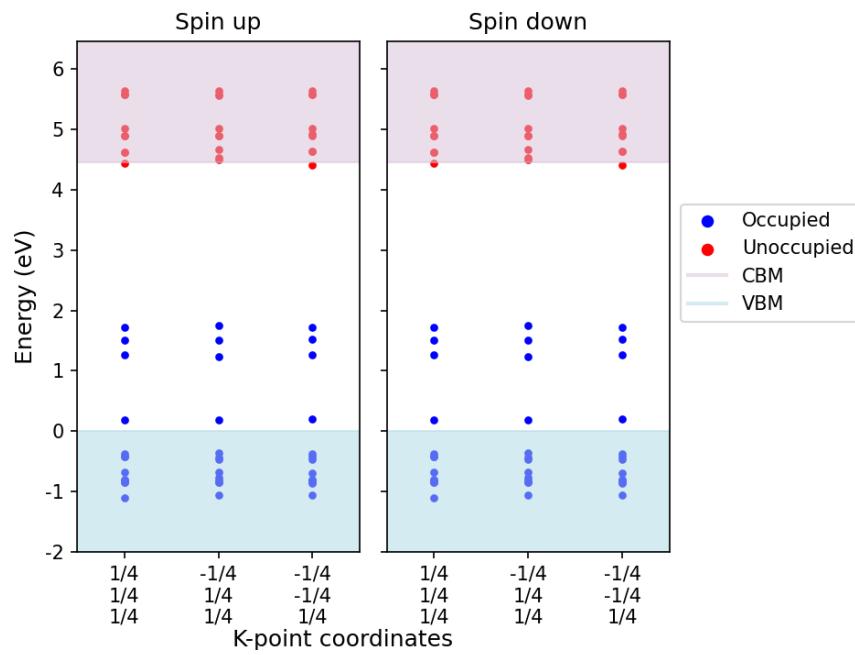


Figure 150: Kohn-Sham states.

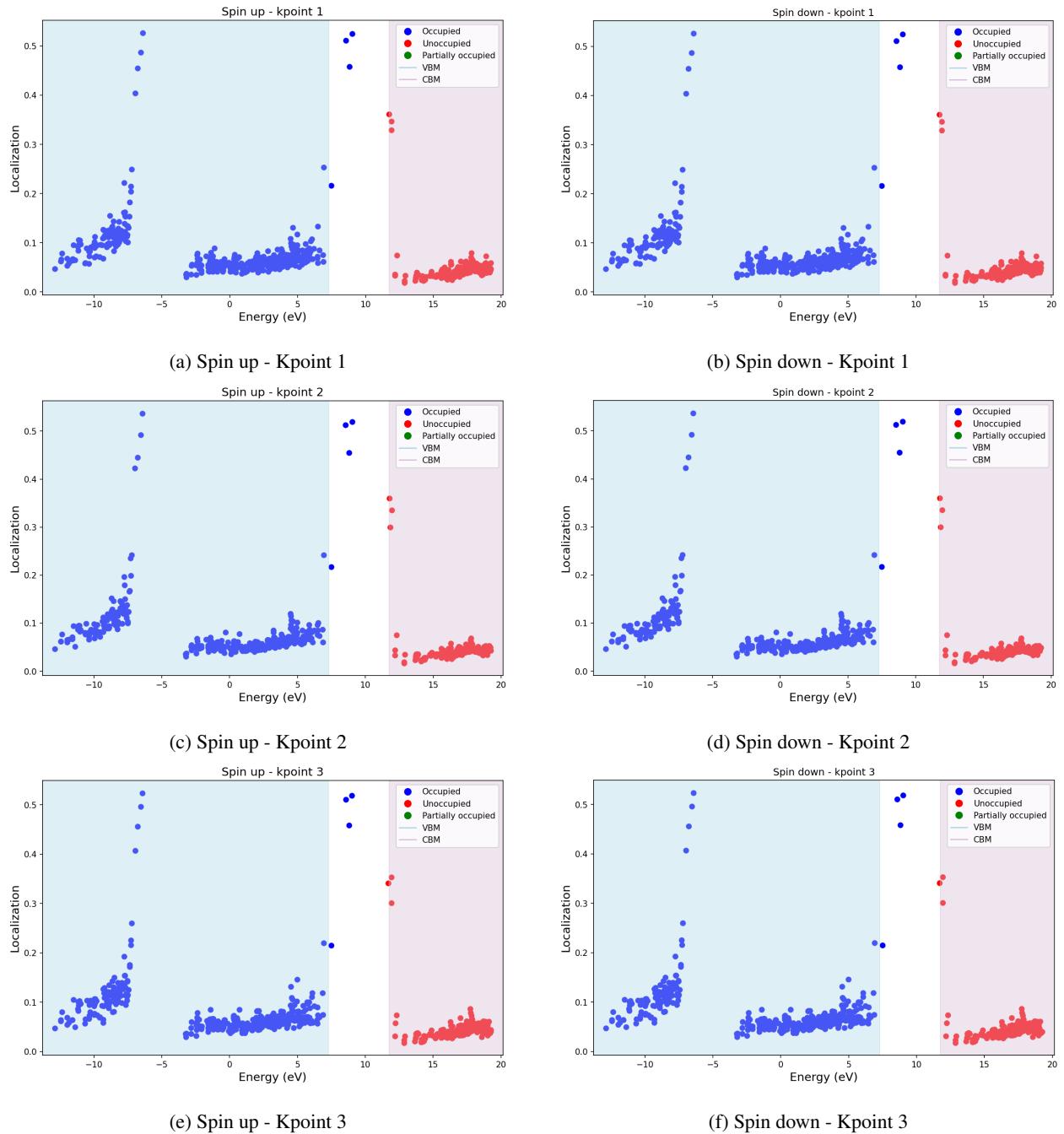


Figure 151: Localization factor using projected orbitals (s, p, and d).

6.72 Complex: $(V_B - V_N)^{-3}$

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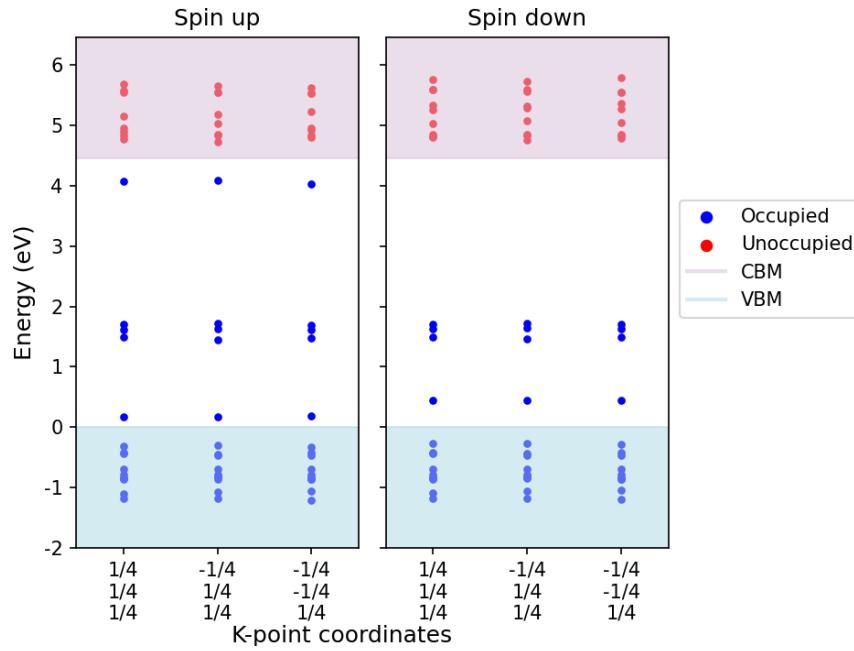


Figure 152: Kohn-Sham states.

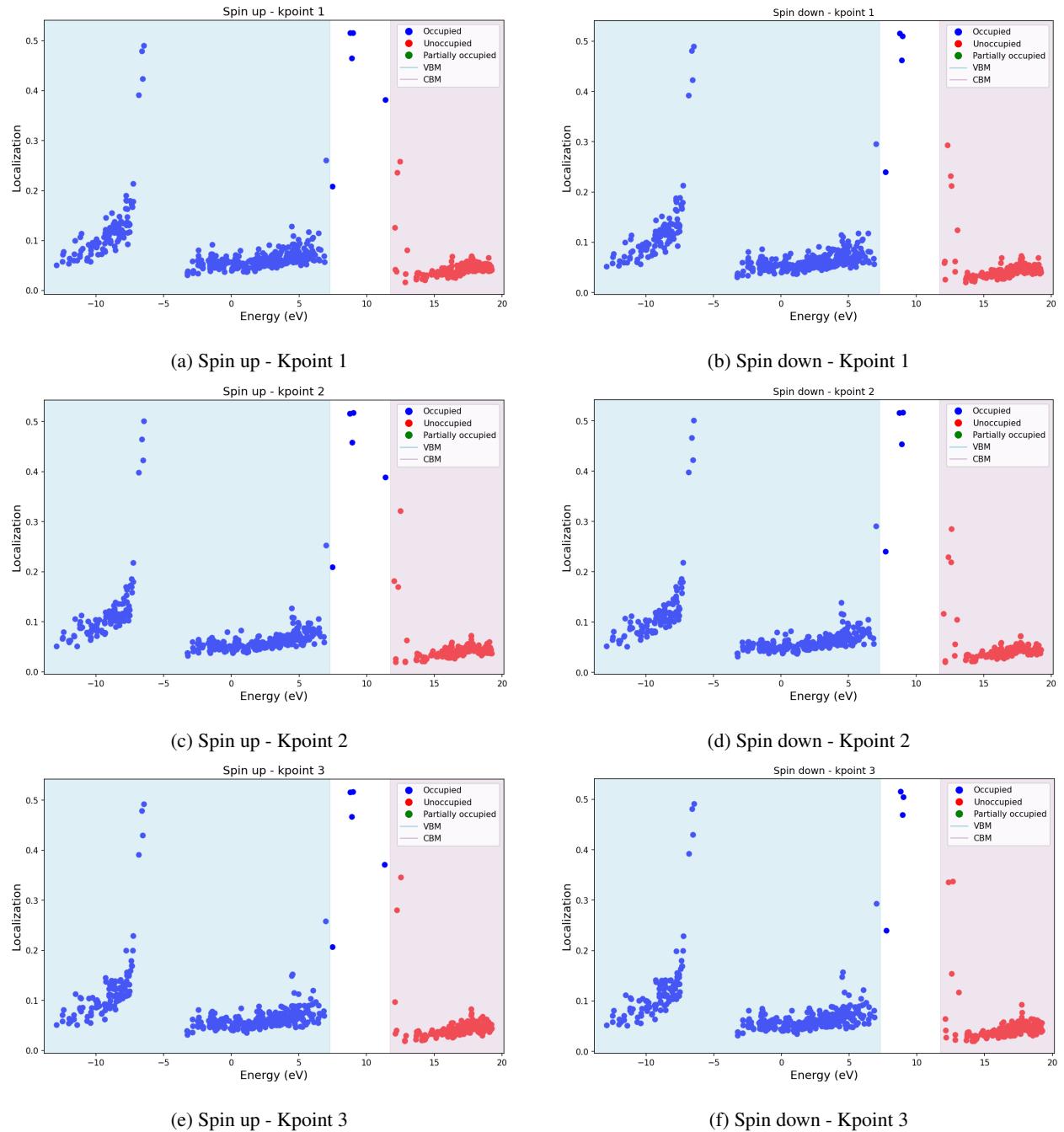


Figure 153: Localization factor using projected orbitals (s, p, and d).

6.73 Complex: $(V_B - V_N)^{-4}$

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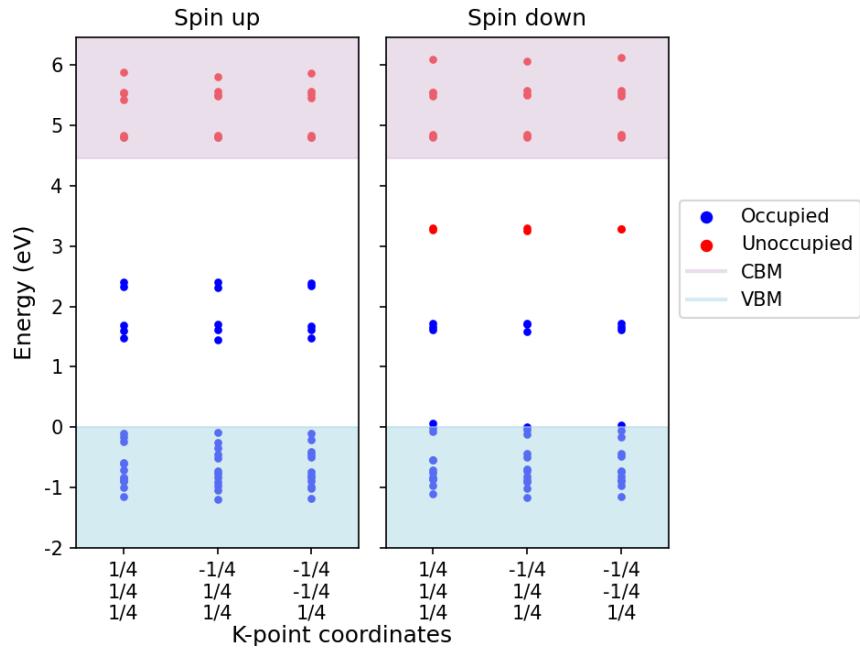


Figure 154: Kohn-Sham states.

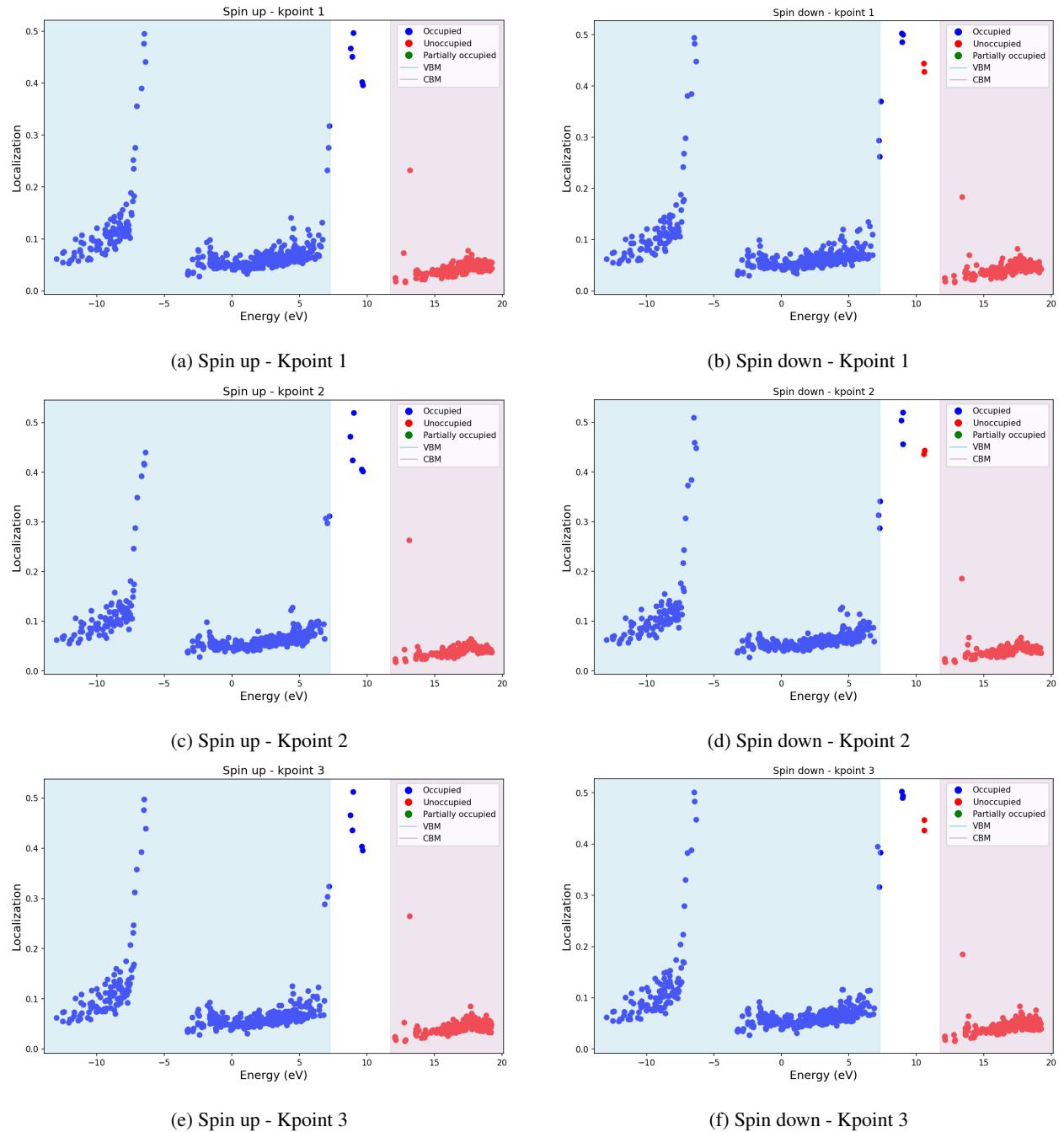


Figure 155: Localization factor using projected orbitals (s, p, and d).

6.74 Complex: $(C_B - V_N)^0$

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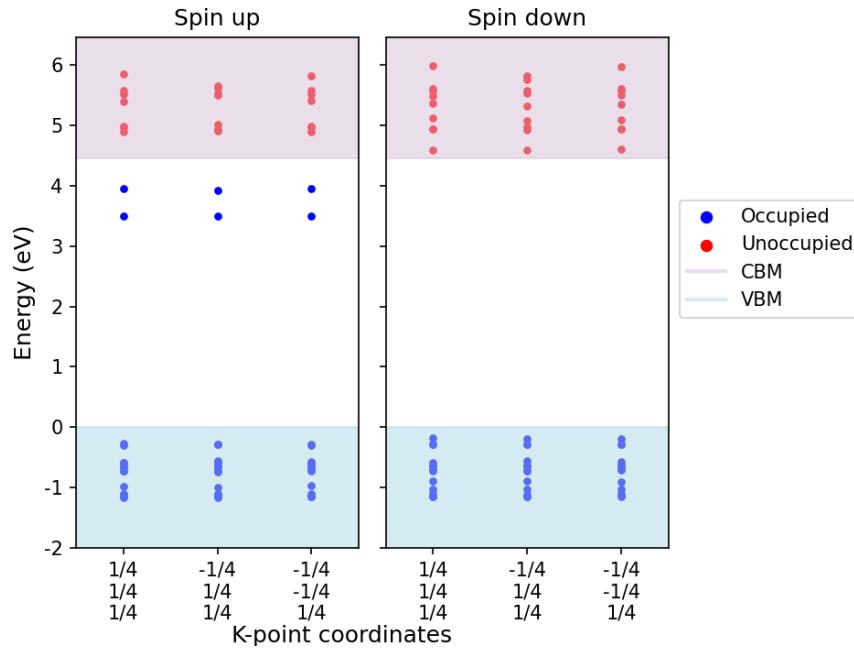


Figure 156: Kohn-Sham states.

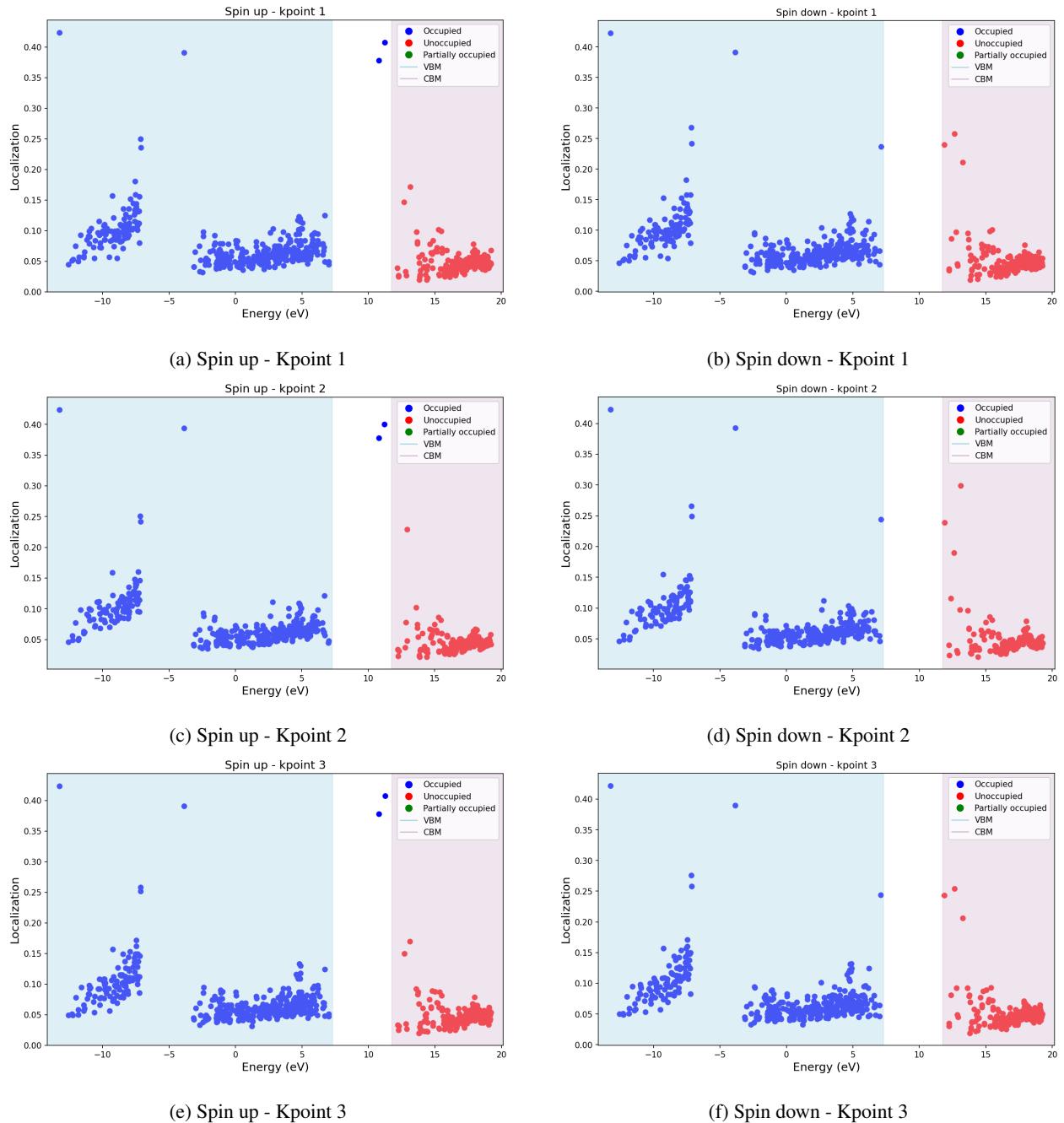


Figure 157: Localization factor using projected orbitals (s, p, and d).

6.75 Complex: $(C_B - V_N)^{+1}$

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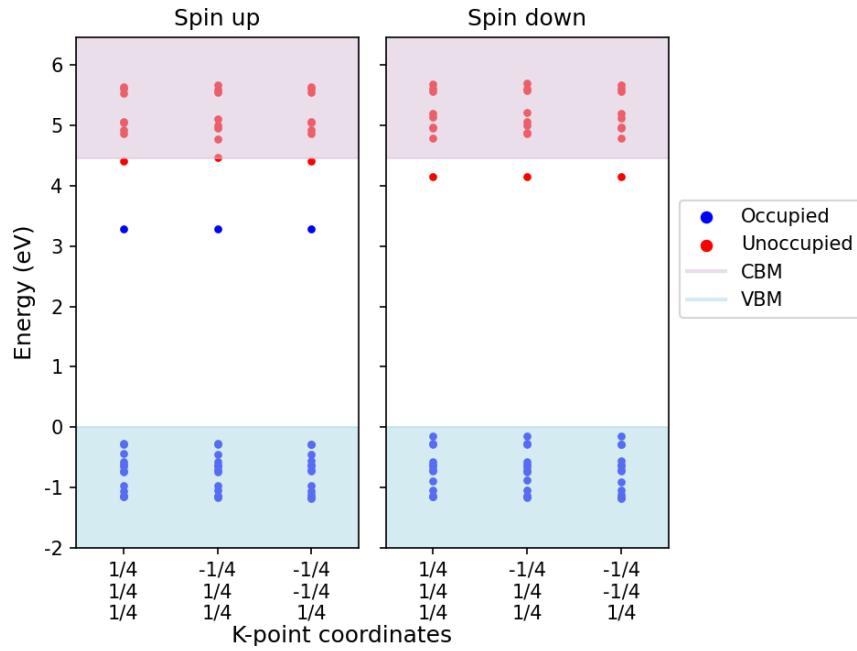


Figure 158: Kohn-Sham states.

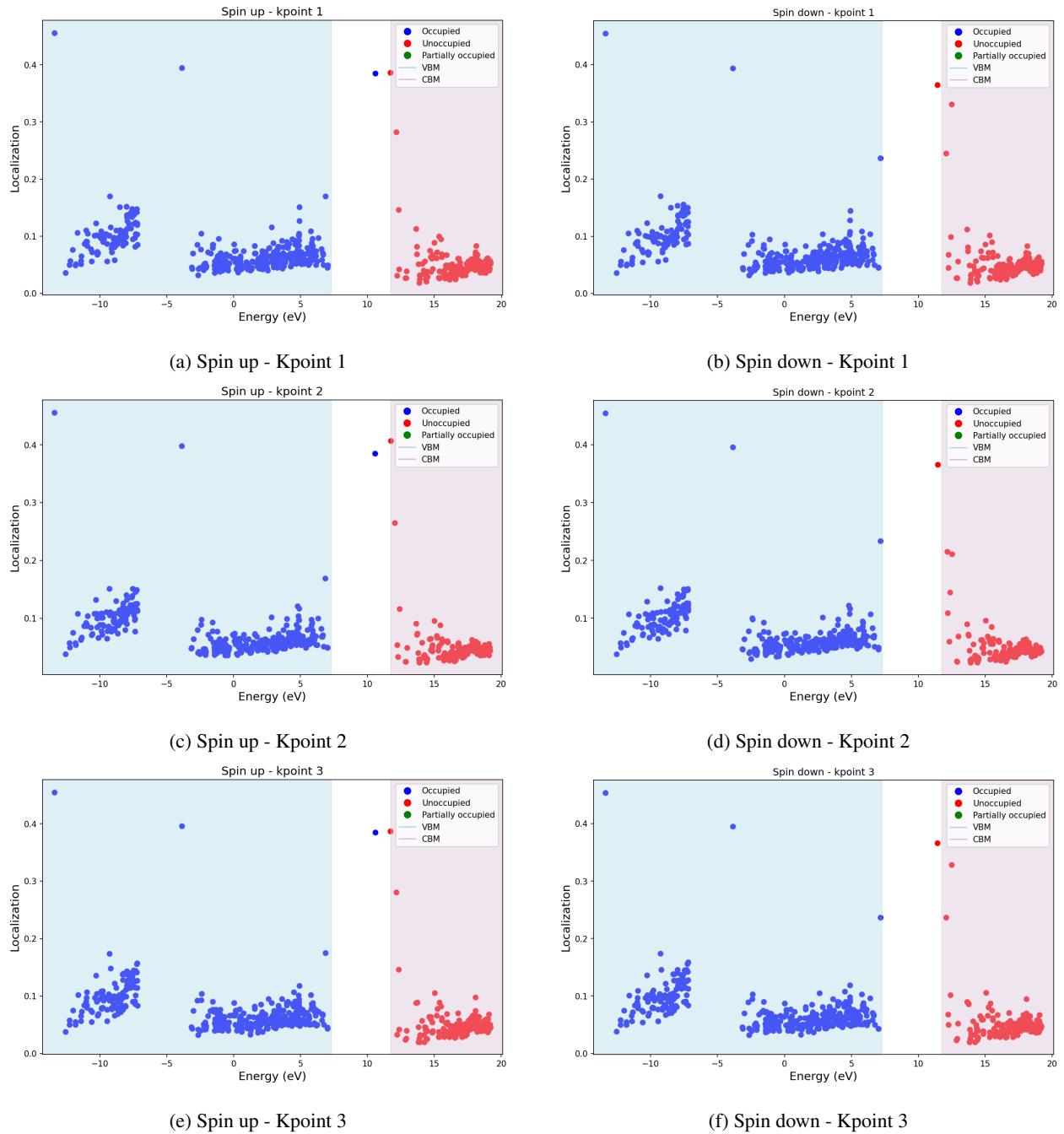


Figure 159: Localization factor using projected orbitals (s, p, and d).

6.76 Complex: $(C_B - V_N)^{+2}$

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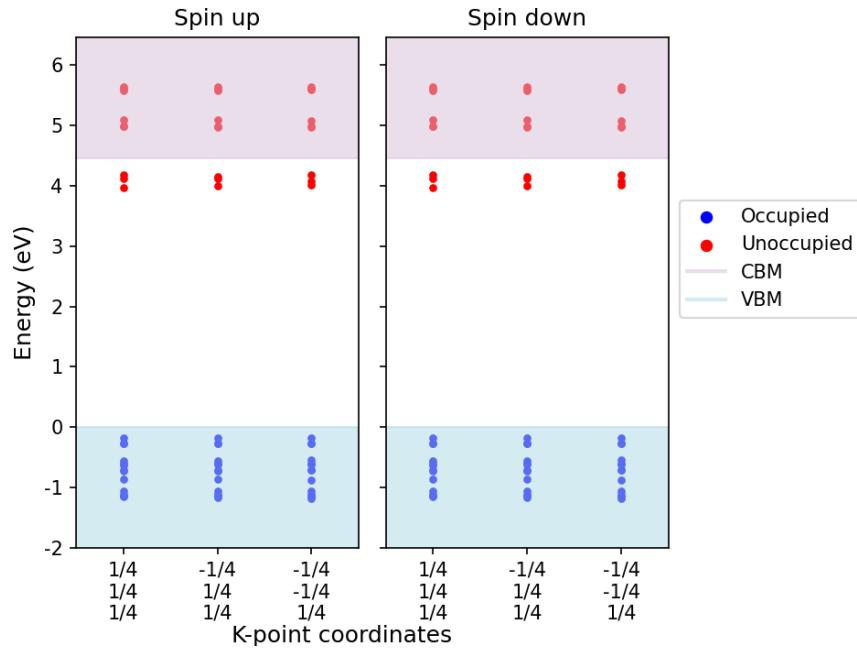


Figure 160: Kohn-Sham states.

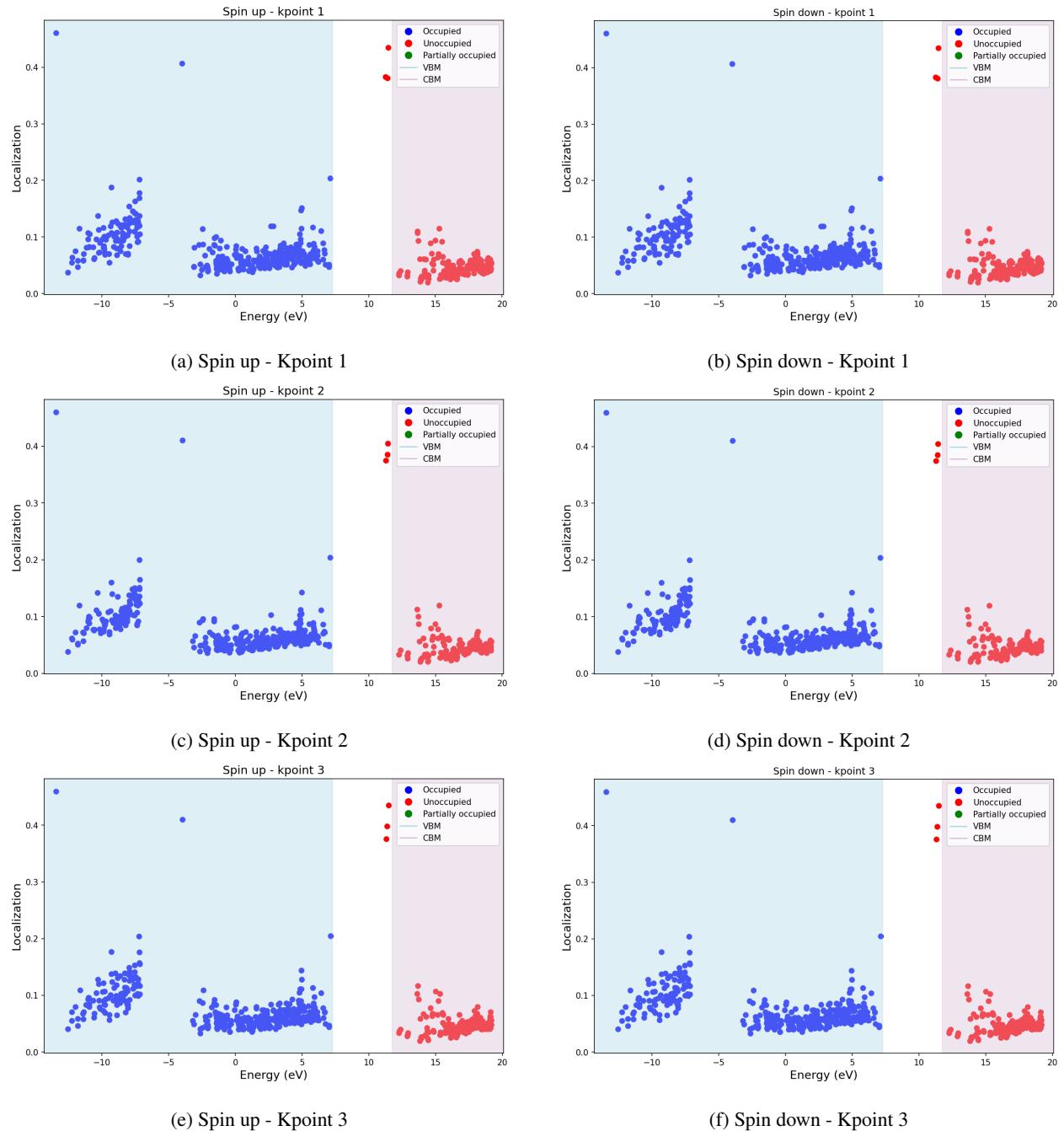


Figure 161: Localization factor using projected orbitals (s, p, and d).

6.77 Complex: $(C_B - V_N)^{+3}$

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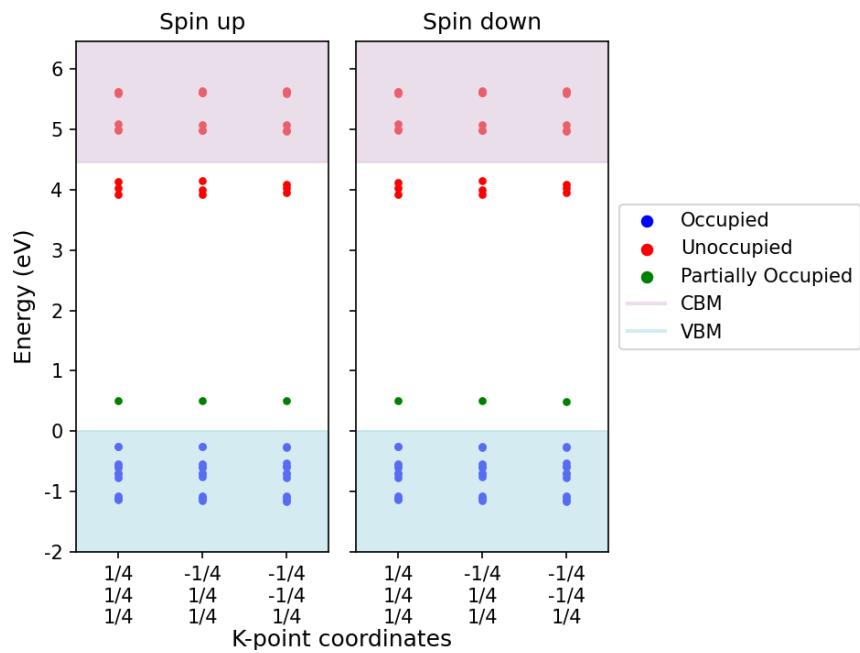


Figure 162: Kohn-Sham states.

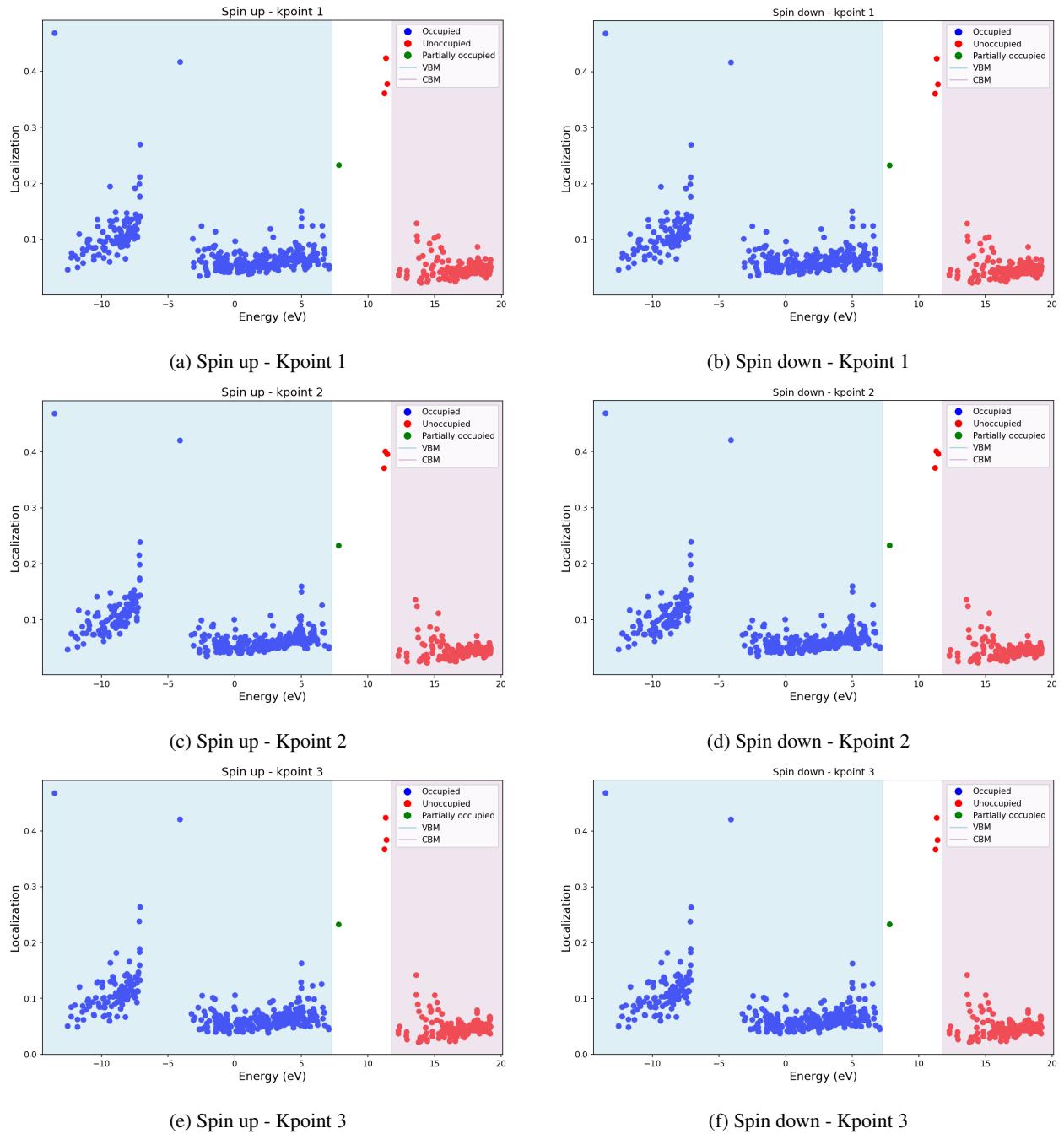


Figure 163: Localization factor using projected orbitals (s, p, and d).

6.78 Complex: $(C_B - V_N)^{+4}$

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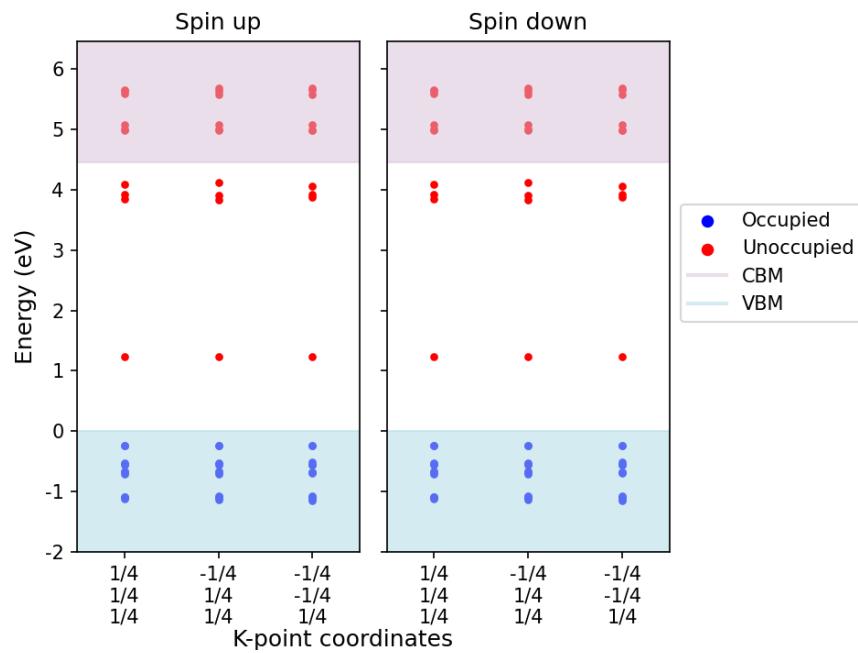


Figure 164: Kohn-Sham states.

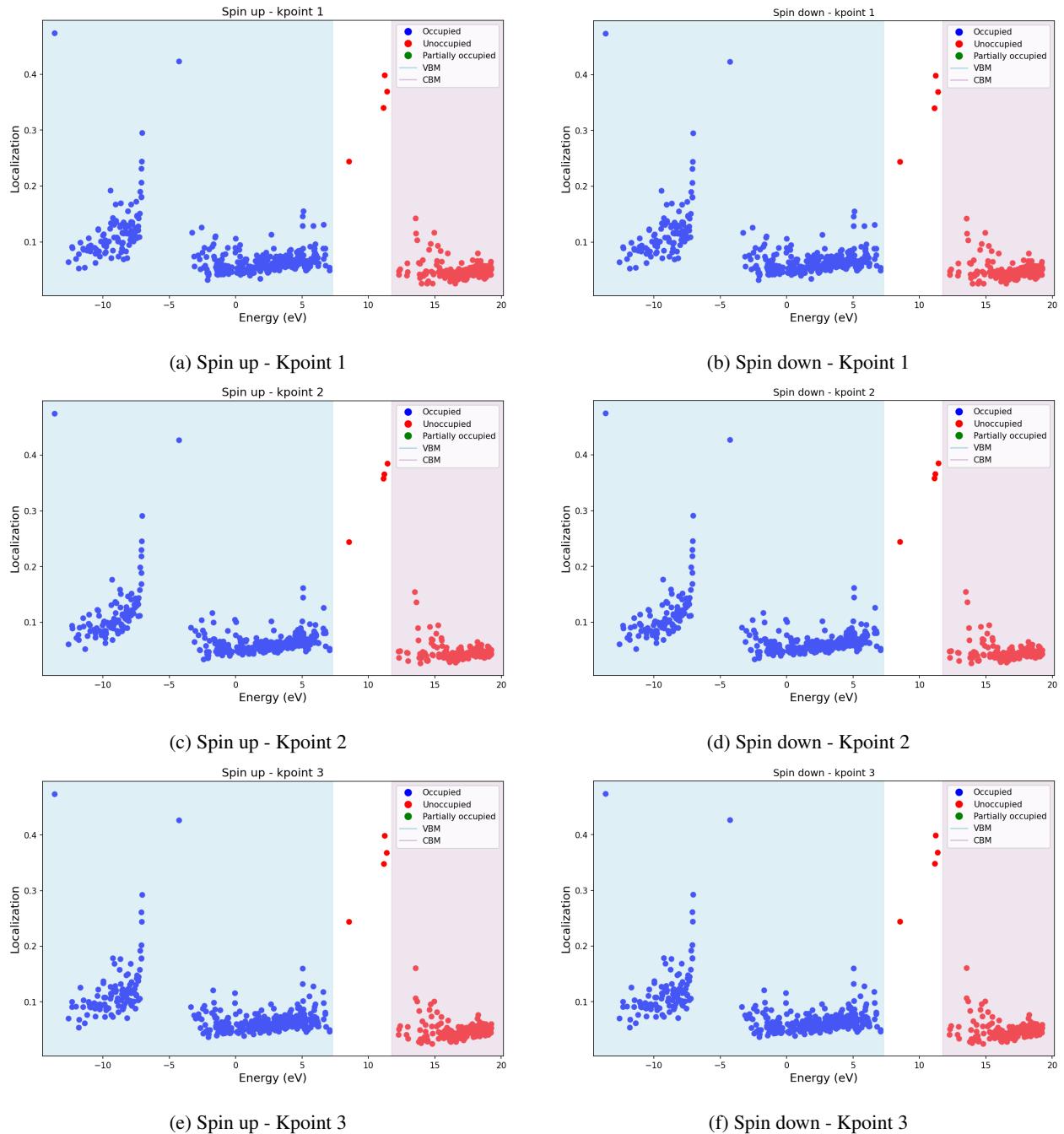


Figure 165: Localization factor using projected orbitals (s, p, and d).

6.79 Complex: $(C_B - V_N)^{-1}$

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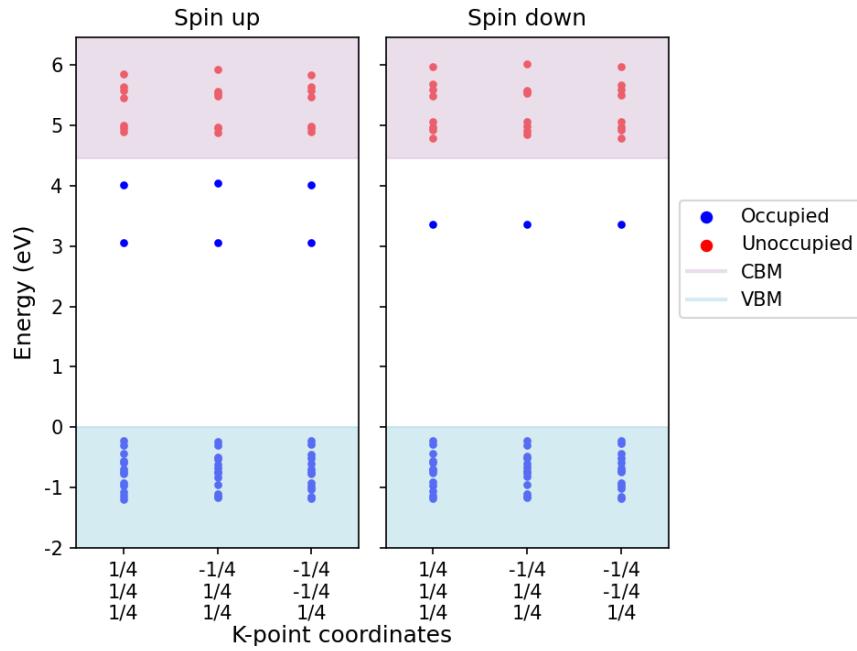


Figure 166: Kohn-Sham states.

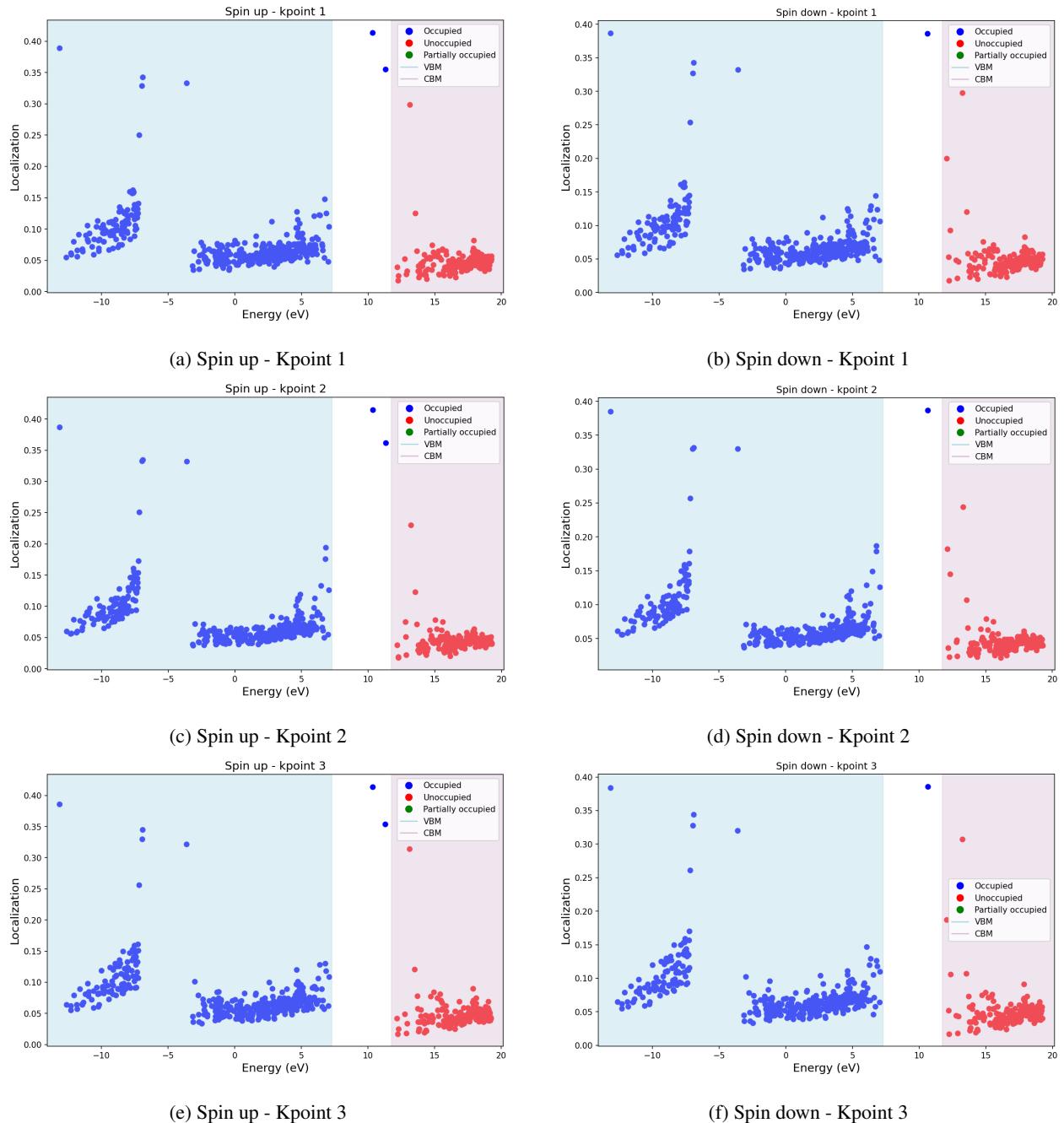


Figure 167: Localization factor using projected orbitals (s, p, and d).

6.80 Complex: $(C_B - V_N)^{-2}$

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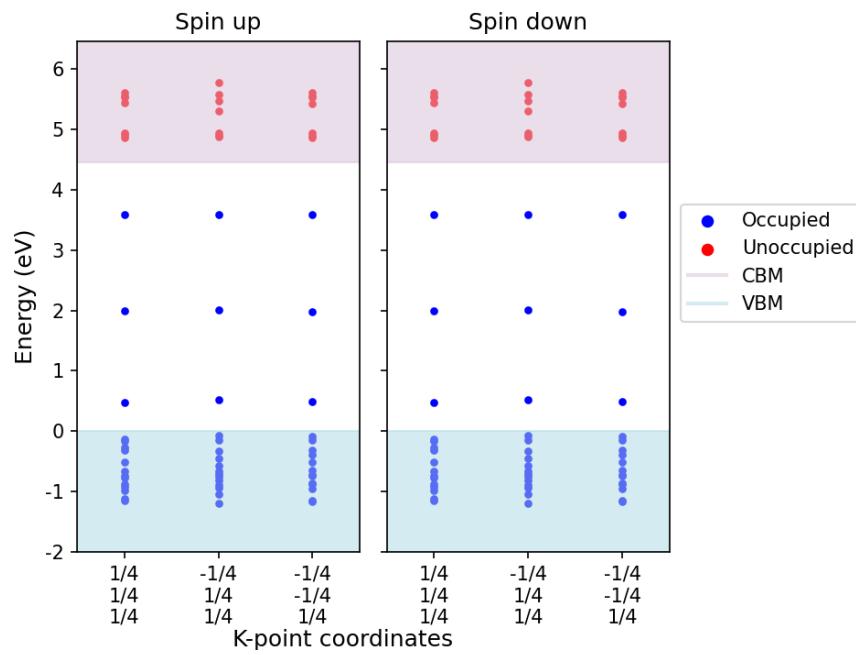


Figure 168: Kohn-Sham states.

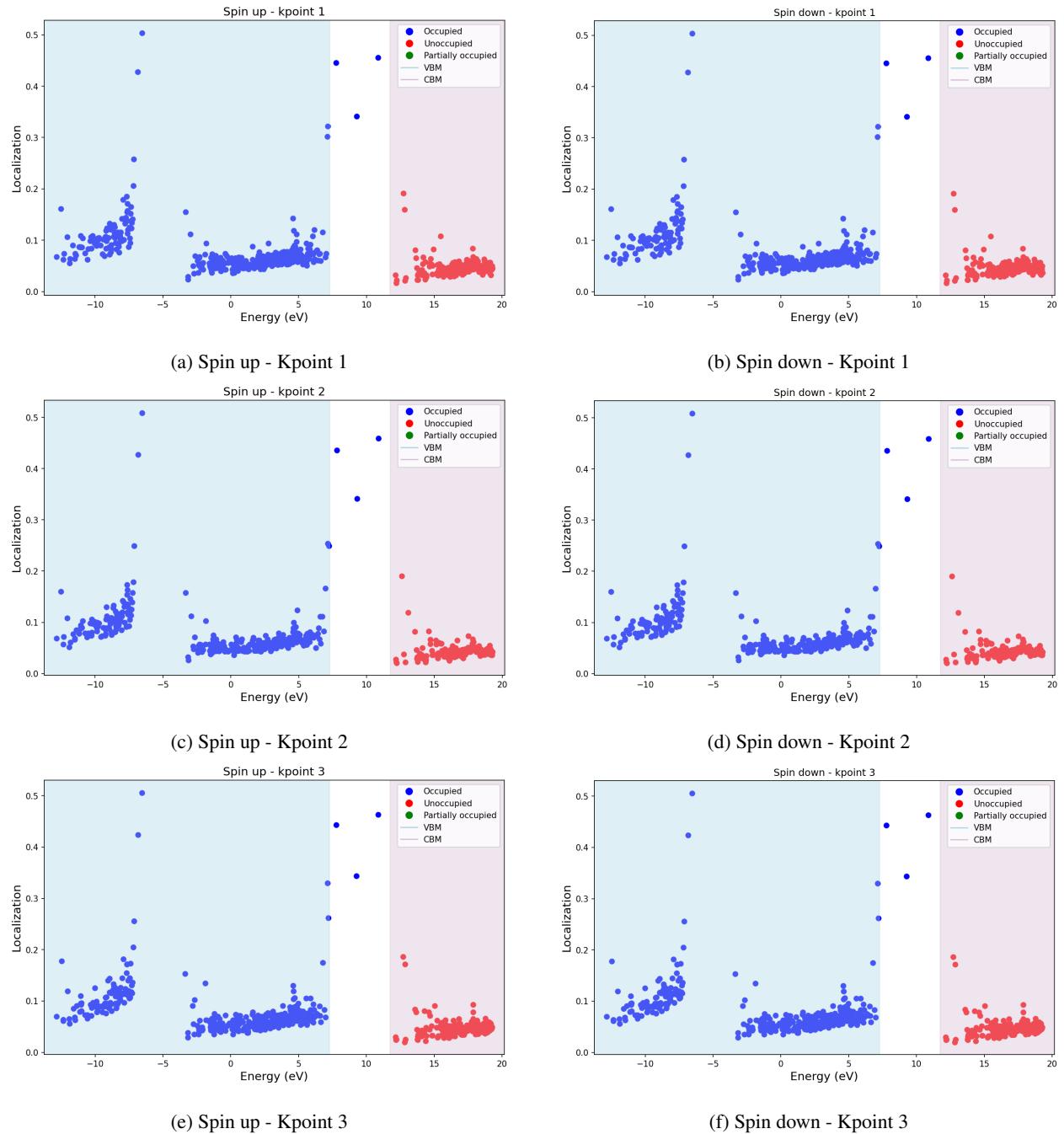


Figure 169: Localization factor using projected orbitals (s, p, and d).

6.81 Complex: $(C_B - V_N)^{-3}$

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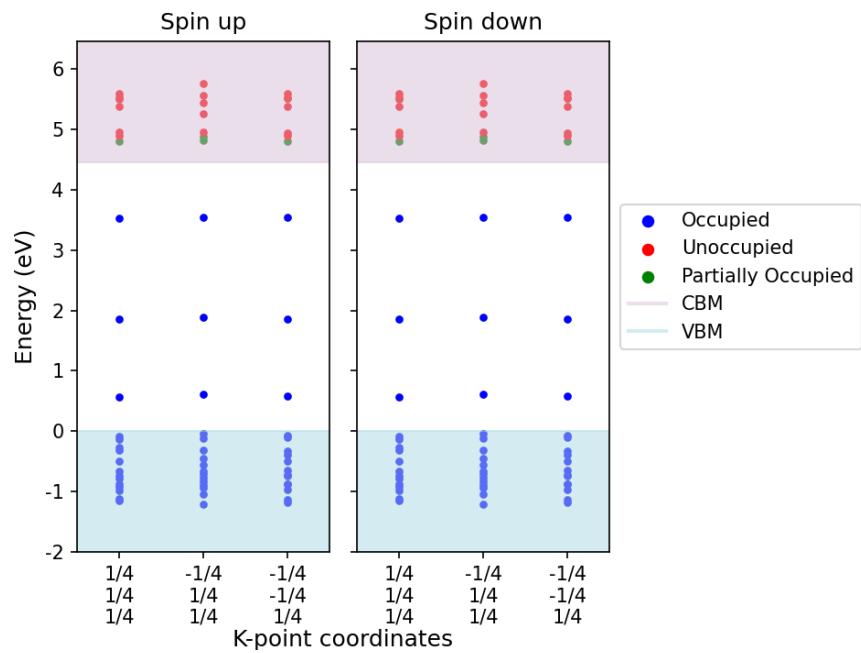


Figure 170: Kohn-Sham states.

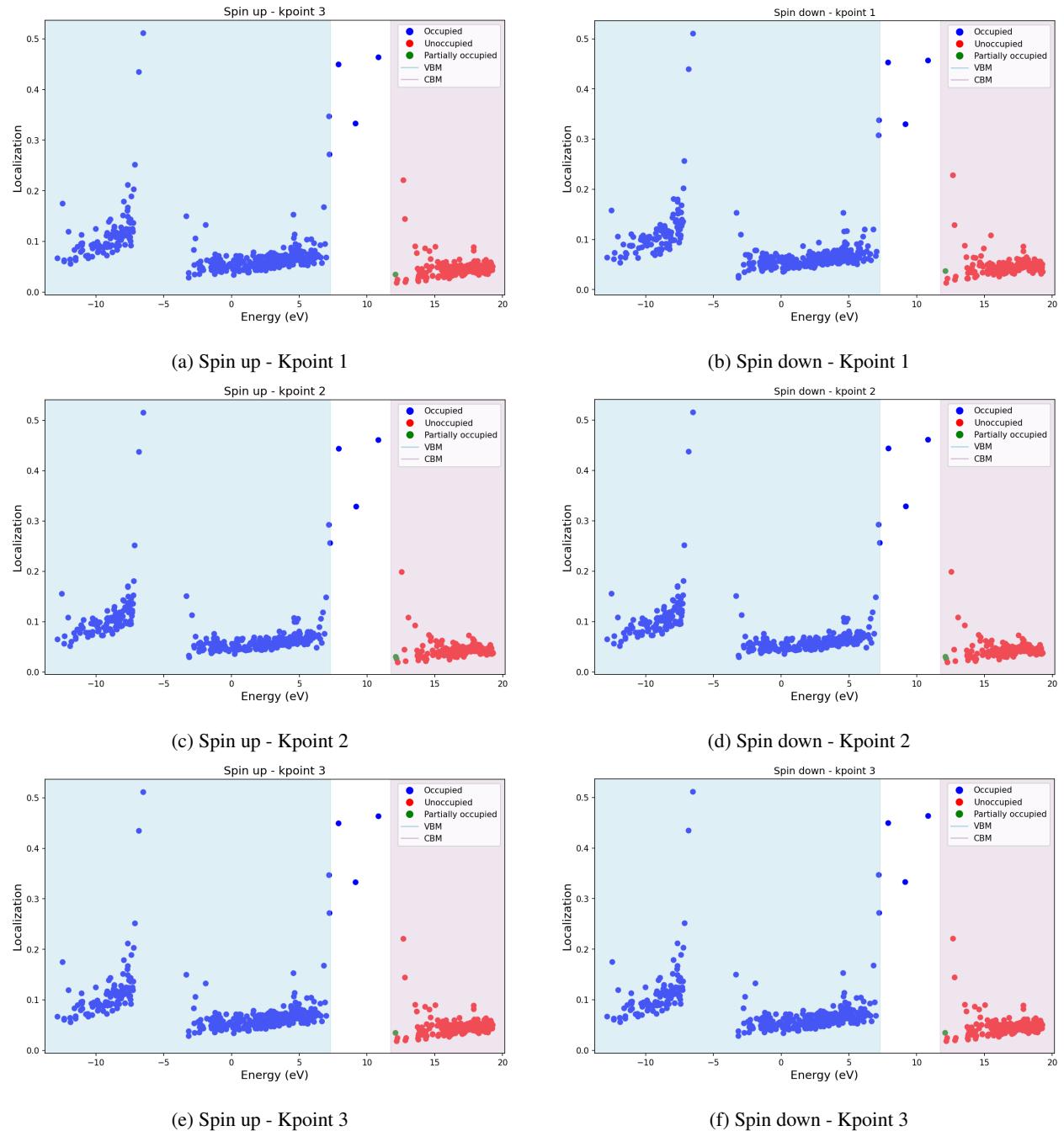


Figure 171: Localization factor using projected orbitals (s, p, and d).

6.82 Complex: $(C_B - V_N)^{-4}$

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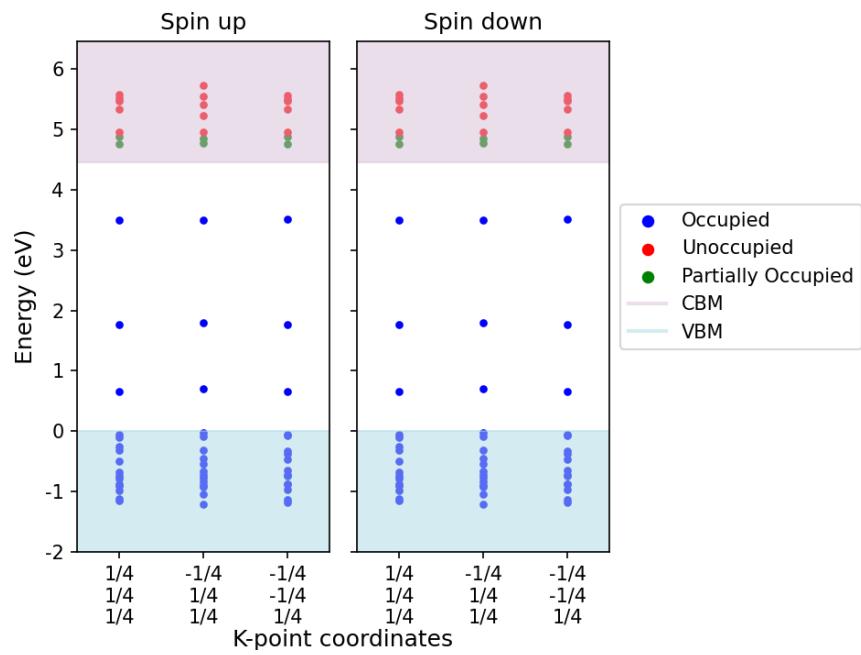


Figure 172: Kohn-Sham states.

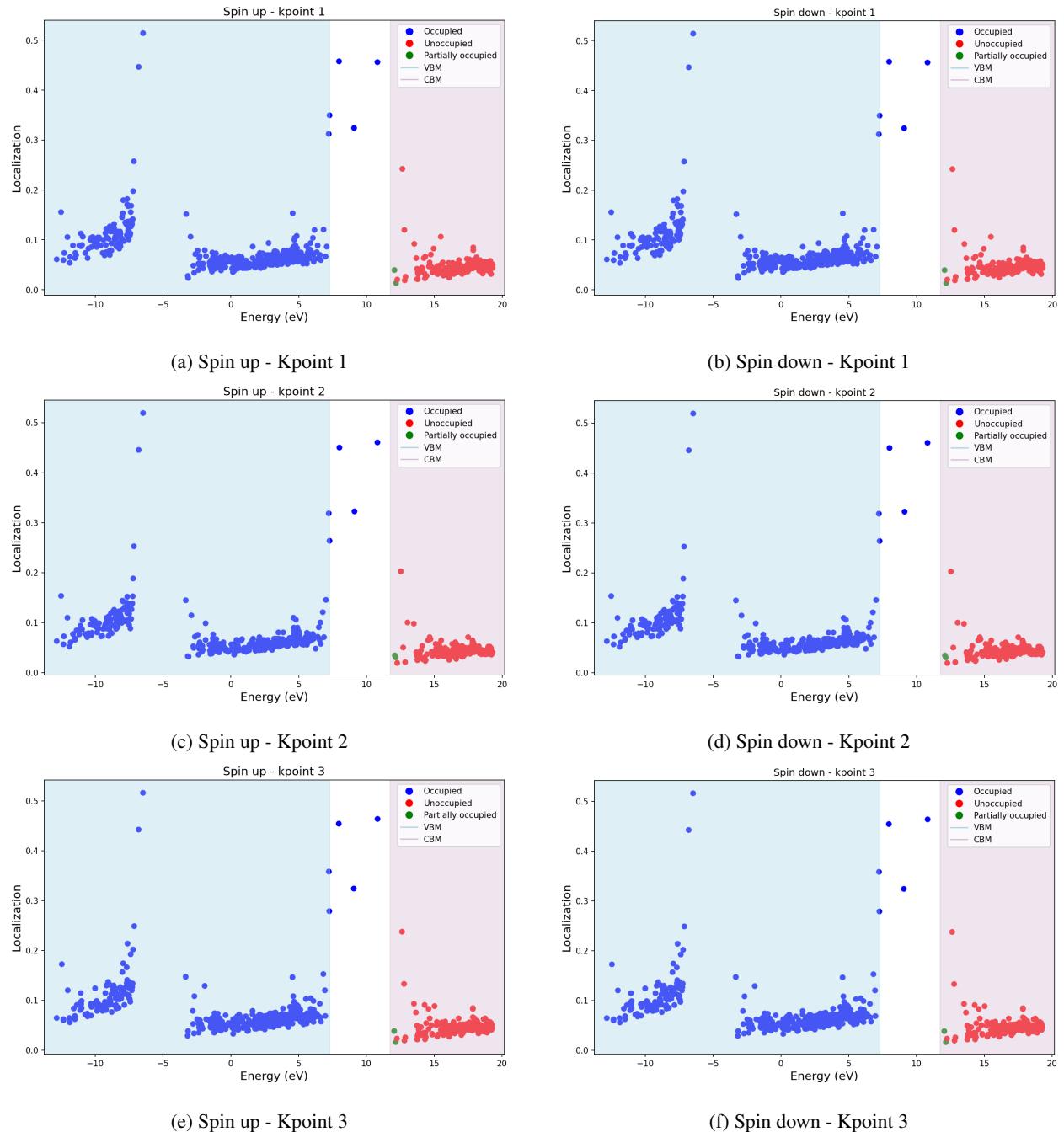


Figure 173: Localization factor using projected orbitals (s, p, and d).

6.83 Complex: $(C_N - V_B)^0$

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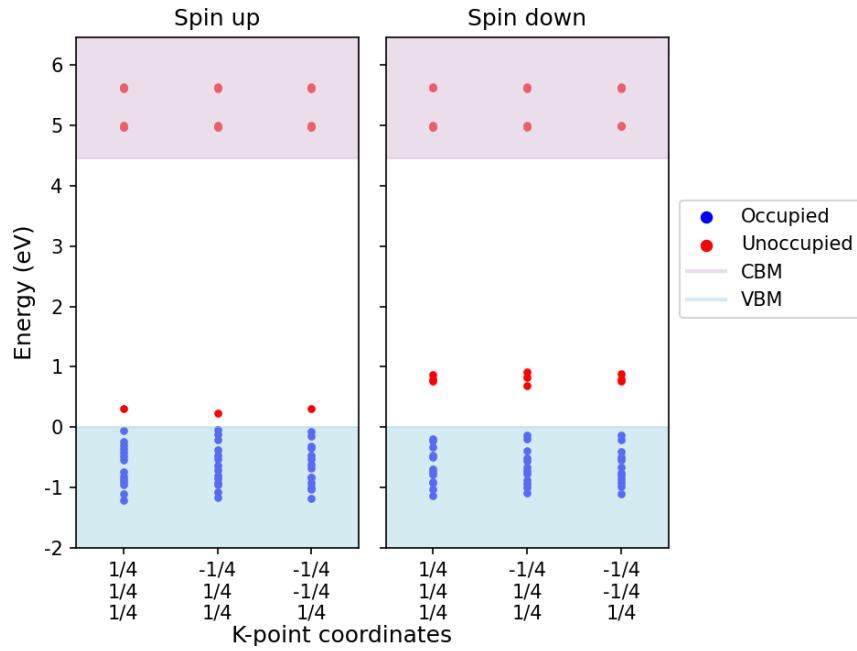


Figure 174: Kohn-Sham states.

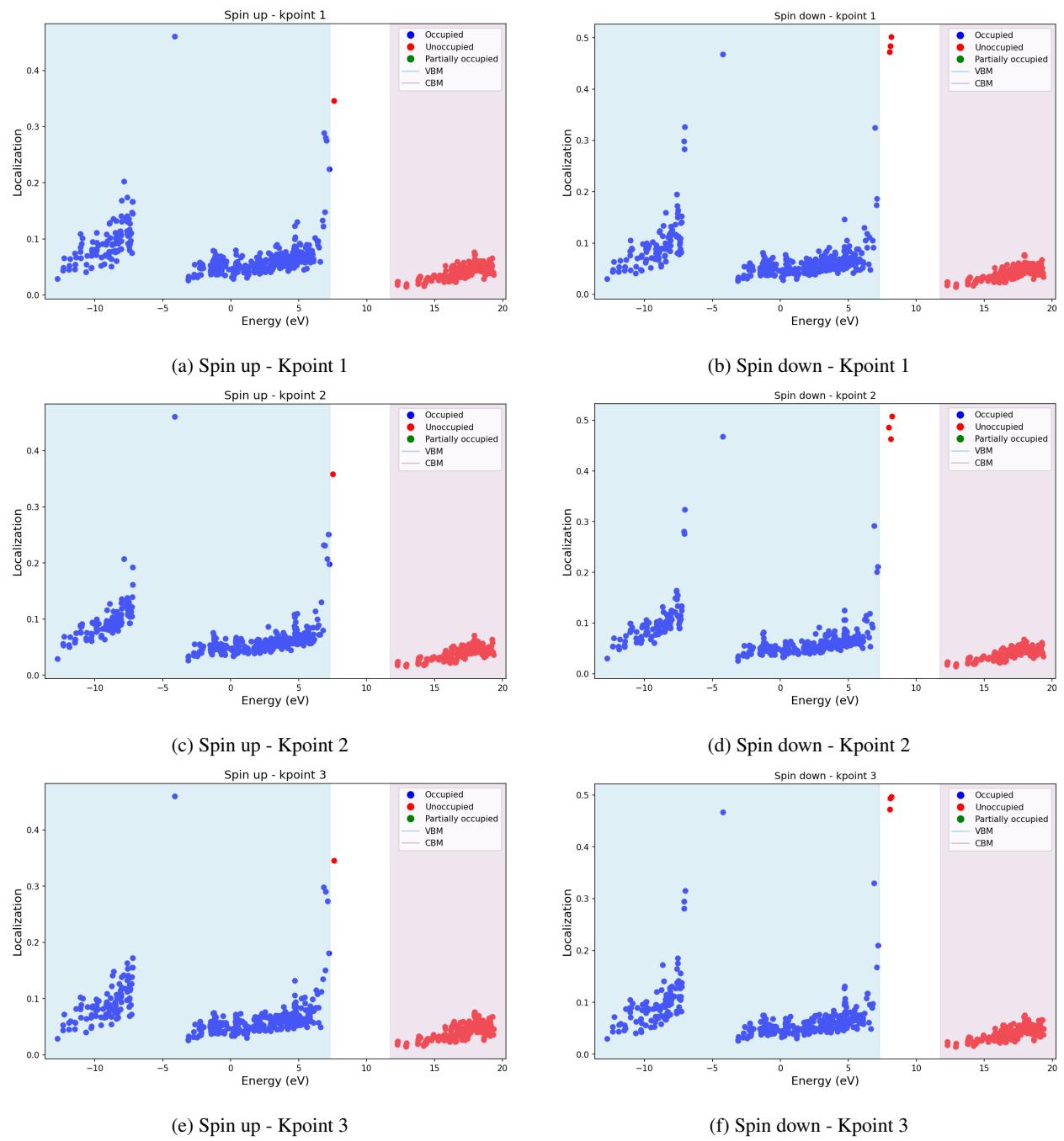


Figure 175: Localization factor using projected orbitals (s, p, and d).

6.84 Complex: $(C_N - V_B)^{+1}$

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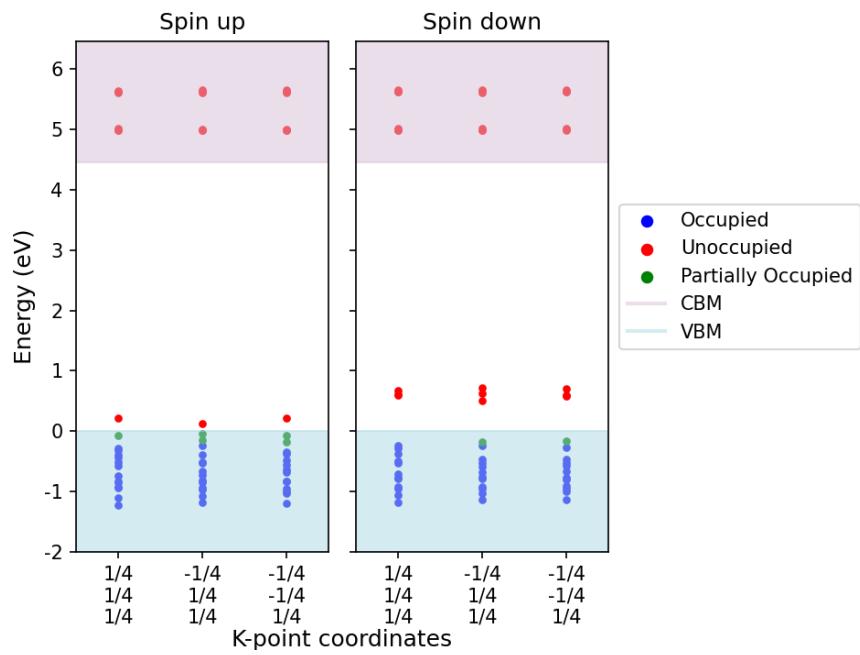


Figure 176: Kohn-Sham states.

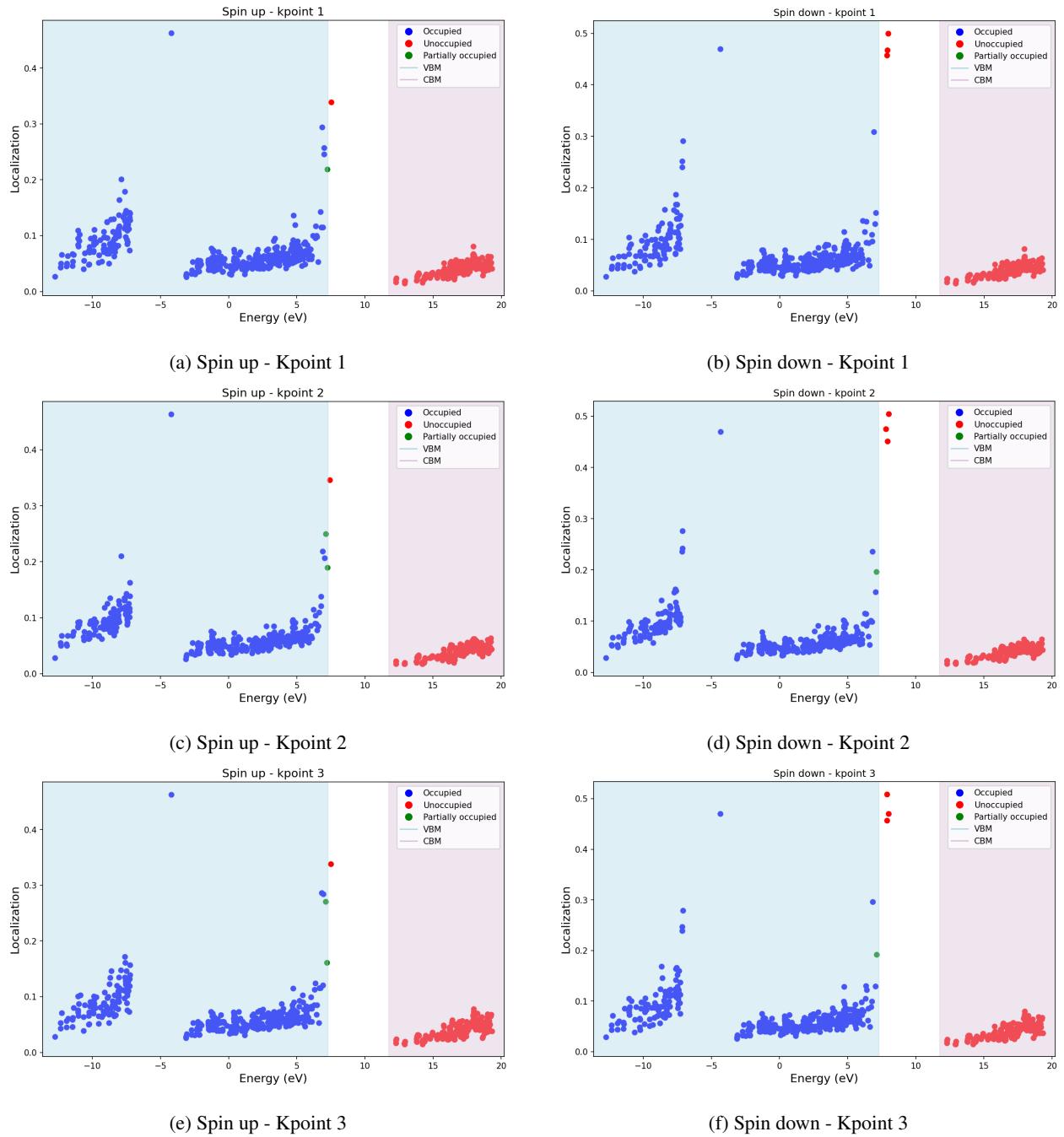


Figure 177: Localization factor using projected orbitals (s, p, and d).

6.85 Complex: $(C_N - V_B)^{+2}$

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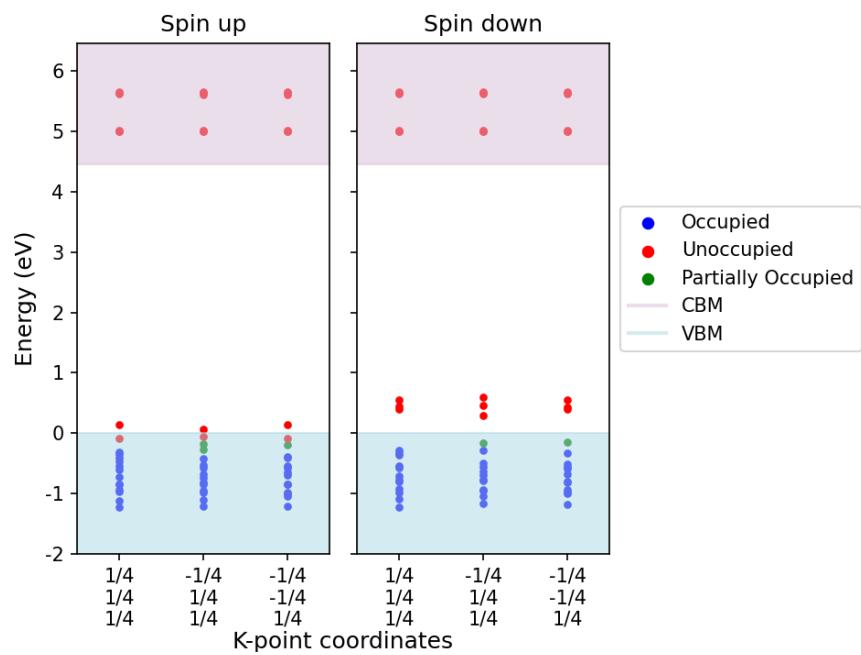


Figure 178: Kohn-Sham states.

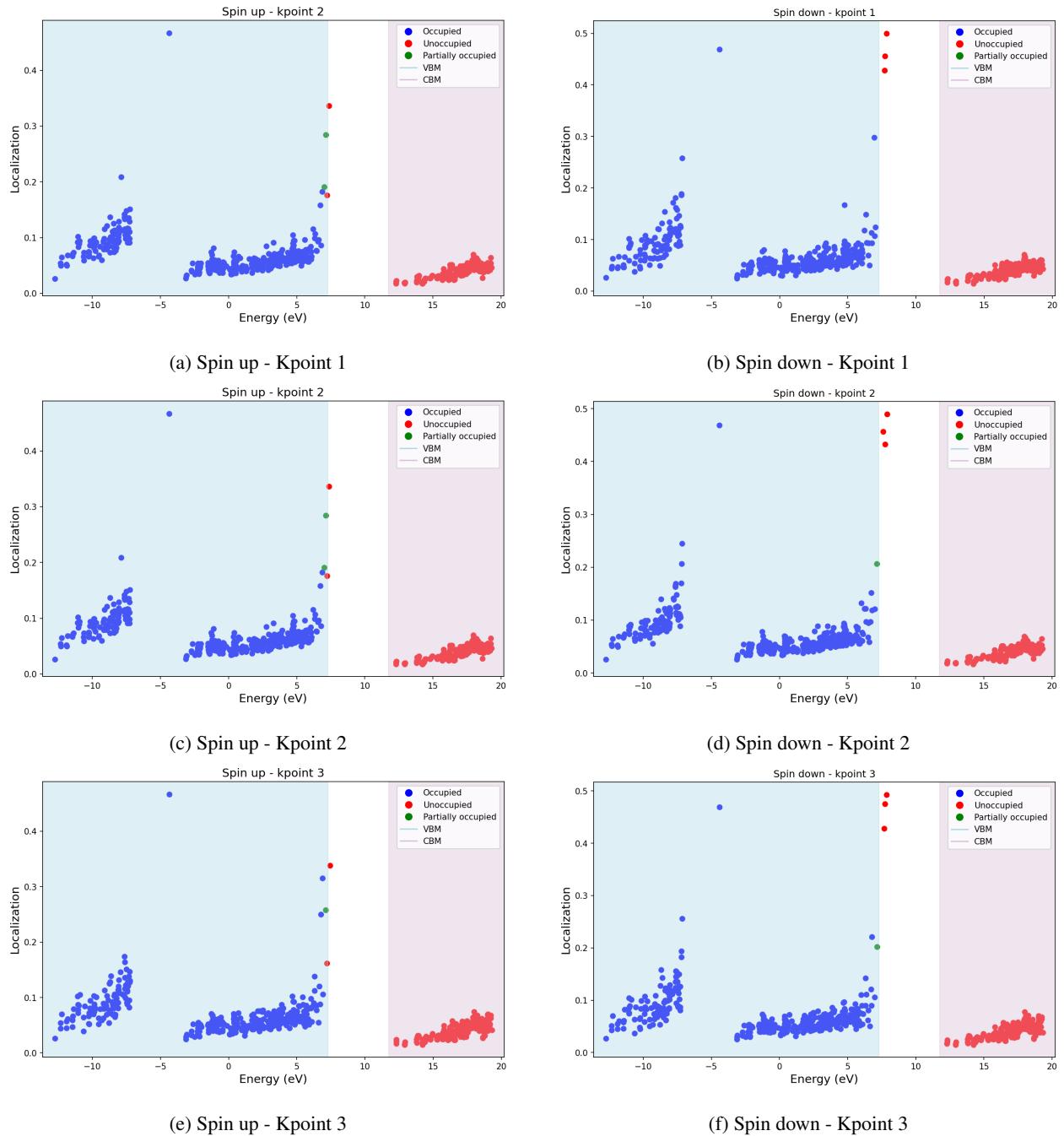


Figure 179: Localization factor using projected orbitals (s, p, and d).

6.86 Complex: $(C_N - V_B)^{+3}$

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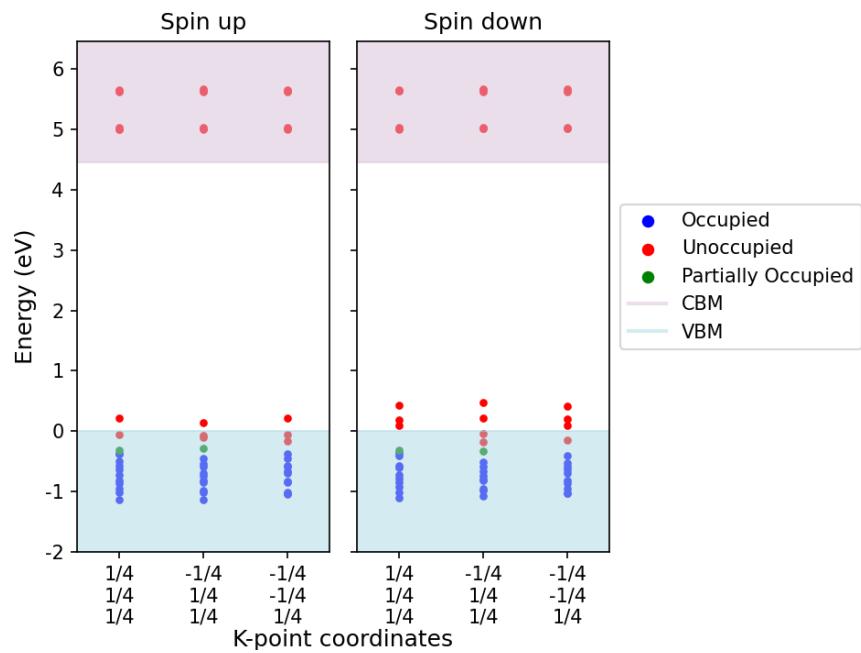


Figure 180: Kohn-Sham states.

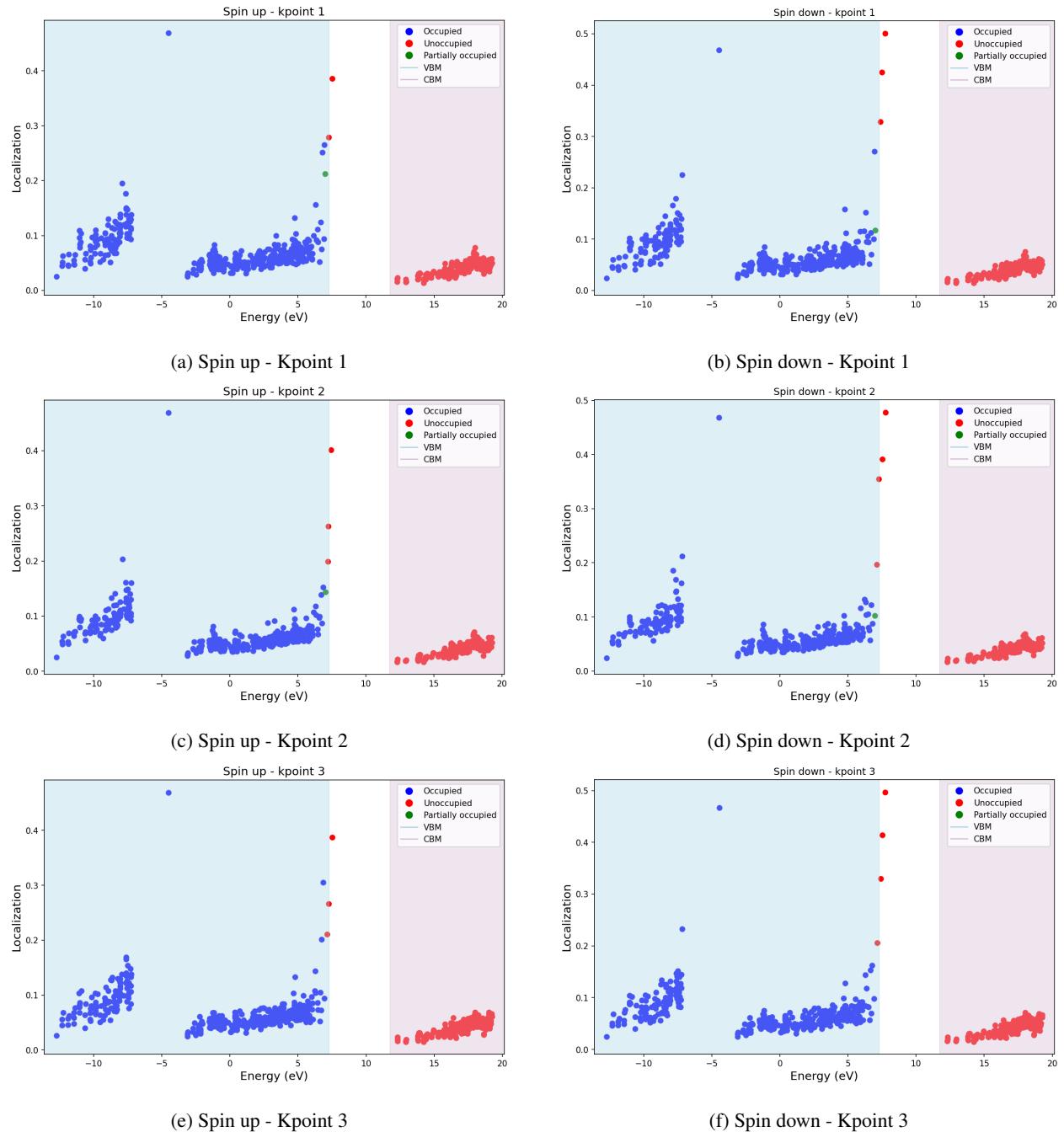


Figure 181: Localization factor using projected orbitals (s, p, and d).

6.87 Complex: $(C_N - V_B)^{+4}$

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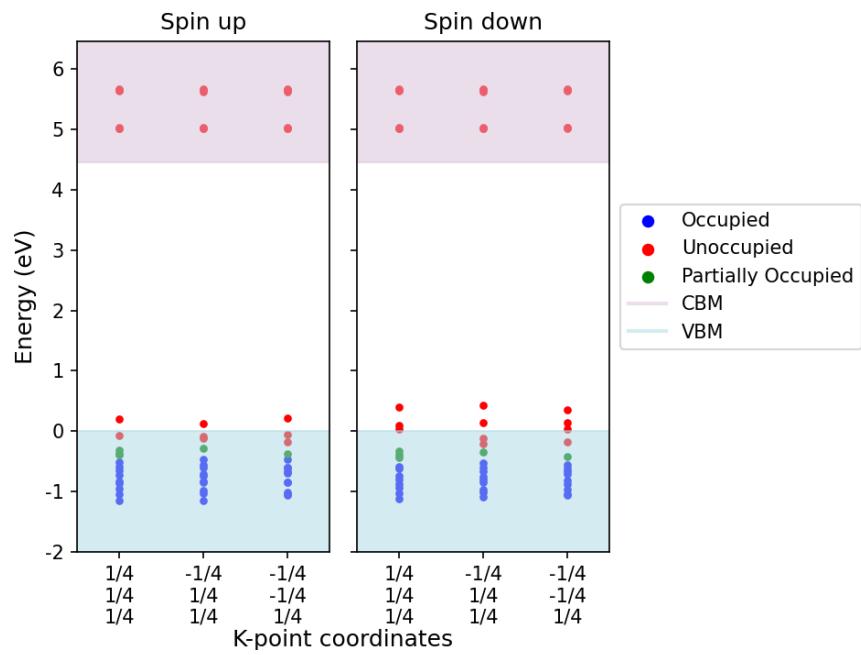


Figure 182: Kohn-Sham states.

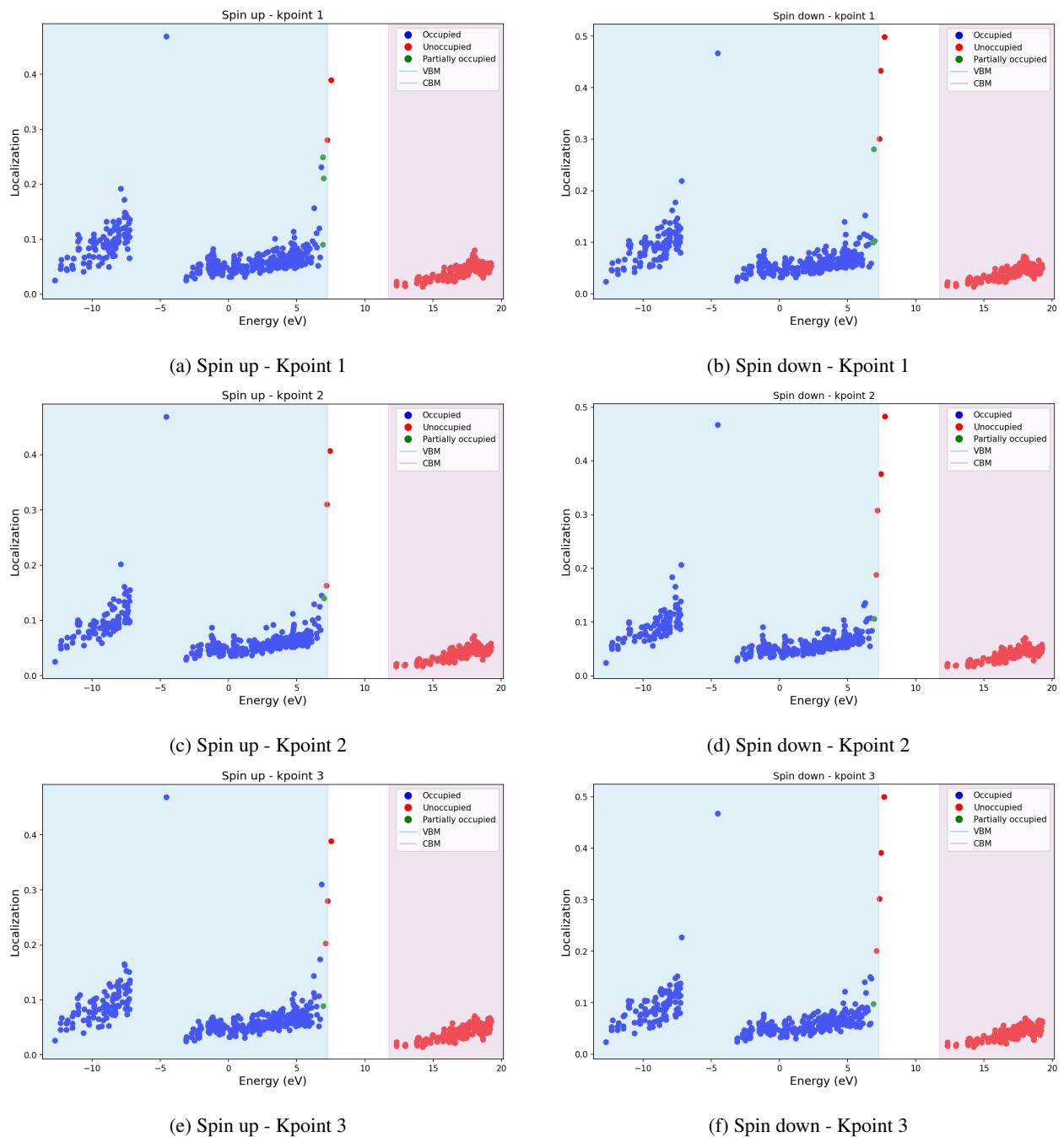


Figure 183: Localization factor using projected orbitals (s, p, and d).

6.88 Complex: $(C_N - V_B)^{-1}$

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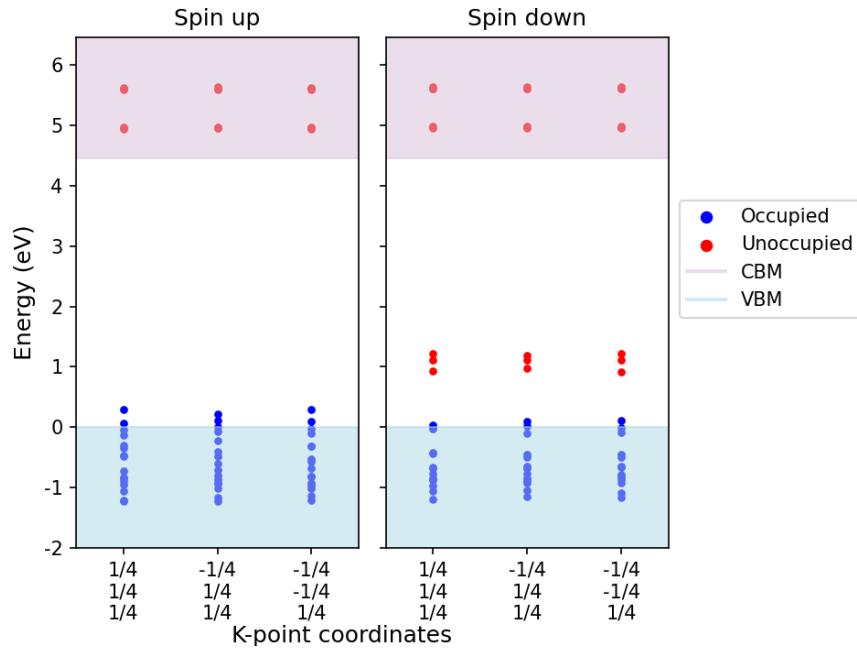


Figure 184: Kohn-Sham states.

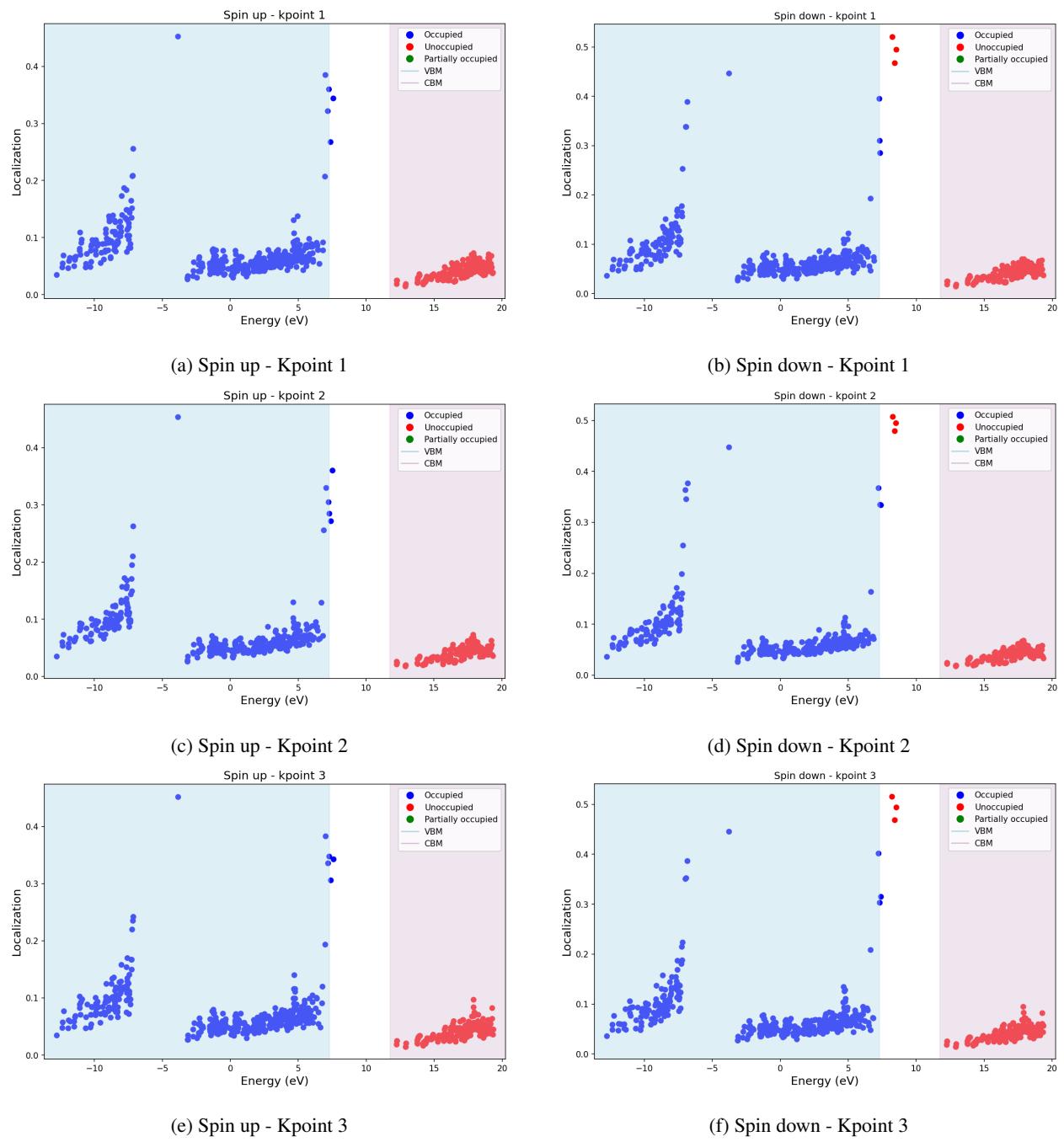


Figure 185: Localization factor using projected orbitals (s, p, and d).

6.89 Complex: $(C_N - V_B)^{-2}$

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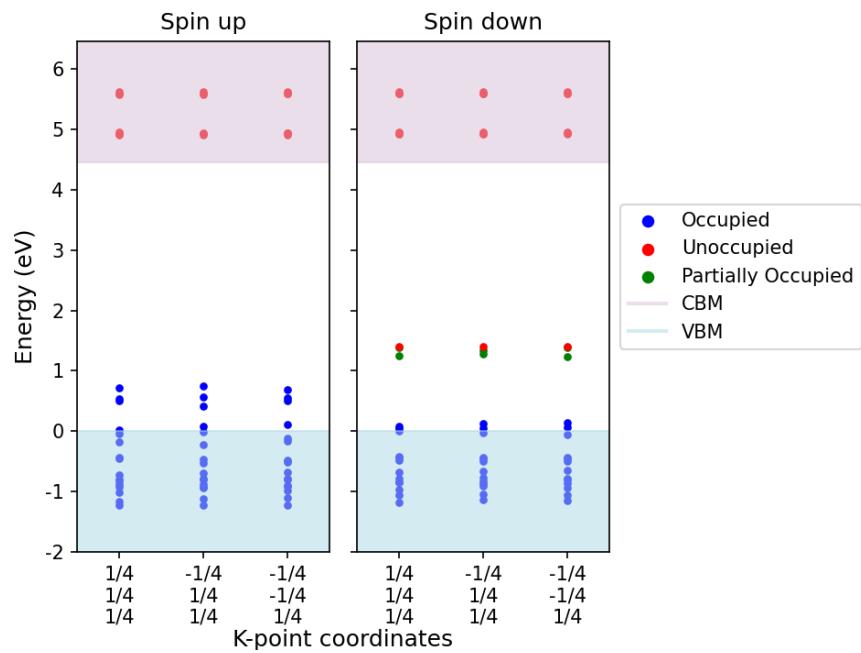


Figure 186: Kohn-Sham states.

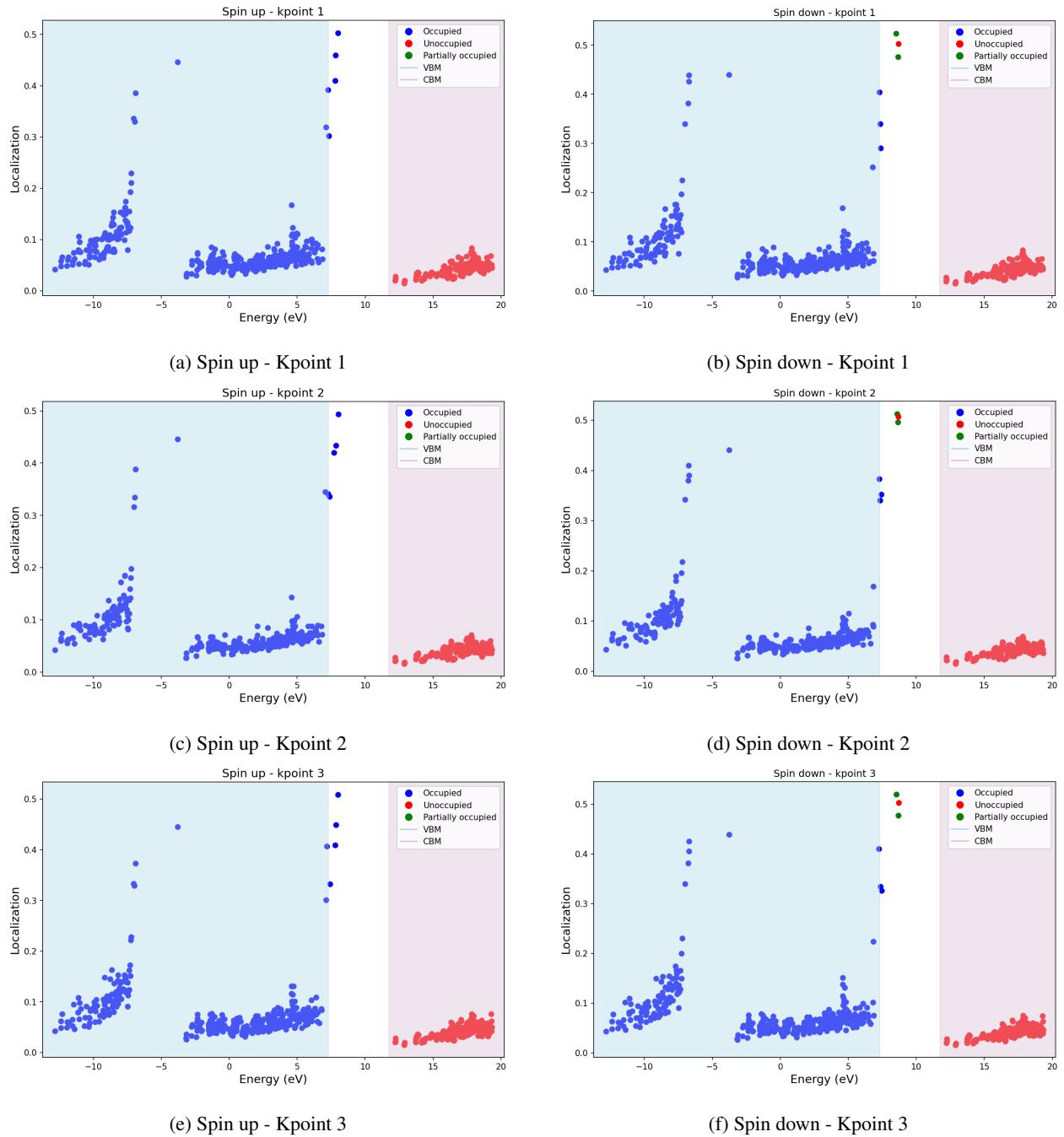


Figure 187: Localization factor using projected orbitals (s, p, and d).

6.90 Complex: $(C_N - V_B)^{-3}$

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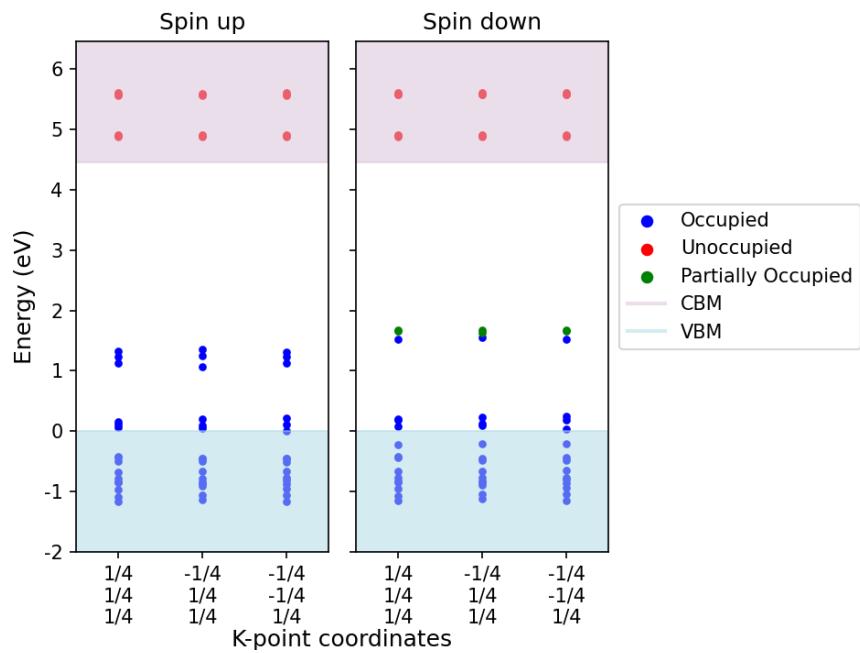


Figure 188: Kohn-Sham states.

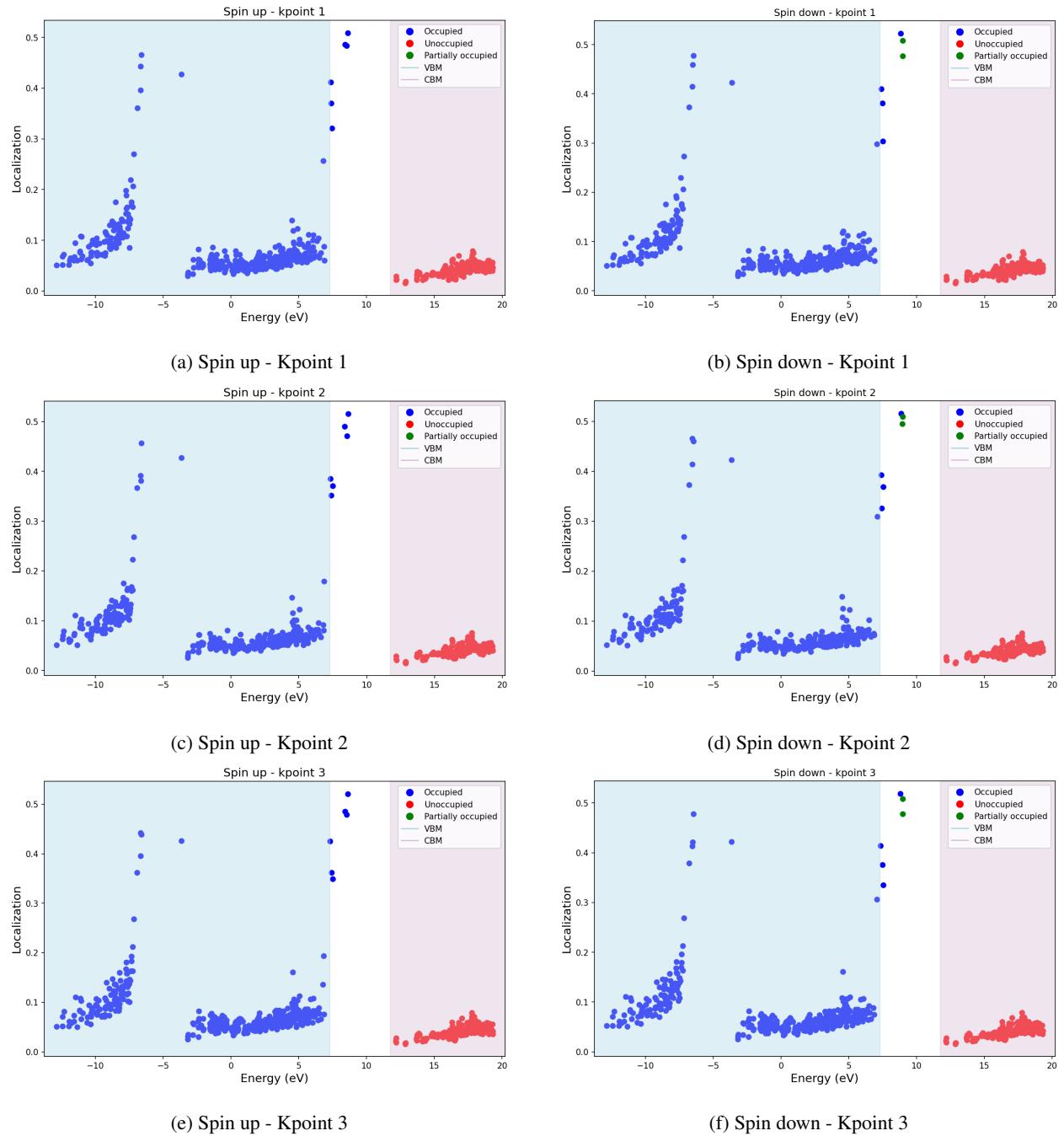


Figure 189: Localization factor using projected orbitals (s, p, and d).

6.91 Complex: $(C_N - V_B)^{-4}$

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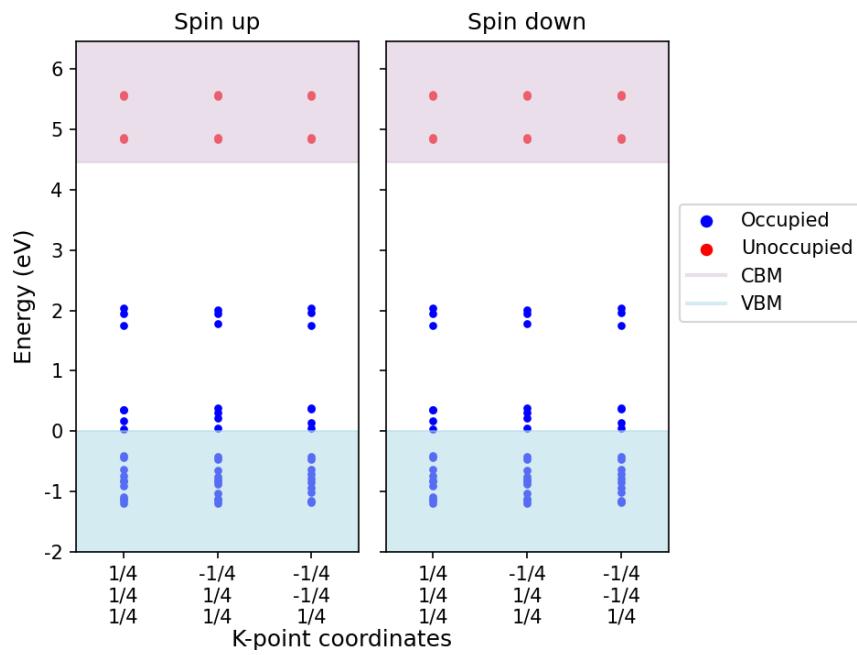


Figure 190: Kohn-Sham states.

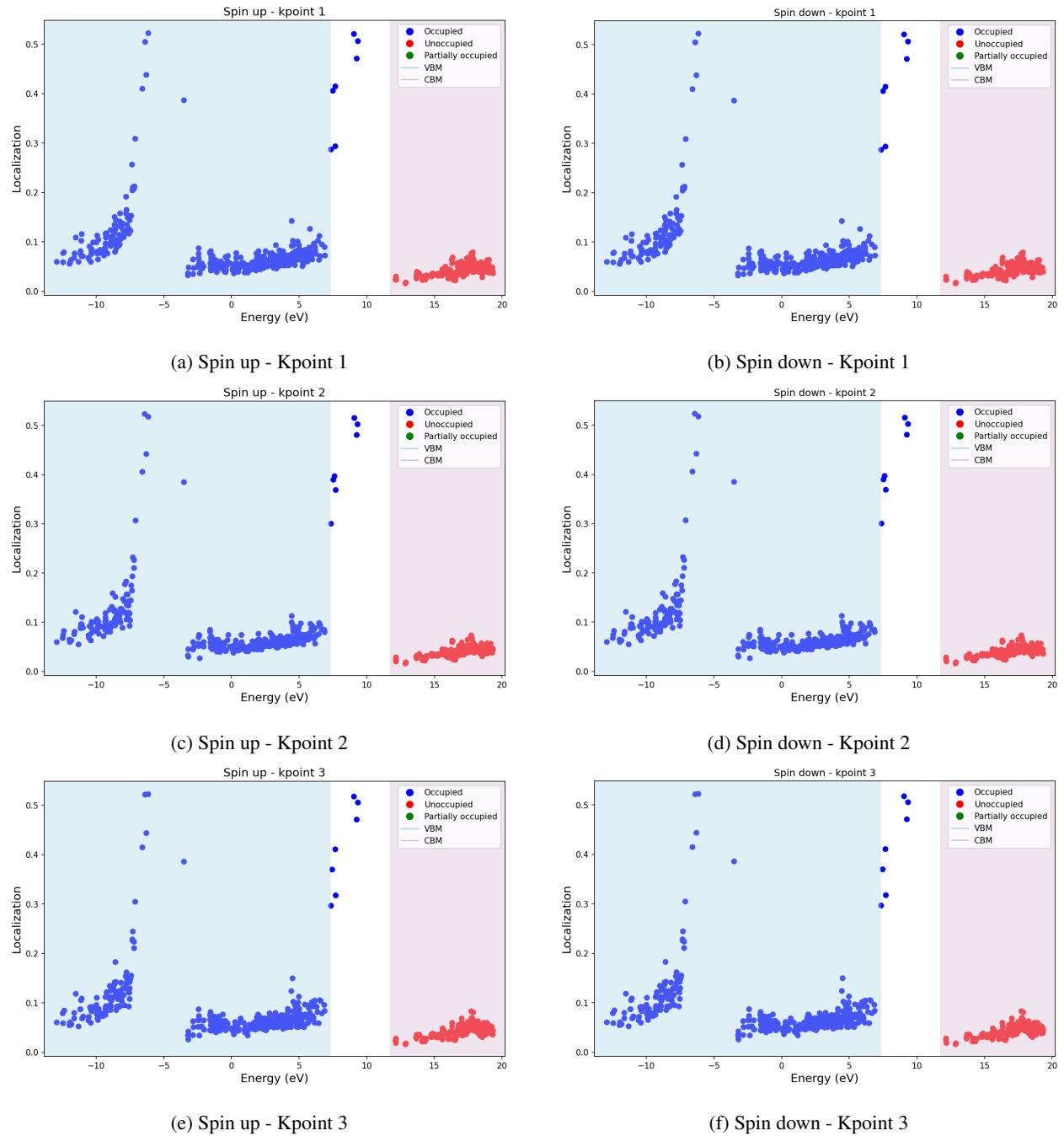


Figure 191: Localization factor using projected orbitals (s, p, and d).

6.92 Substitutional: C_B^0

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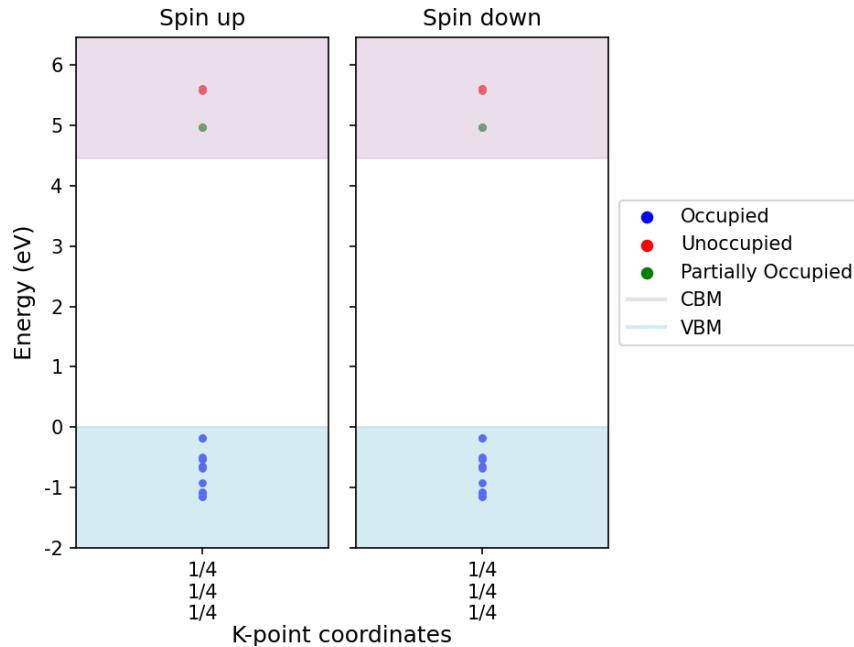


Figure 192: Kohn-Sham states.

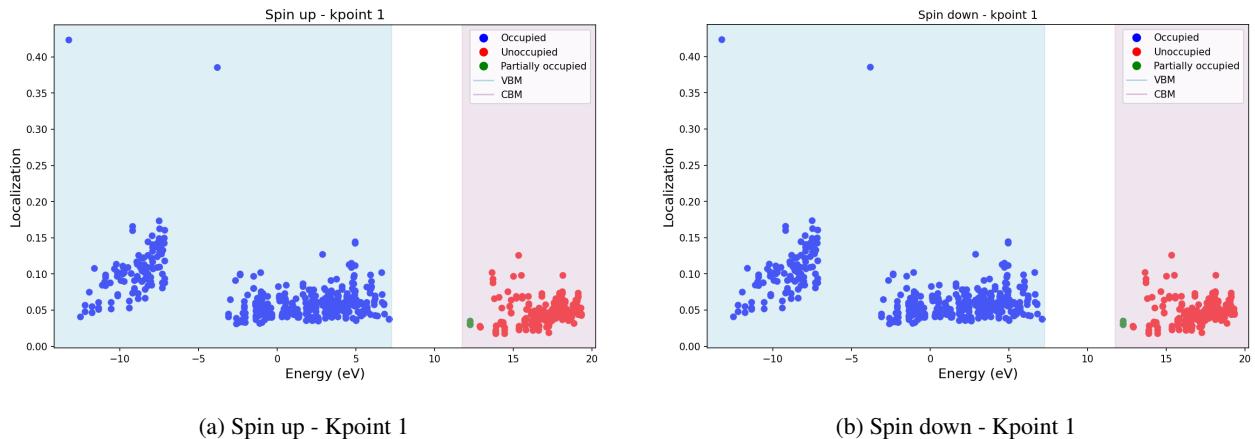


Figure 193: Localization factor using projected orbitals (s, p and d).

6.93 Substitutional: C_B^{+1}

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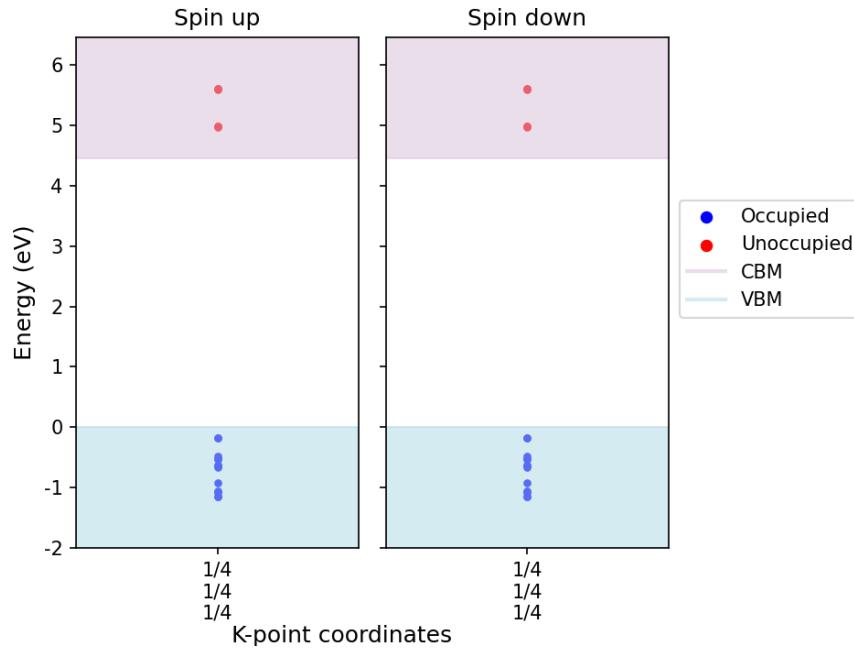


Figure 194: Kohn-Sham states.

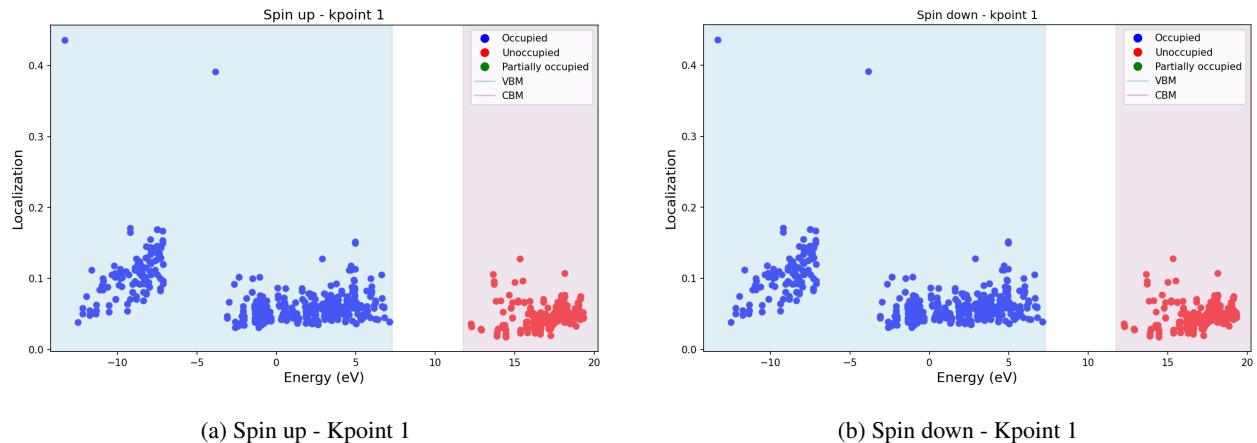


Figure 195: Localization factor using projected orbitals (s, p and d).

6.94 Substitutional: C_B^{+2}

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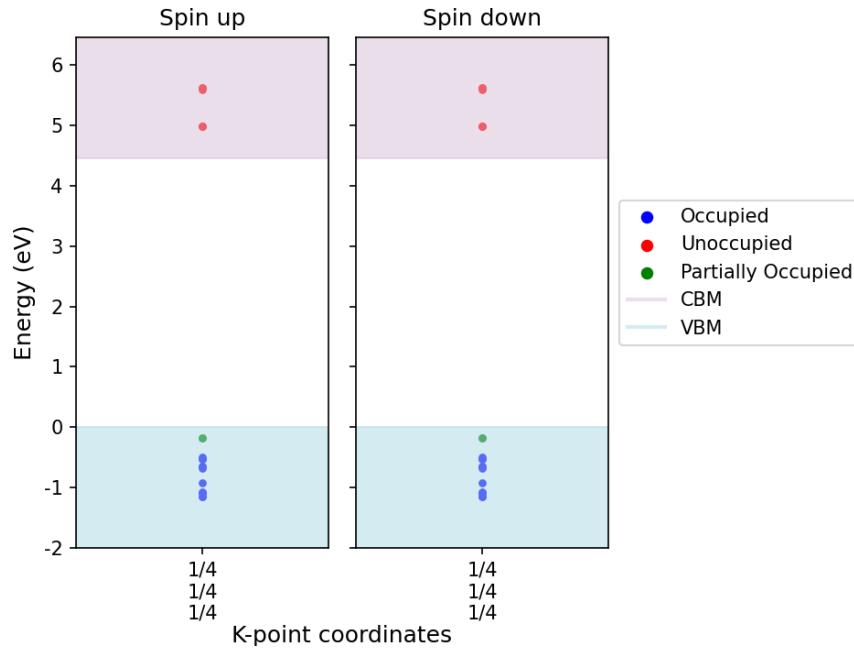


Figure 196: Kohn-Sham states.

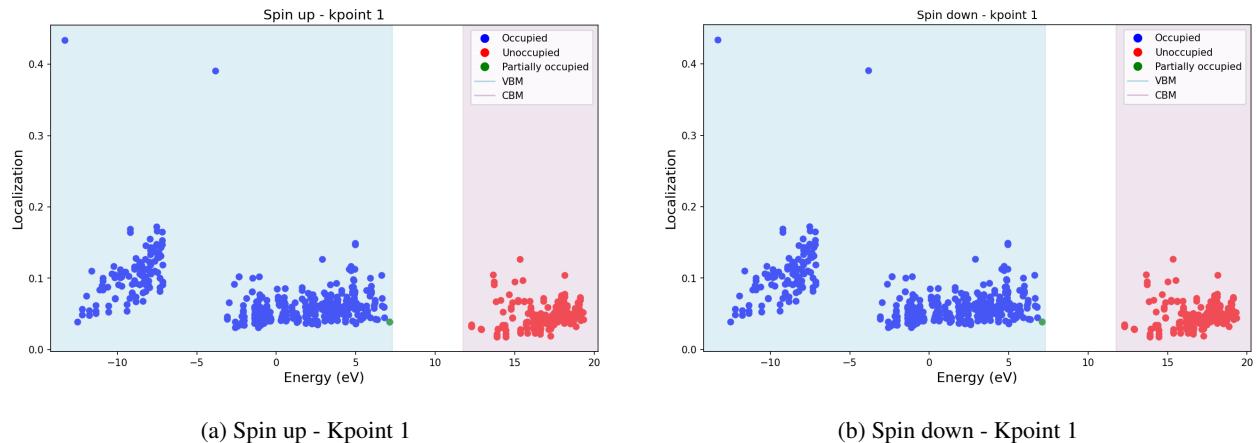


Figure 197: Localization factor using projected orbitals (s, p and d).

6.95 Substitutional: C_B^{-1}

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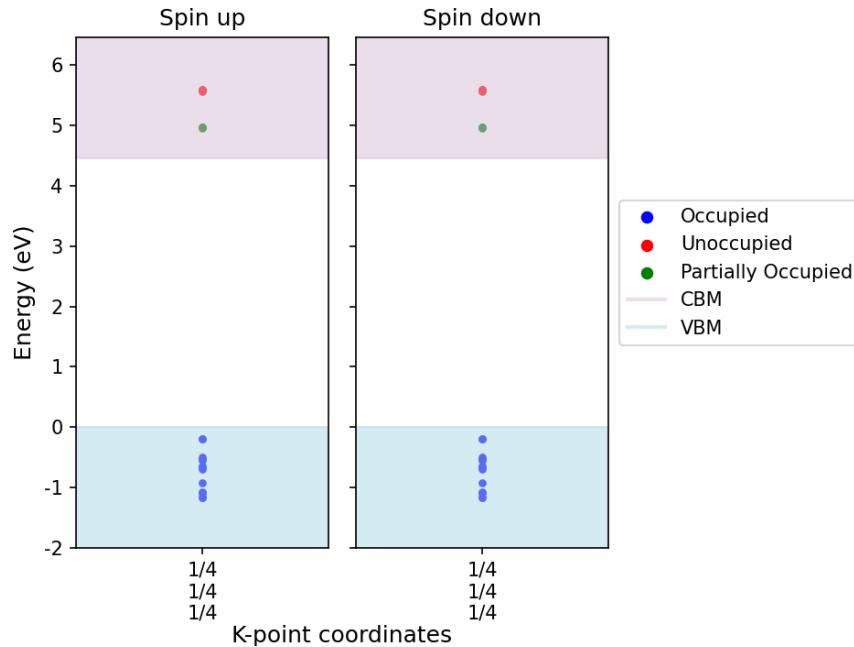


Figure 198: Kohn-Sham states.

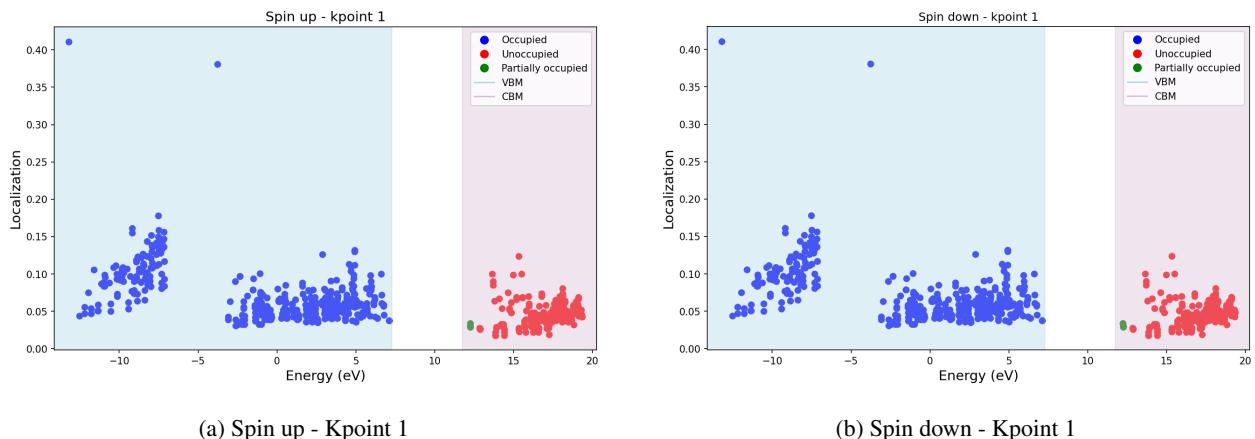


Figure 199: Localization factor using projected orbitals (s, p and d).

6.96 Substitutional: C_B^{-2}

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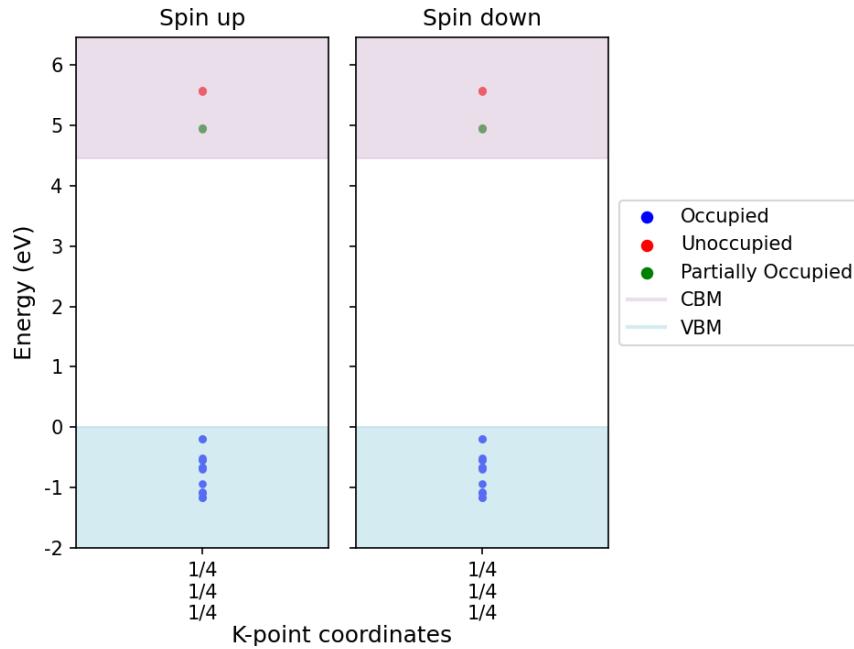


Figure 200: Kohn-Sham states.

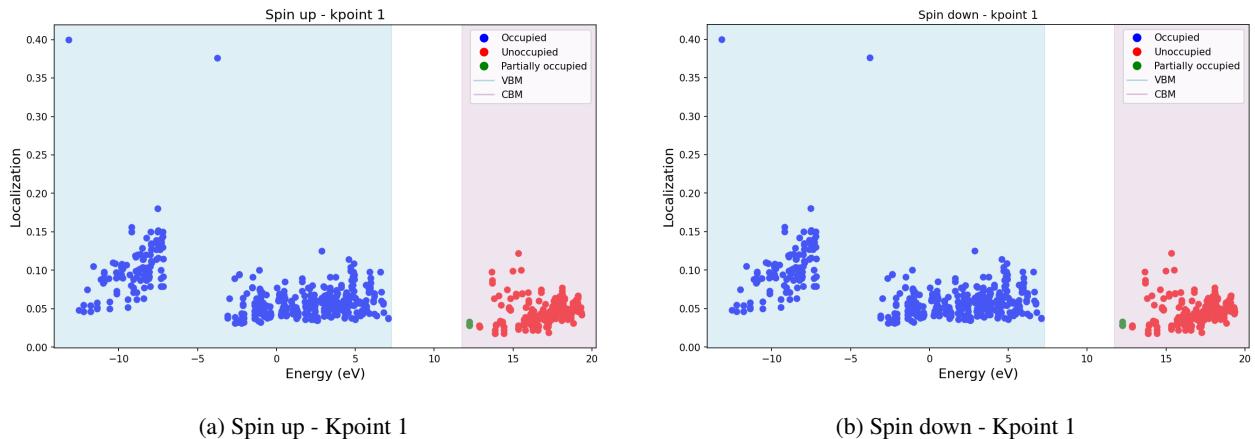


Figure 21: Localization factor using projected orbitals (s, p and d).

6.97 Substitutional: C_N^0

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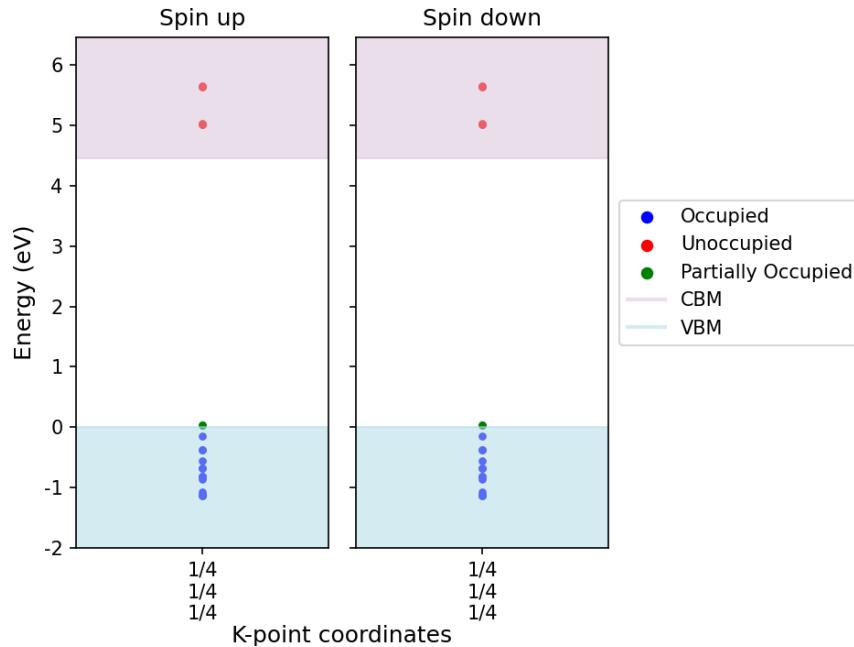


Figure 202: Kohn-Sham states.

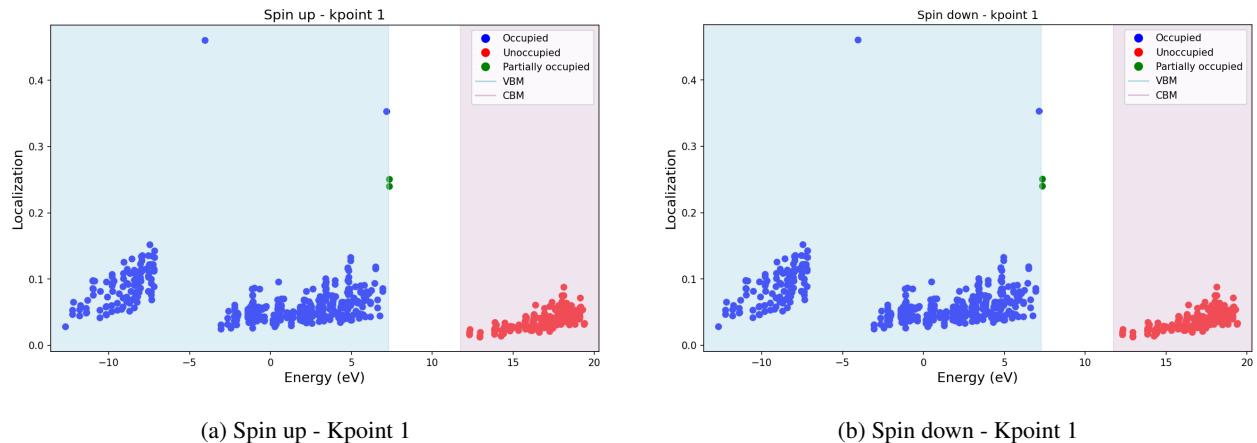


Figure 203: Localization factor using projected orbitals (s, p and d).

6.98 Substitutional: C_N^{+1}

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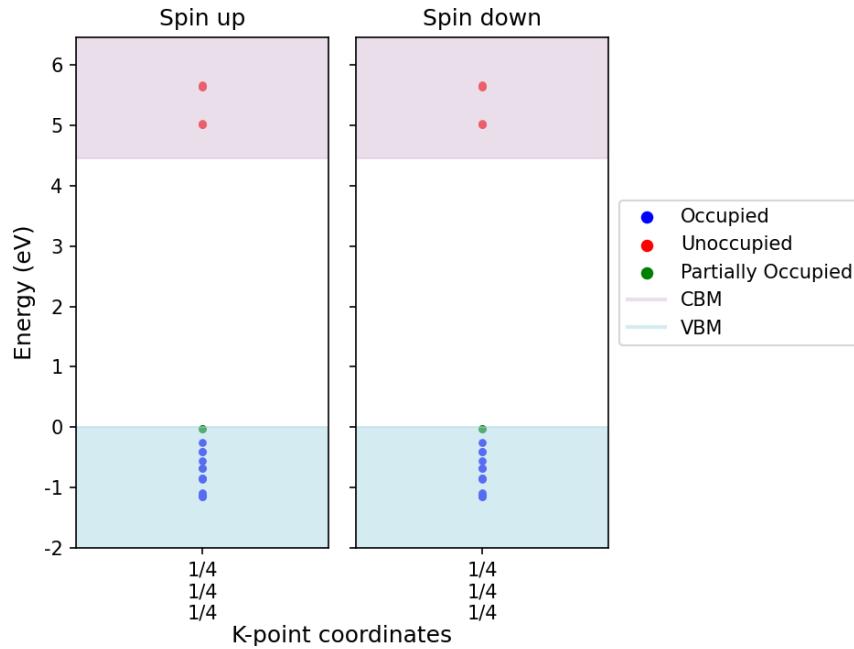


Figure 204: Kohn-Sham states.

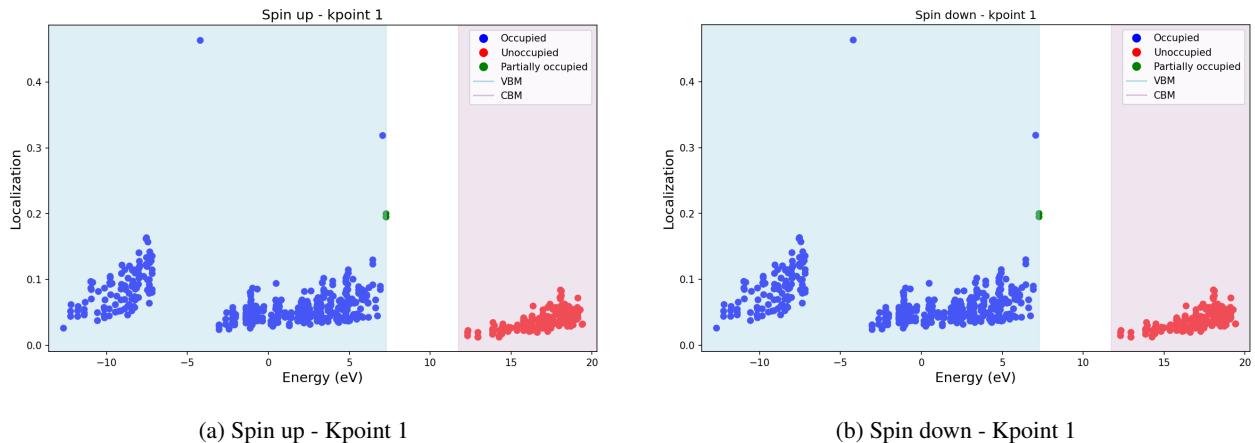


Figure 205: Localization factor using projected orbitals (s, p and d).

6.99 Substitutional: C_N^{+2}

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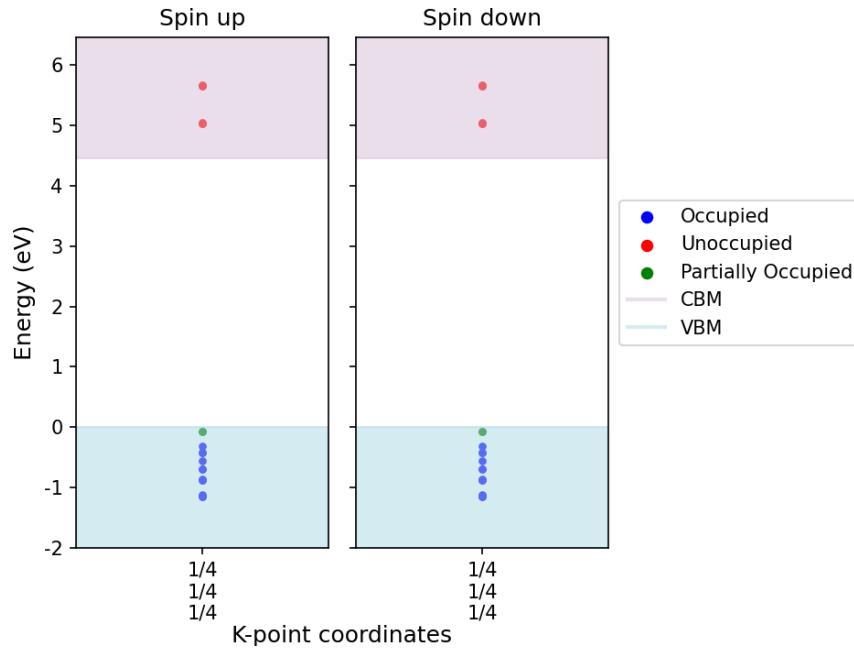


Figure 206: Kohn-Sham states.

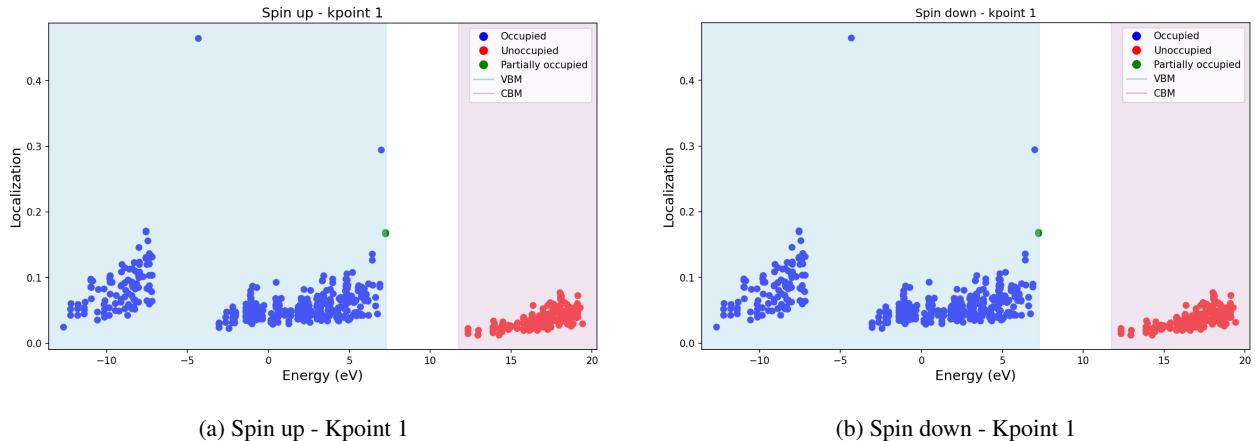


Figure 207: Localization factor using projected orbitals (s, p and d).

6.100 Substitutional: C_N^{-1}

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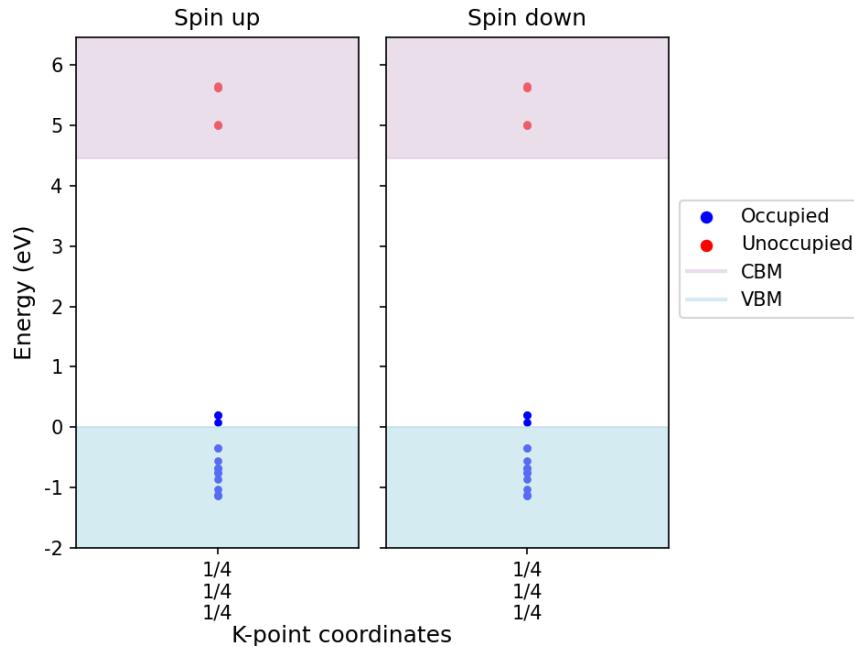


Figure 208: Kohn-Sham states.

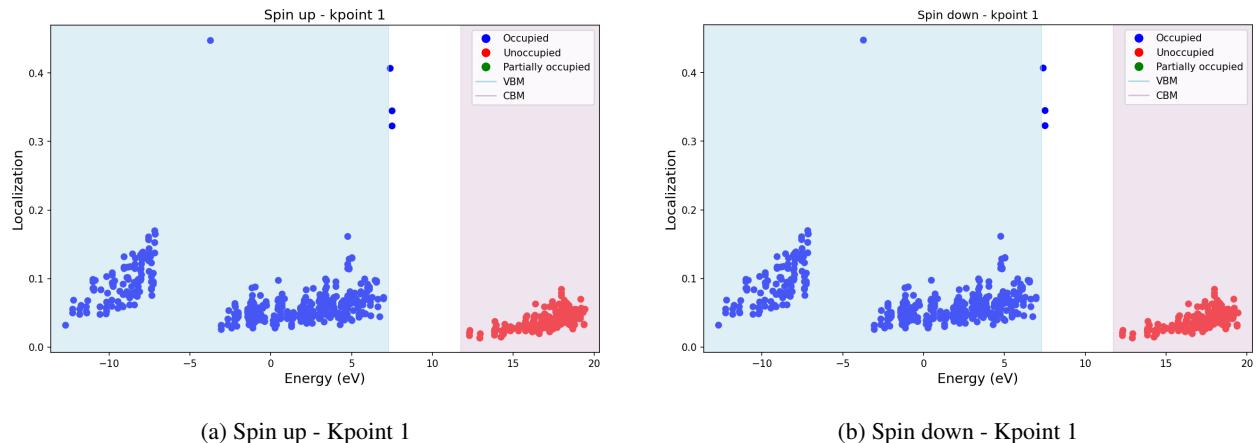


Figure 209: Localization factor using projected orbitals (s, p and d).

6.101 Substitutional: C_N^{-2}

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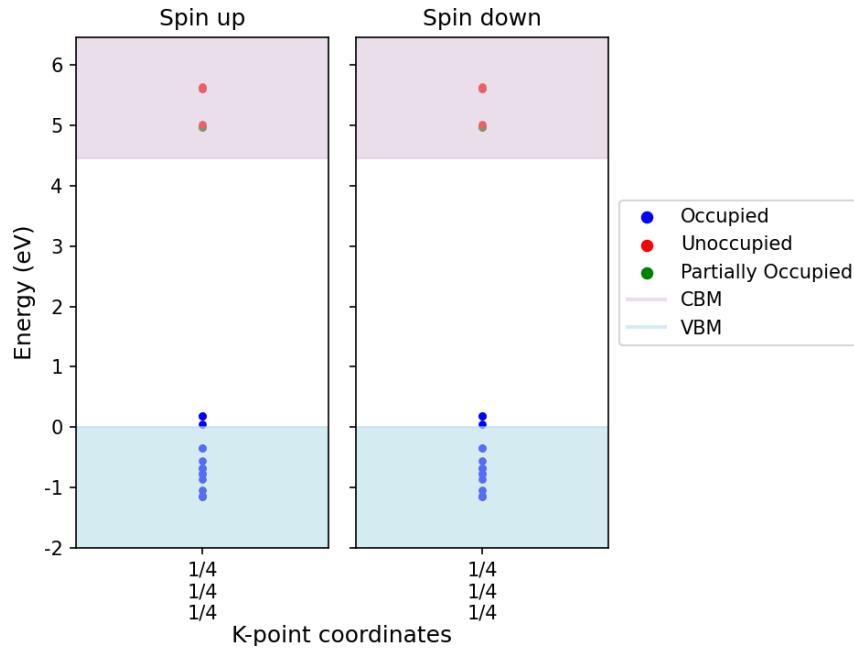


Figure 210: Kohn-Sham states.

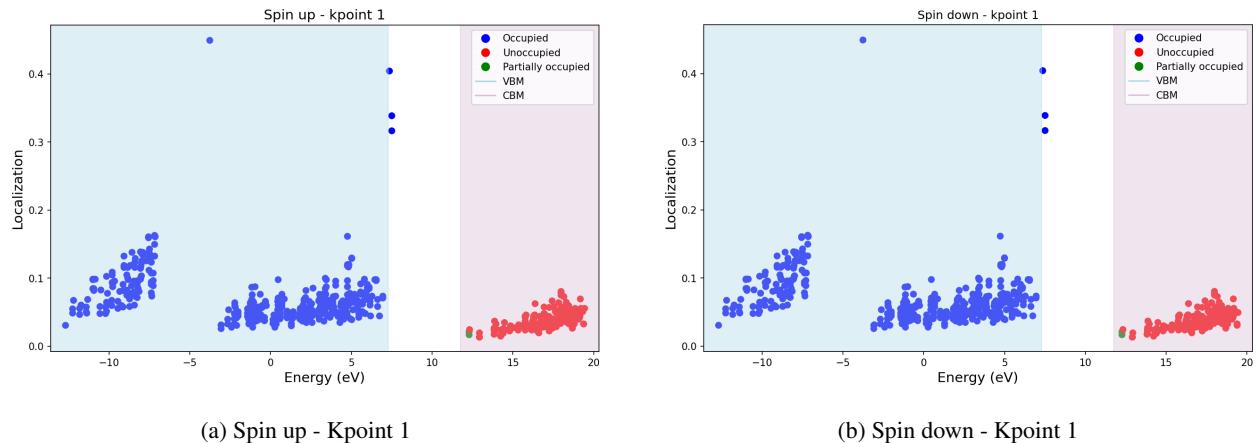


Figure 211: Localization factor using projected orbitals (s, p and d).

6.102 Substitutional: O_B^0

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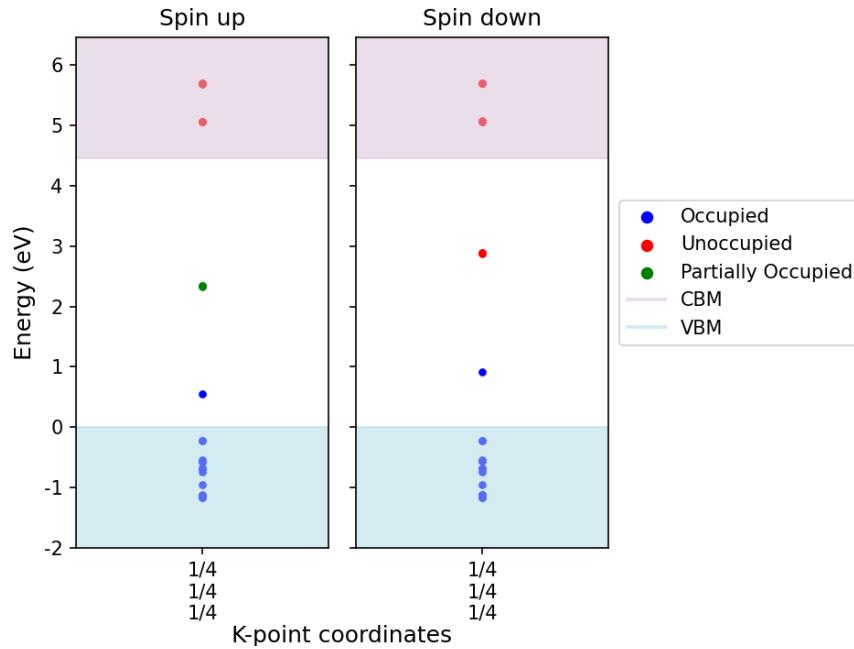


Figure 212: Kohn-Sham states.

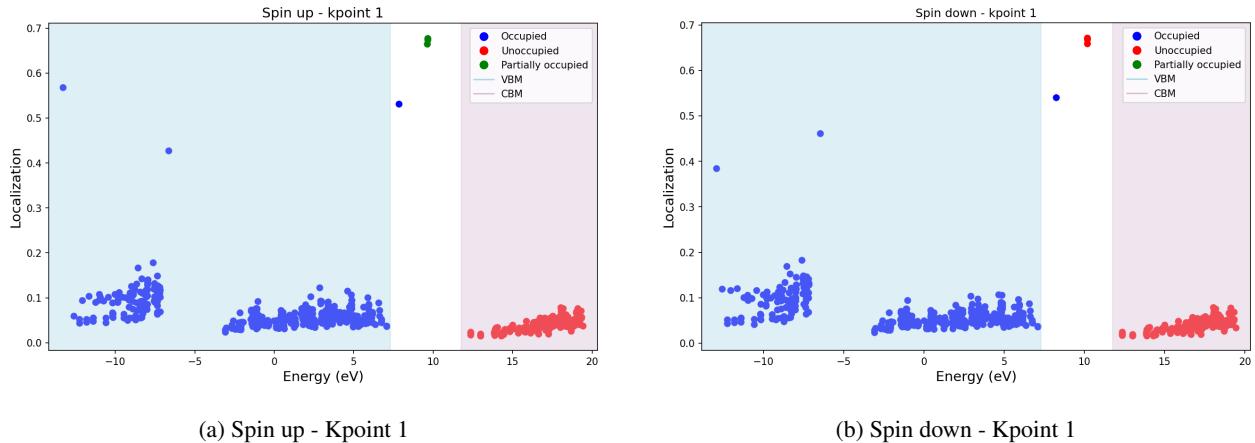


Figure 213: Localization factor using projected orbitals (s, p and d).

6.103 Substitutional: O_B^{+1}

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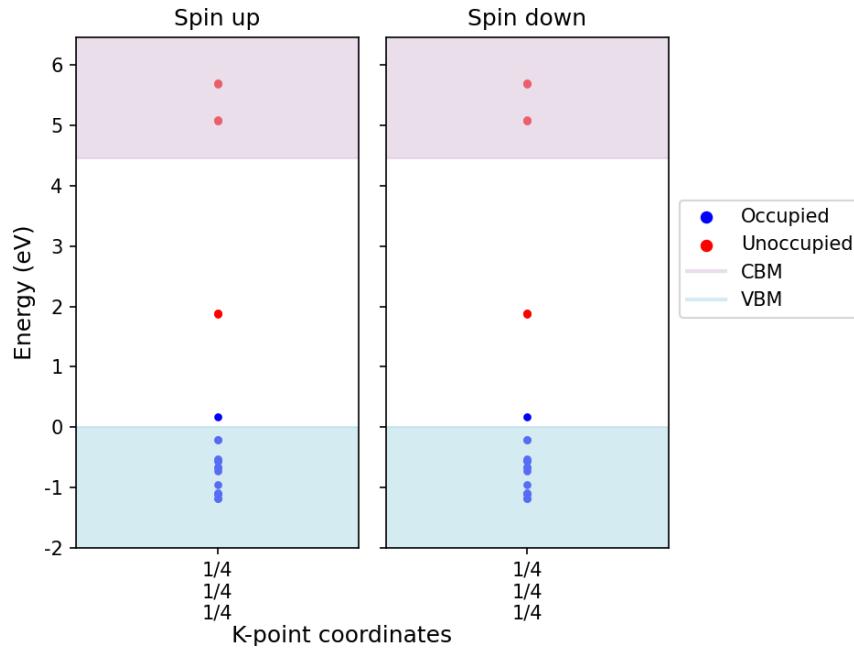


Figure 214: Kohn-Sham states.

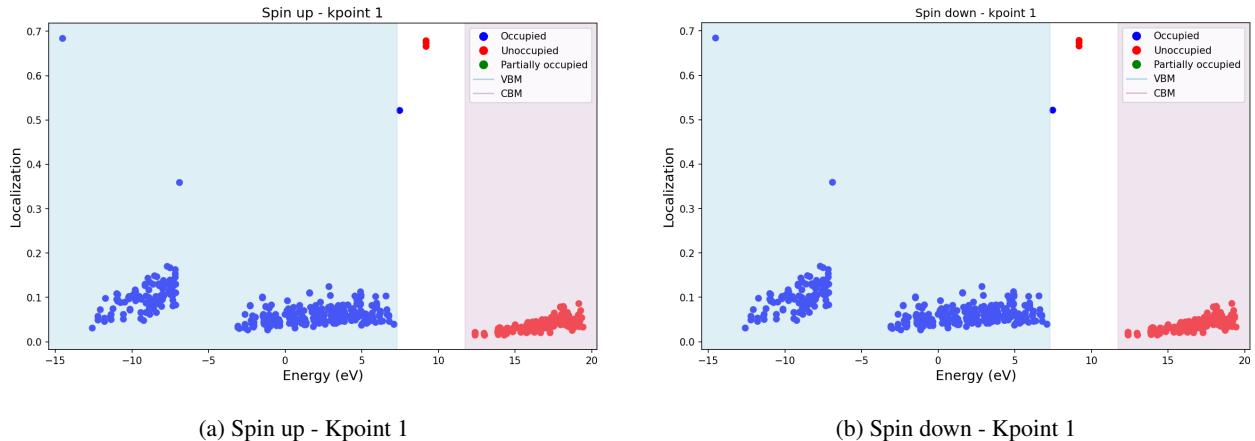


Figure 215: Localization factor using projected orbitals (s, p and d).

6.104 Substitutional: O_B^{+2}

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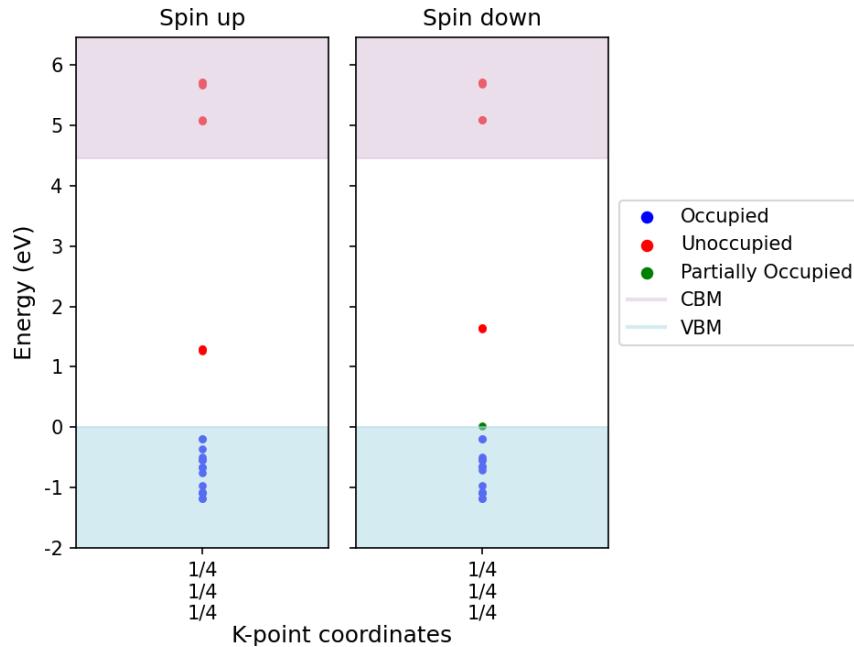


Figure 216: Kohn-Sham states.

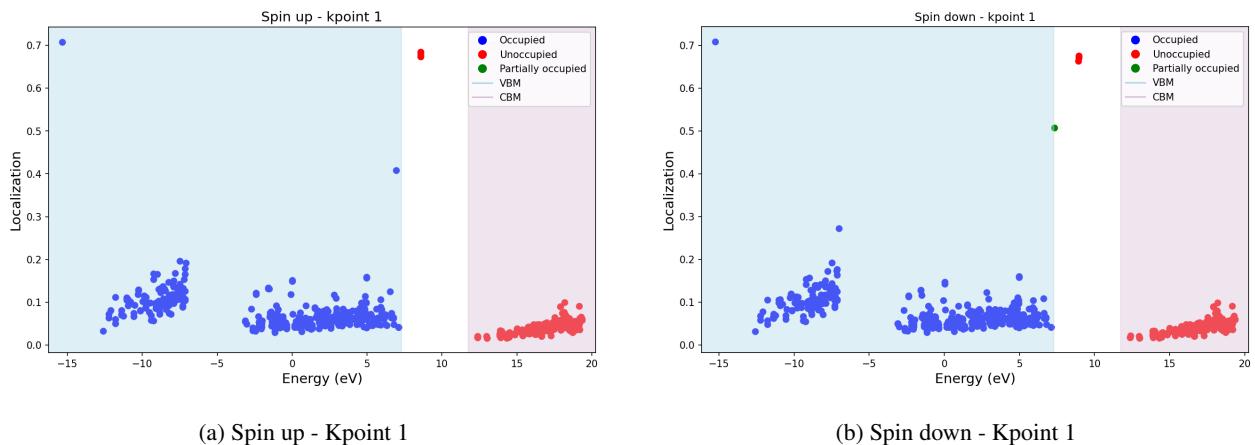


Figure 217: Localization factor using projected orbitals (s, p and d).

6.105 Substitutional: O_B^{-1}

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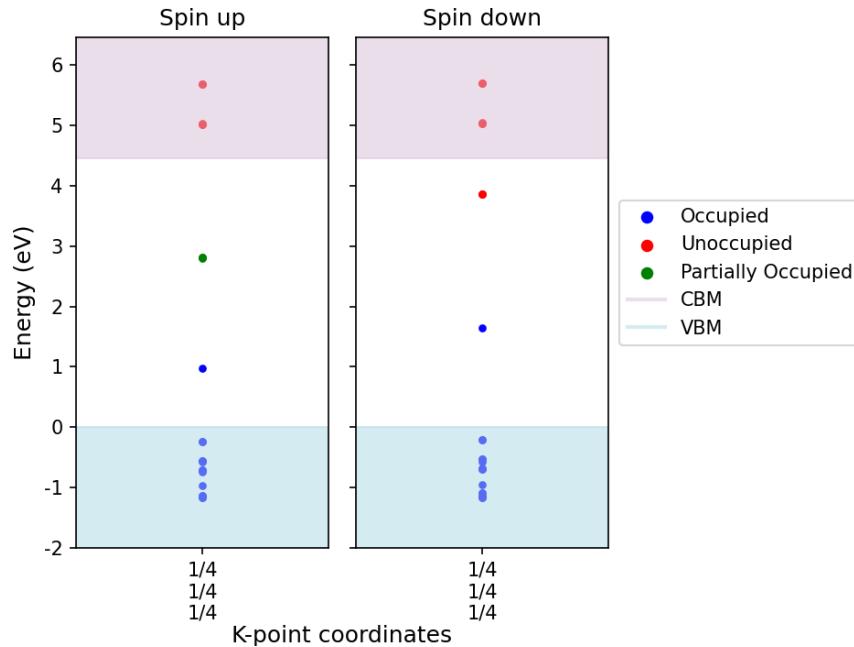


Figure 218: Kohn-Sham states.

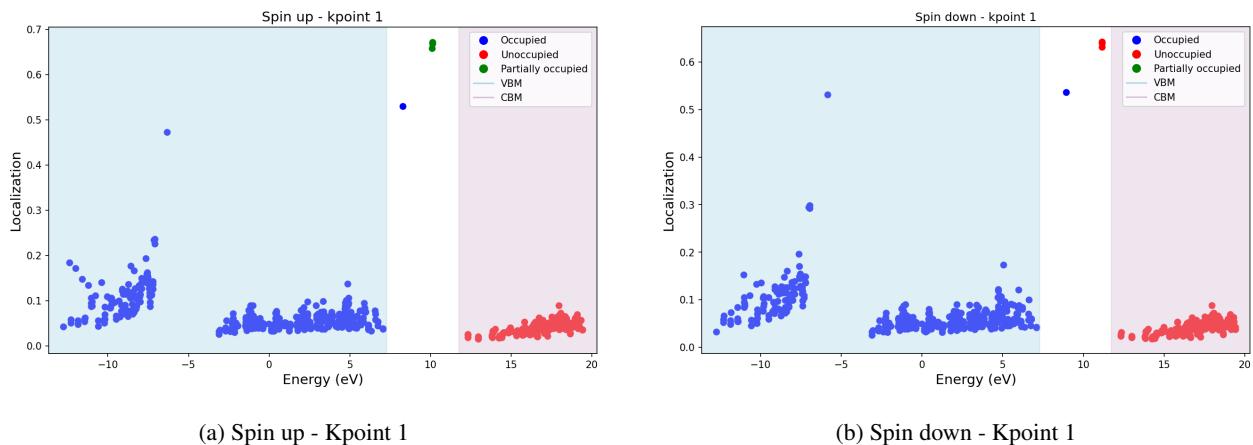


Figure 219: Localization factor using projected orbitals (s, p and d).

6.106 Substitutional: O_B^{-2}

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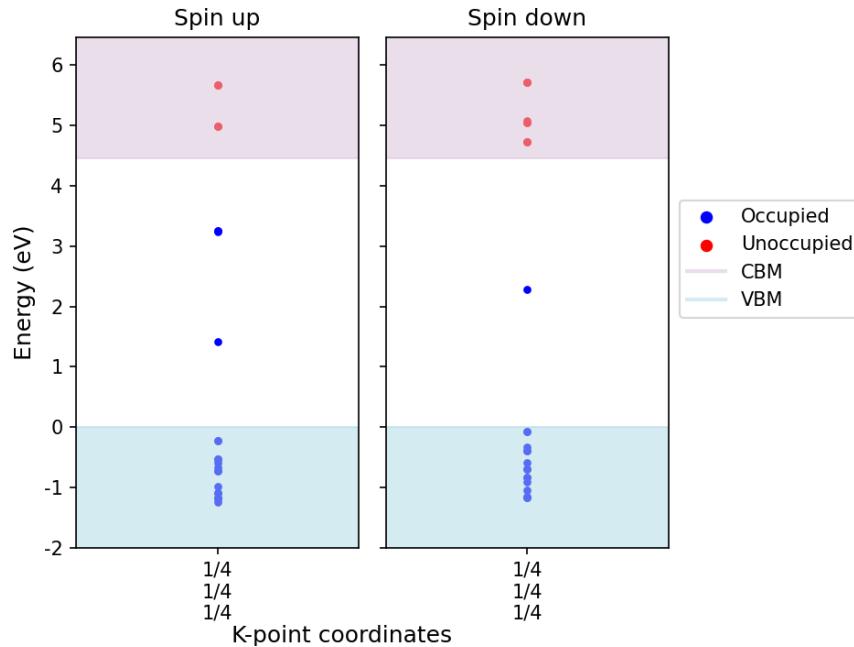


Figure 220: Kohn-Sham states.

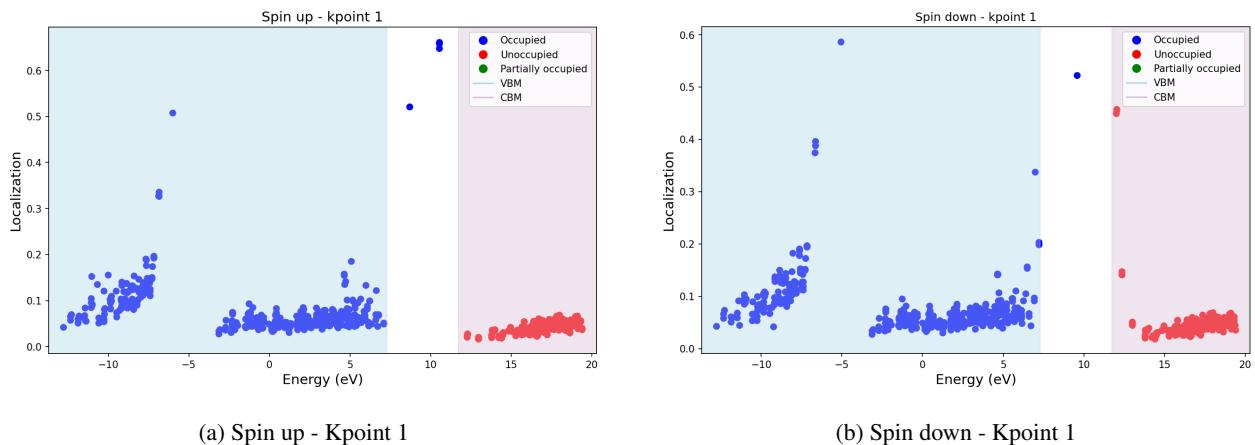


Figure 221: Localization factor using projected orbitals (s, p and d).

6.107 Substitutional: O_N^0

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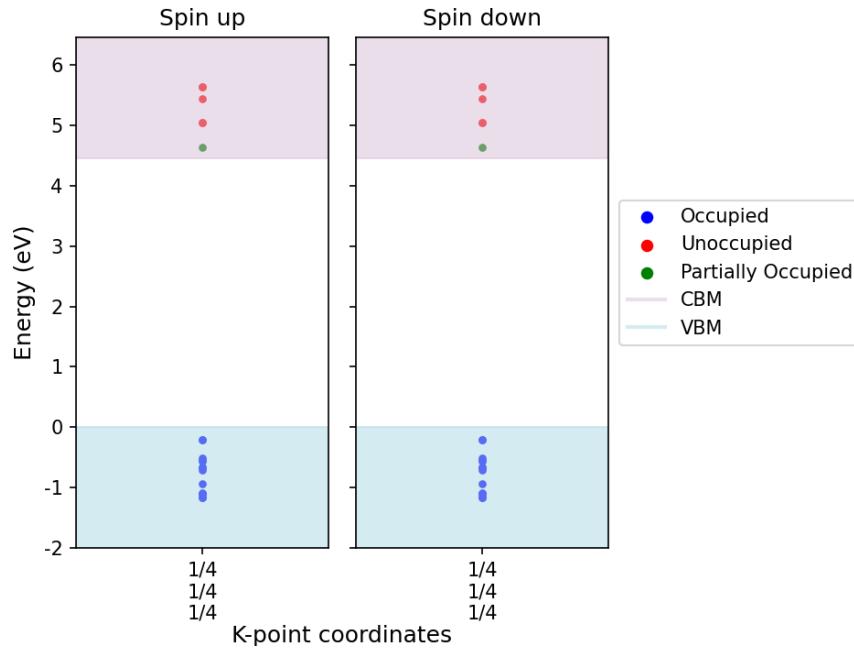


Figure 222: Kohn-Sham states.

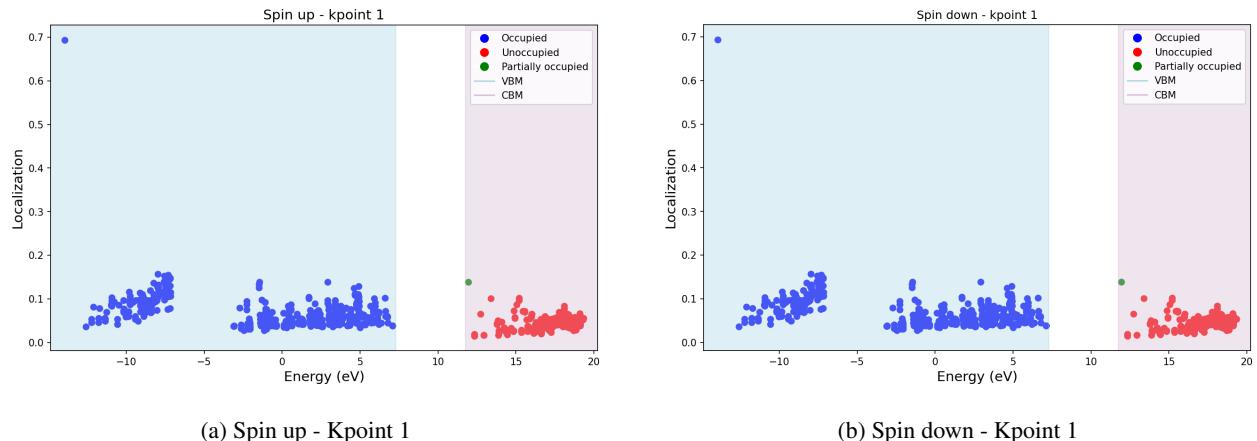


Figure 223: Localization factor using projected orbitals (s, p and d).

6.108 Substitutional: O_N^{+1}

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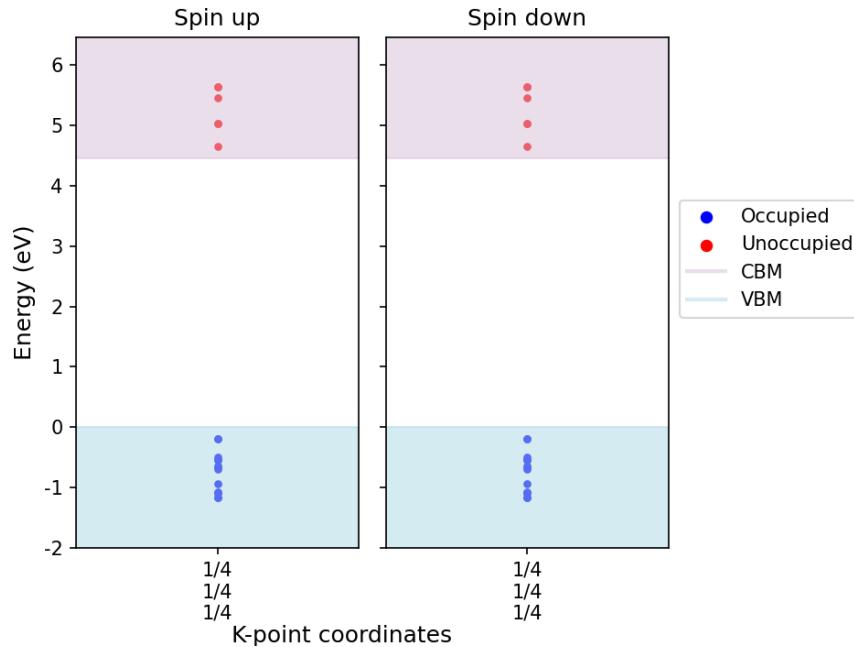


Figure 224: Kohn-Sham states.

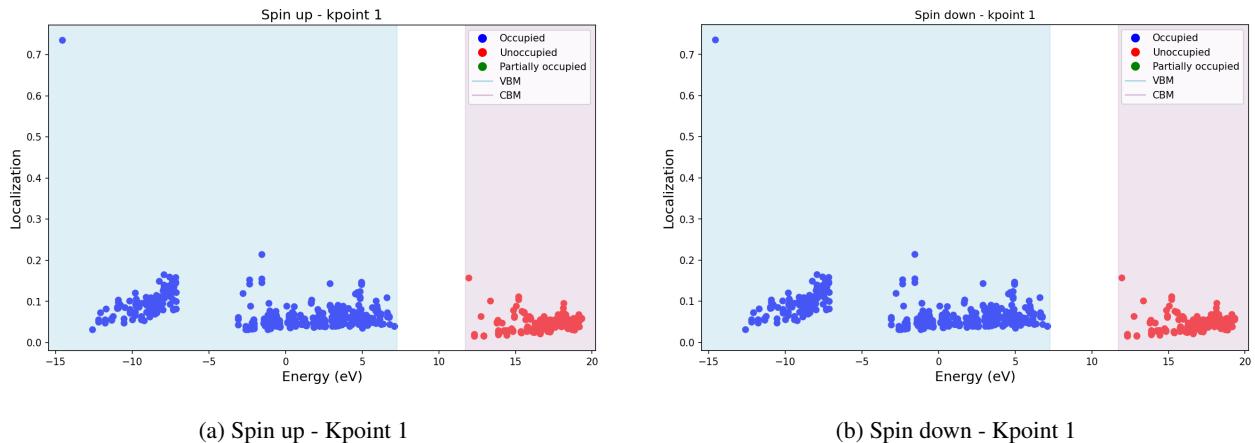


Figure 225: Localization factor using projected orbitals (s, p and d).

6.109 Substitutional: O_N^{+2}

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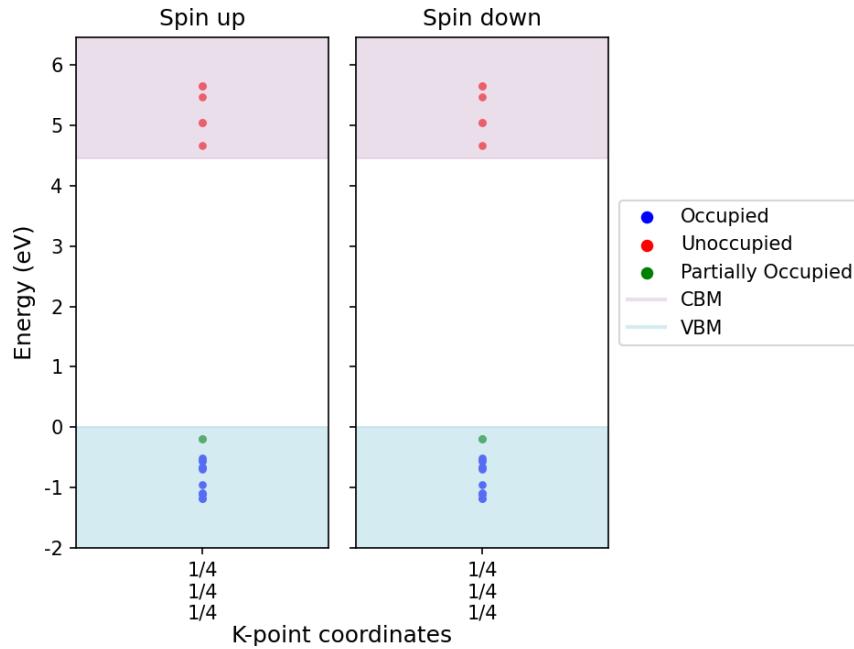


Figure 226: Kohn-Sham states.

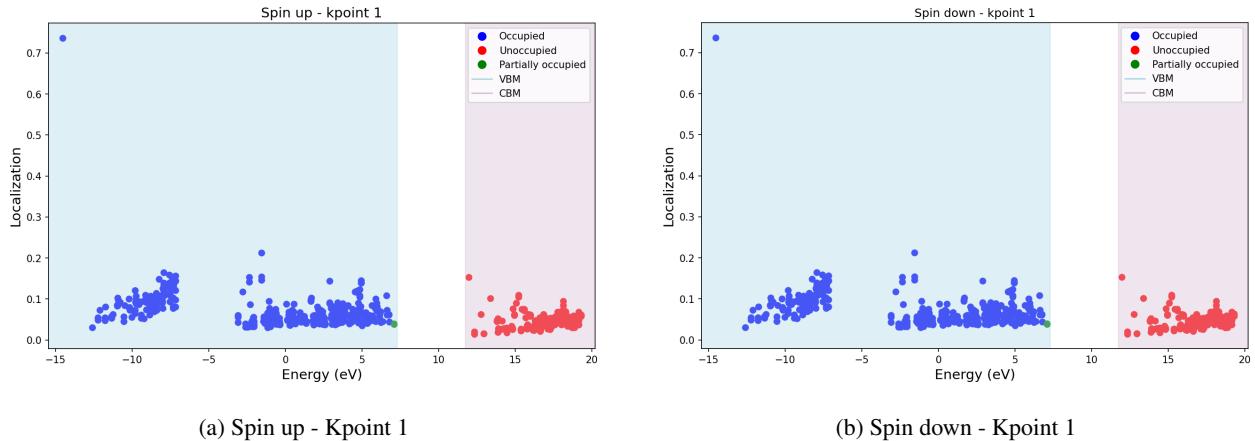


Figure 227: Localization factor using projected orbitals (s, p and d).

6.110 Substitutional: O_N^{-1}

[Go back to the Table 23](#)

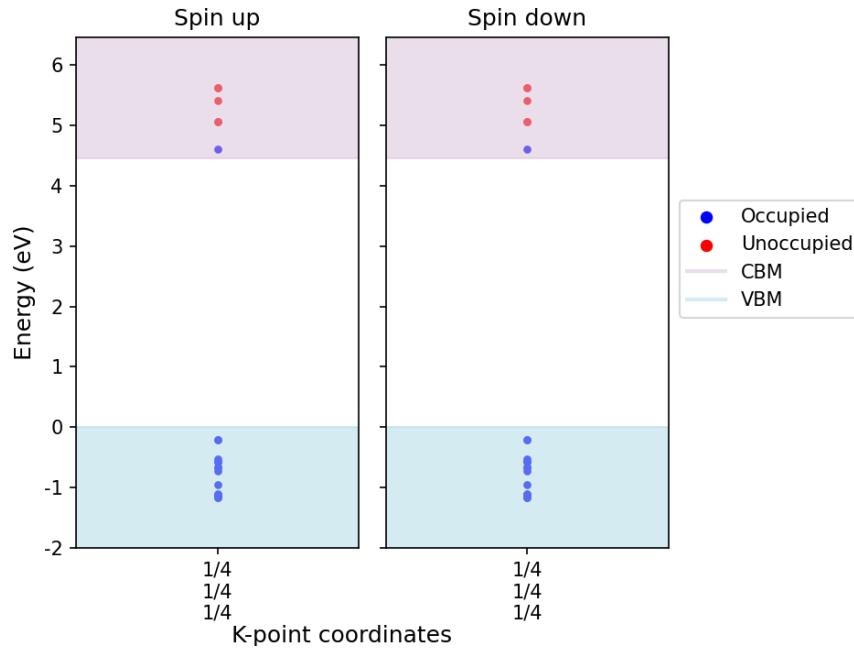


Figure 228: Kohn-Sham states.

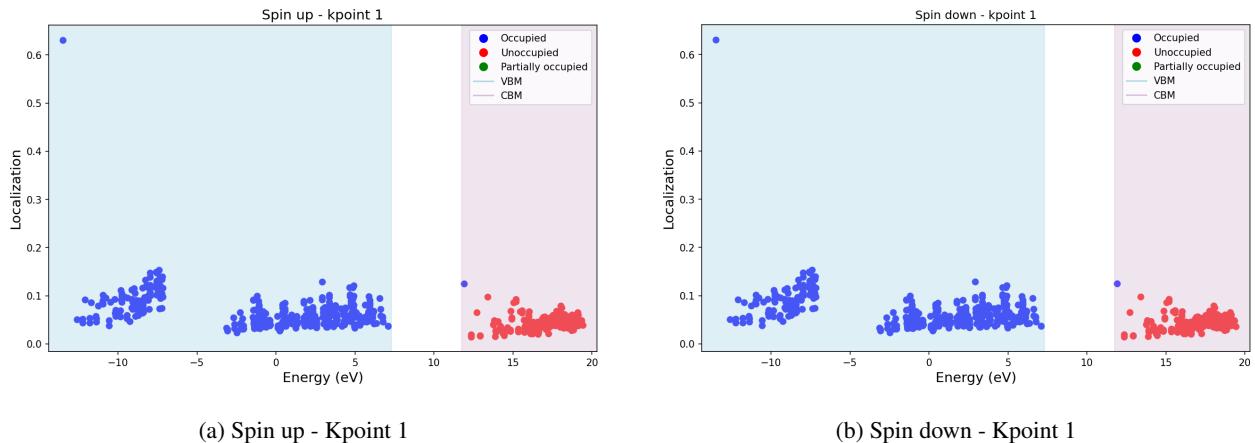


Figure 229: Localization factor using projected orbitals (s, p and d).

6.111 Substitutional: O_N^{-2}

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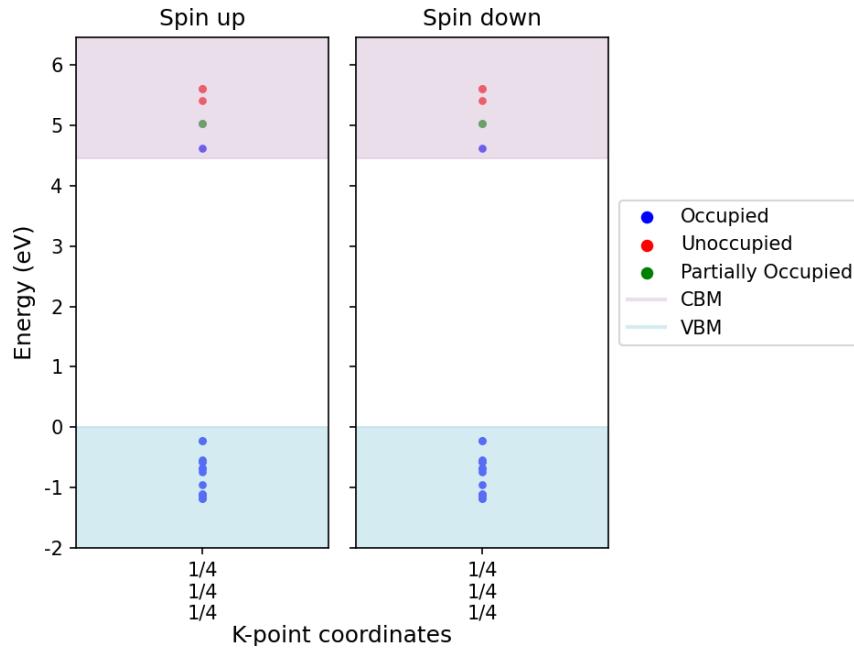


Figure 230: Kohn-Sham states.

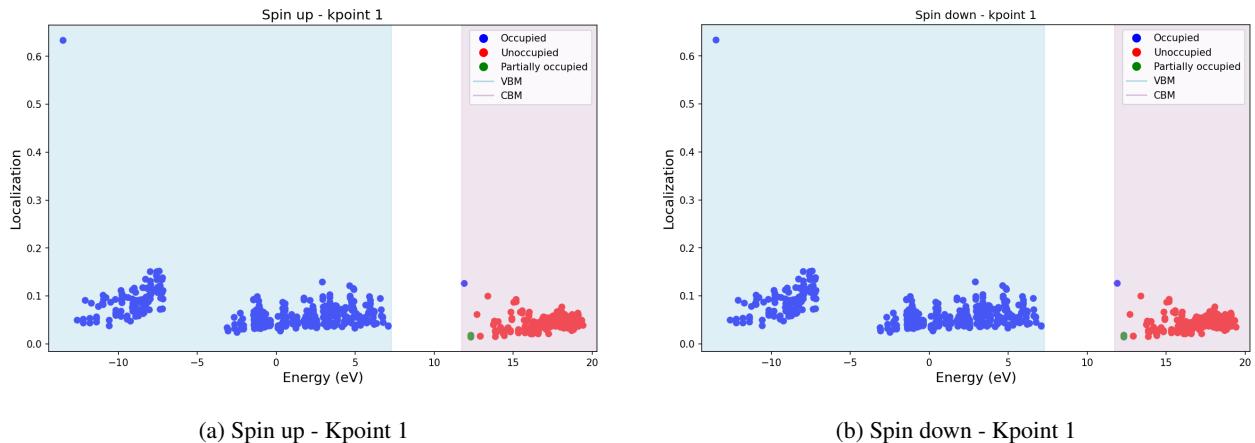


Figure 231: Localization factor using projected orbitals (s, p and d).

6.112 Complex: $(V_B - O_N)^0$

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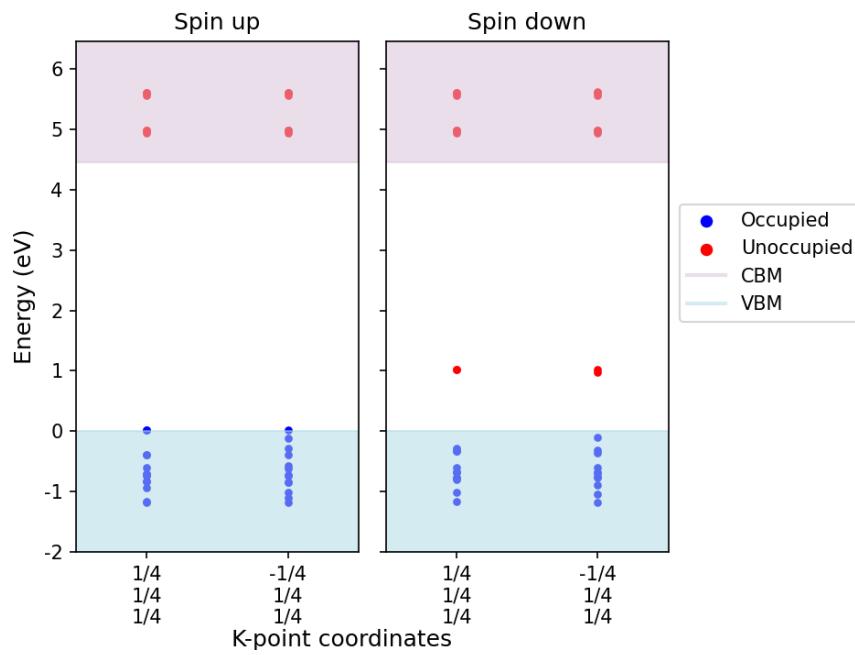


Figure 232: Kohn-Sham states.

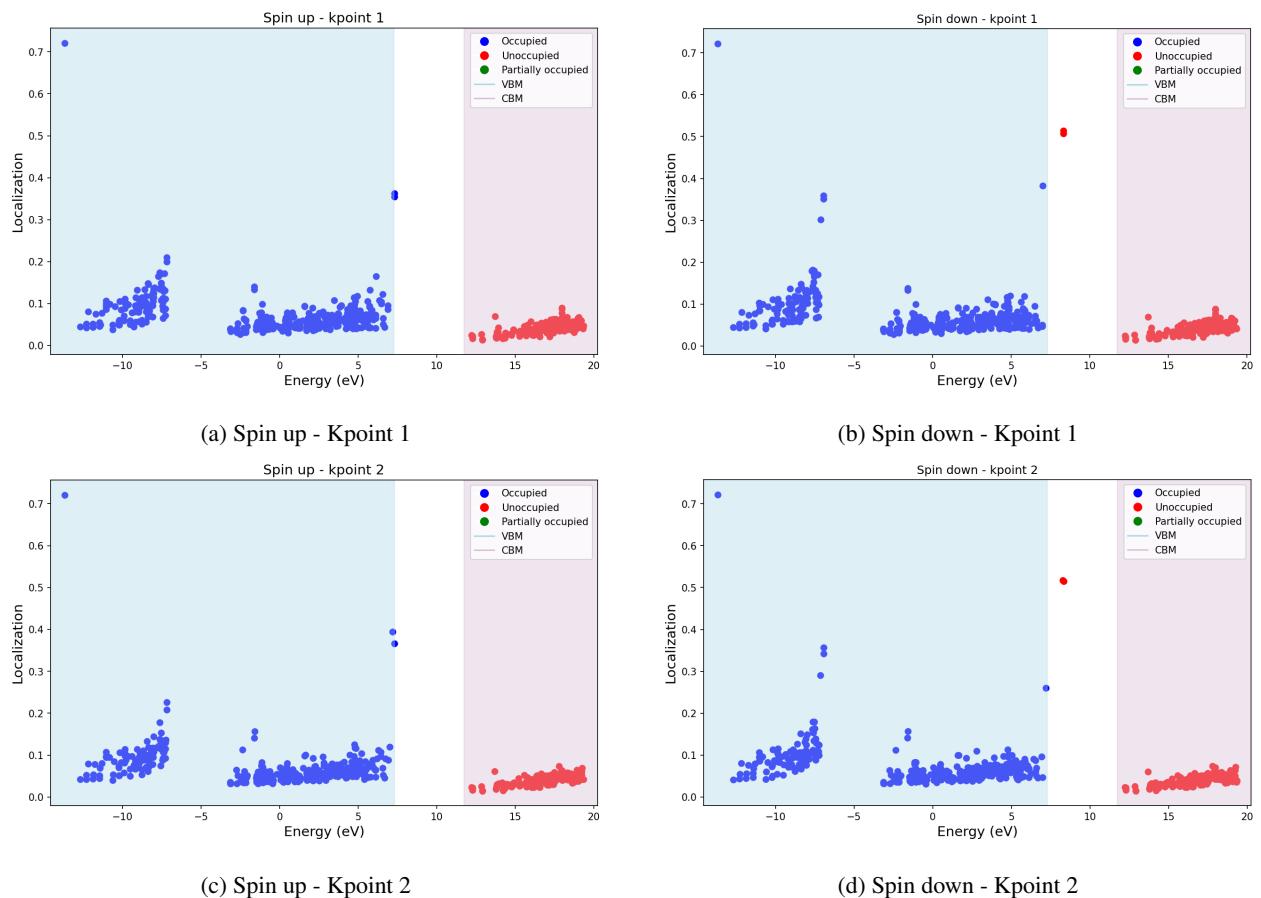


Figure 233: Localization factor using projected orbitals (s, p, and d).

6.113 Complex: $(V_B - O_N)^{+1}$

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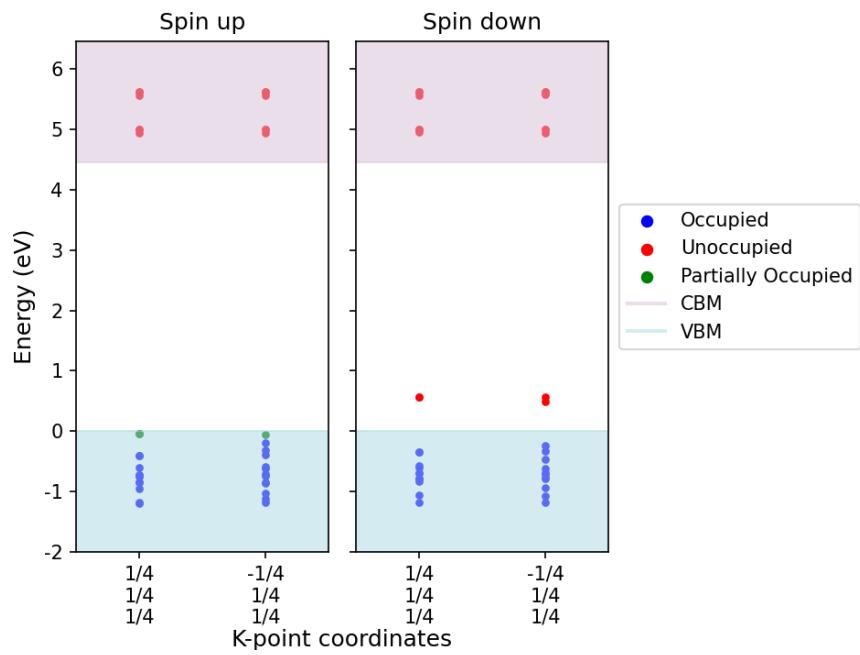


Figure 234: Kohn-Sham states.

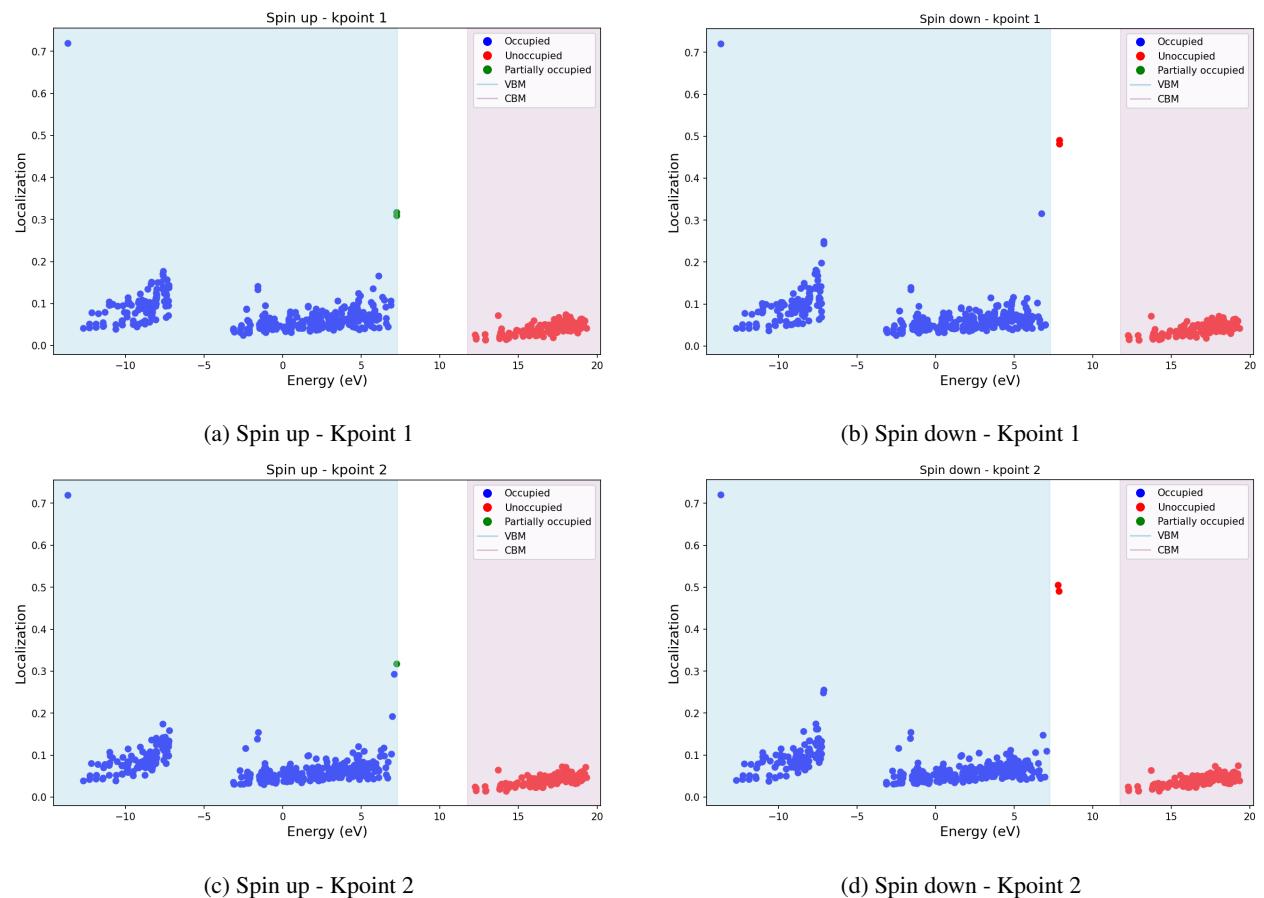


Figure 235: Localization factor using projected orbitals (s, p, and d).

6.114 Complex: $(V_B - O_N)^{+2}$

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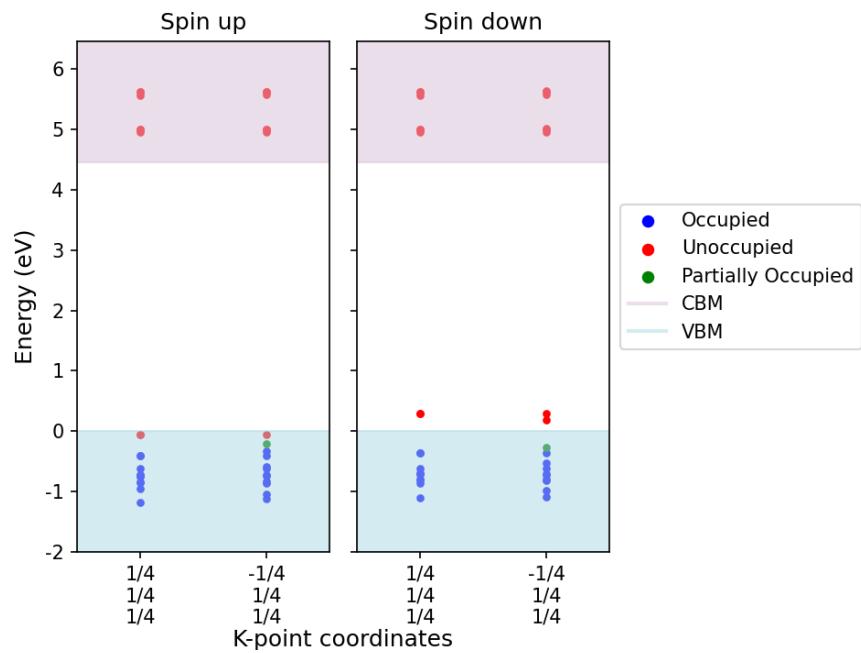


Figure 236: Kohn-Sham states.

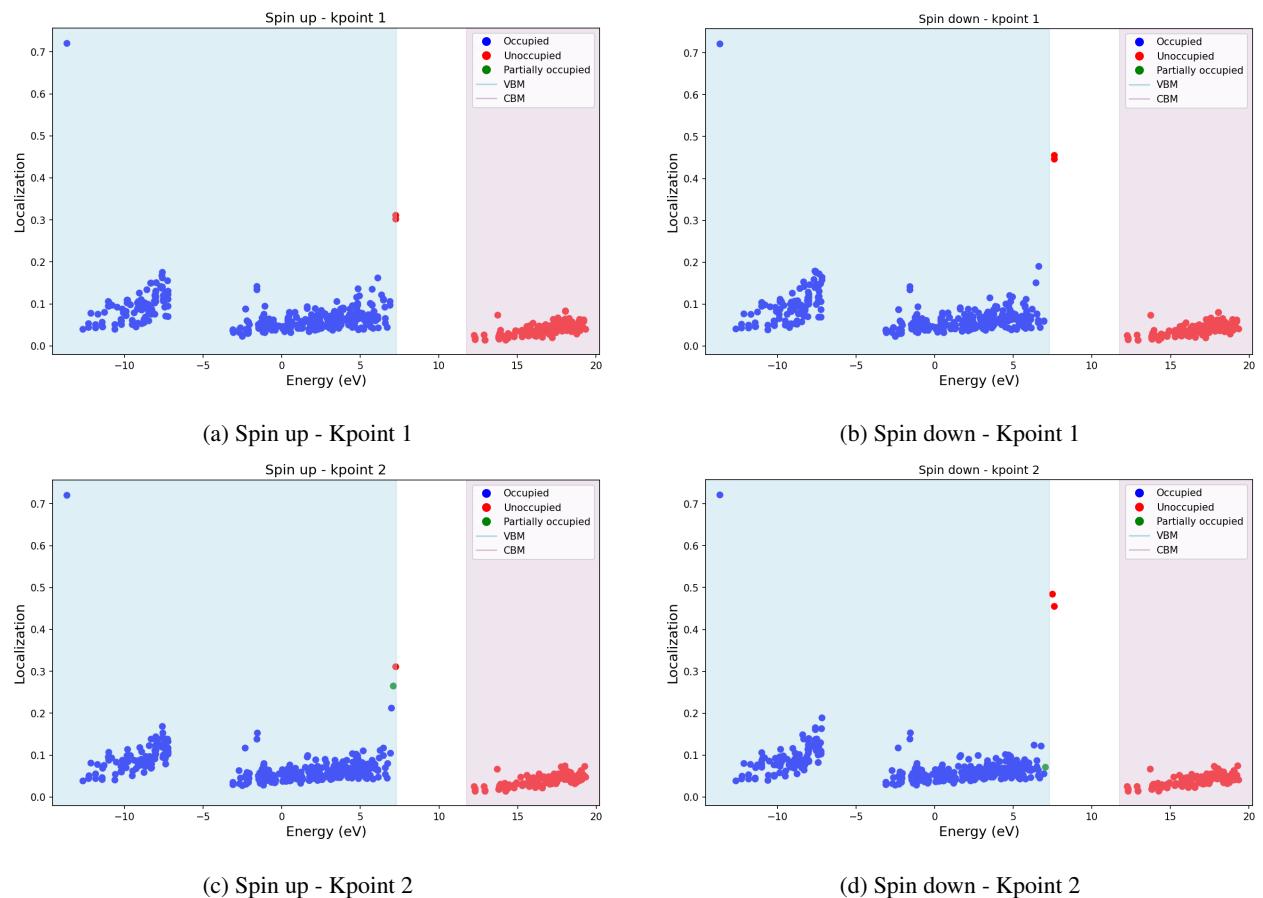


Figure 237: Localization factor using projected orbitals (s, p, and d).

6.115 Complex: $(V_B - O_N)^{-1}$

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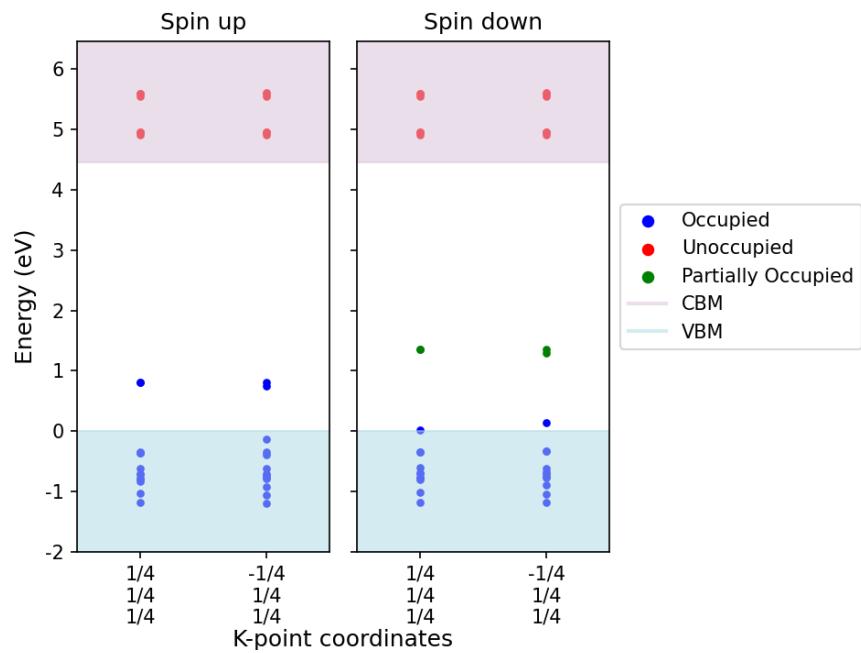


Figure 238: Kohn-Sham states.

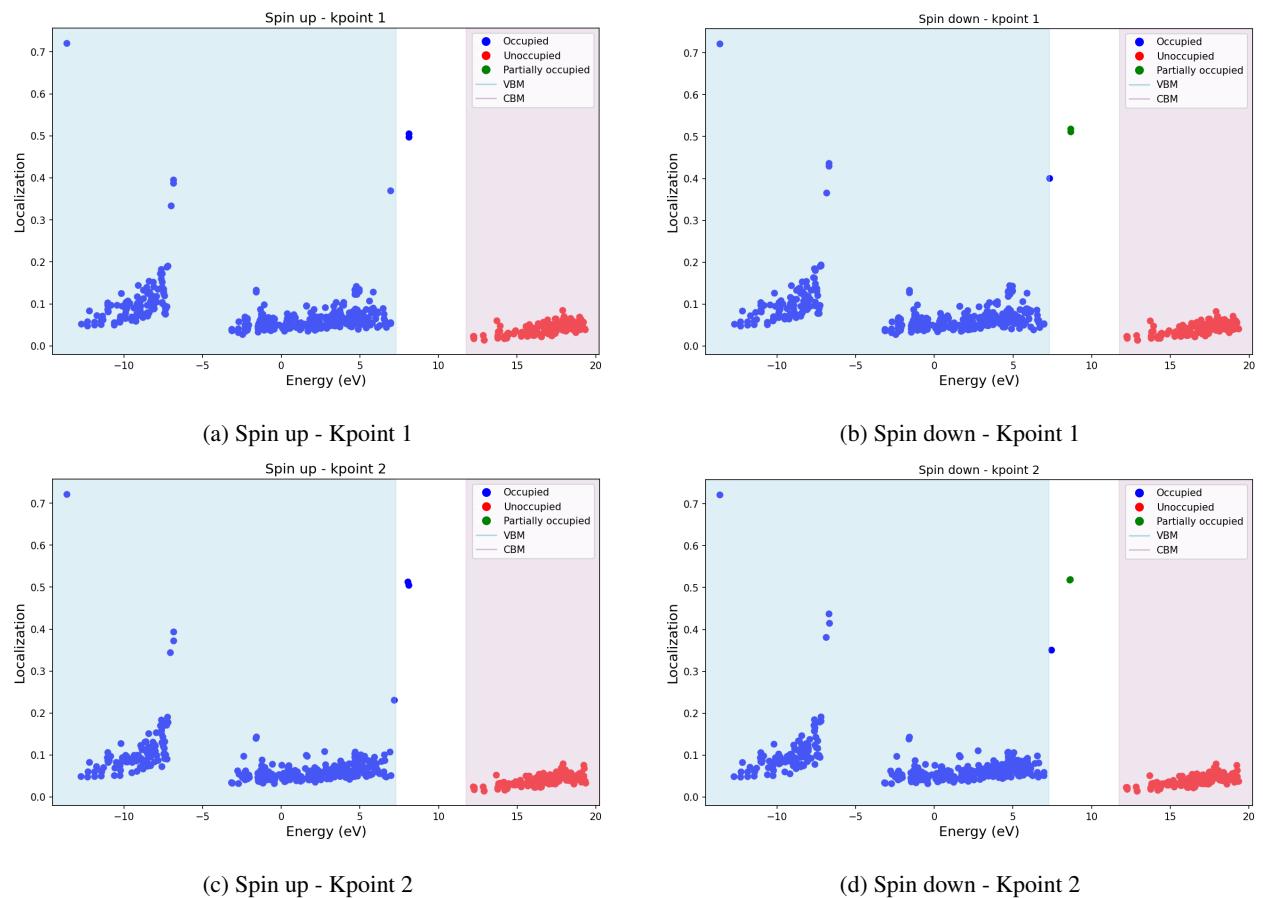


Figure 239: Localization factor using projected orbitals (s, p, and d).

6.116 Complex: $(V_B - O_N)^{-2}$

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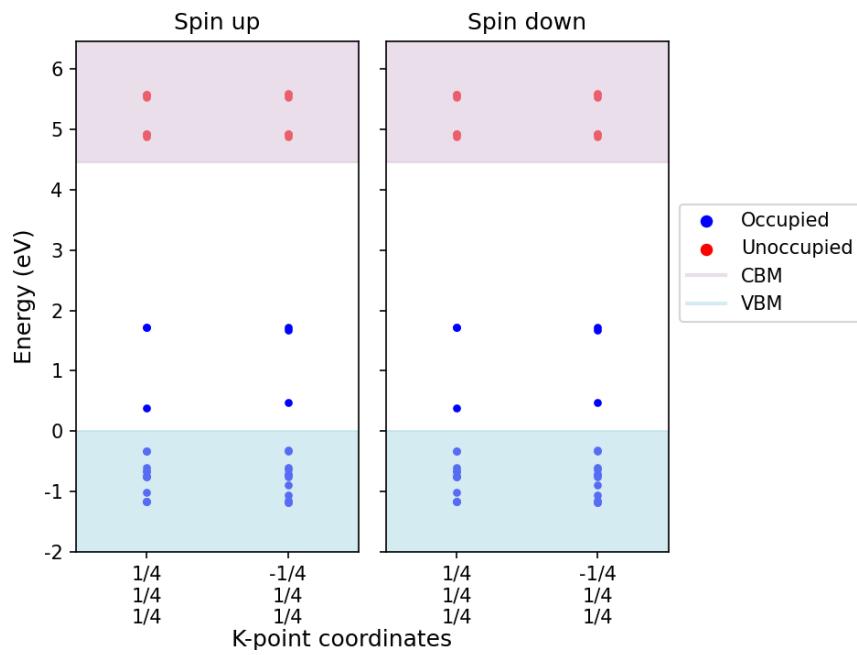


Figure 240: Kohn-Sham states.

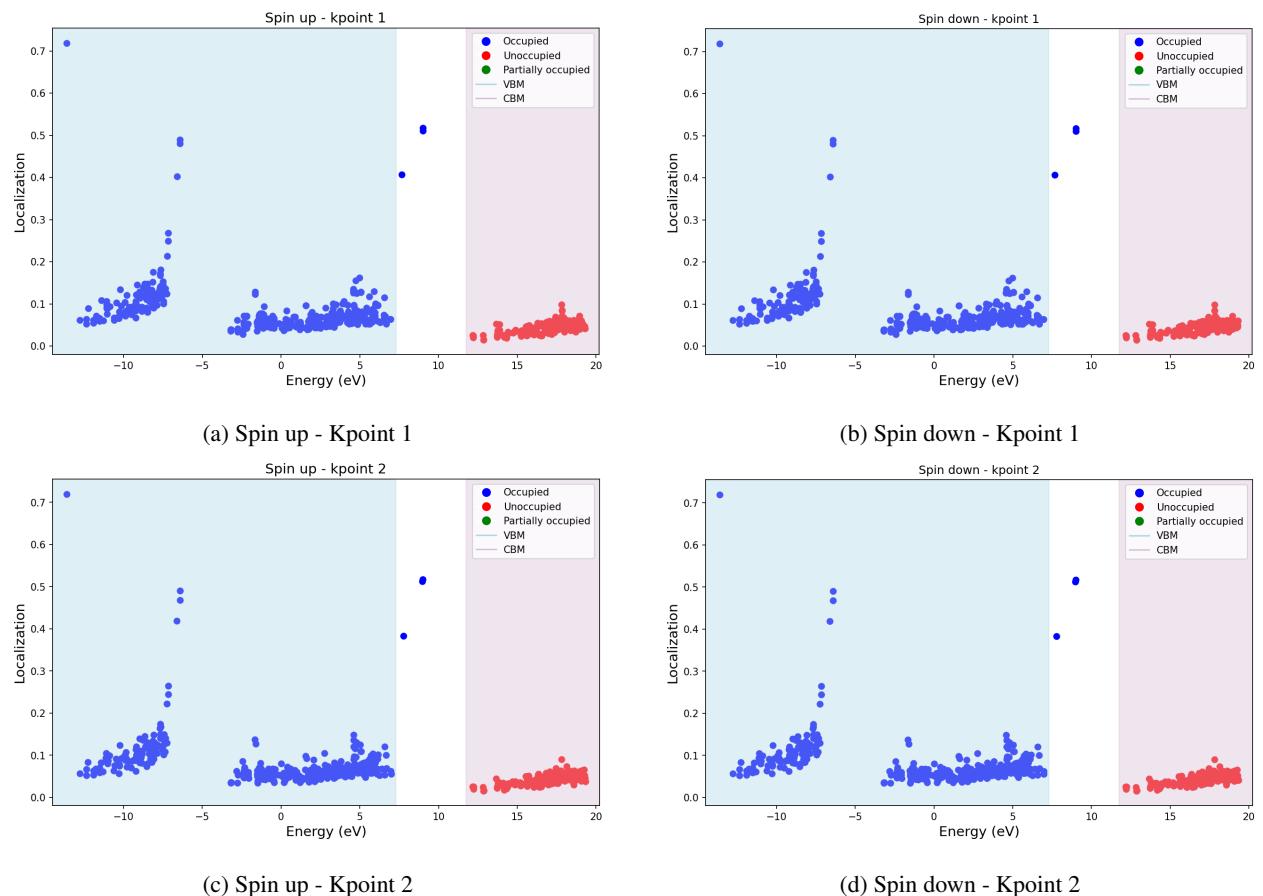


Figure 241: Localization factor using projected orbitals (s, p, and d).

6.117 Complex: $(V_B - O_N)^{-3}$

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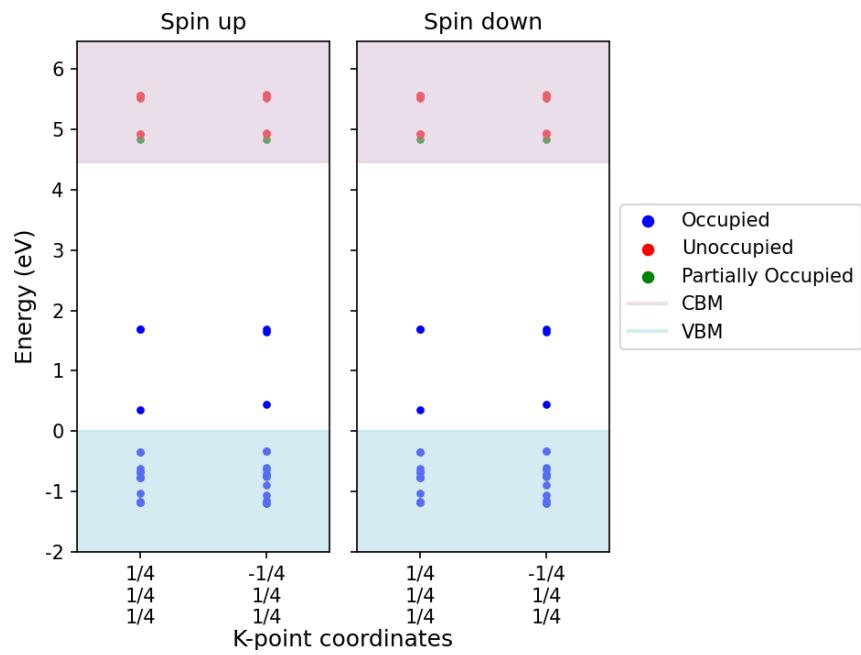


Figure 242: Kohn-Sham states.

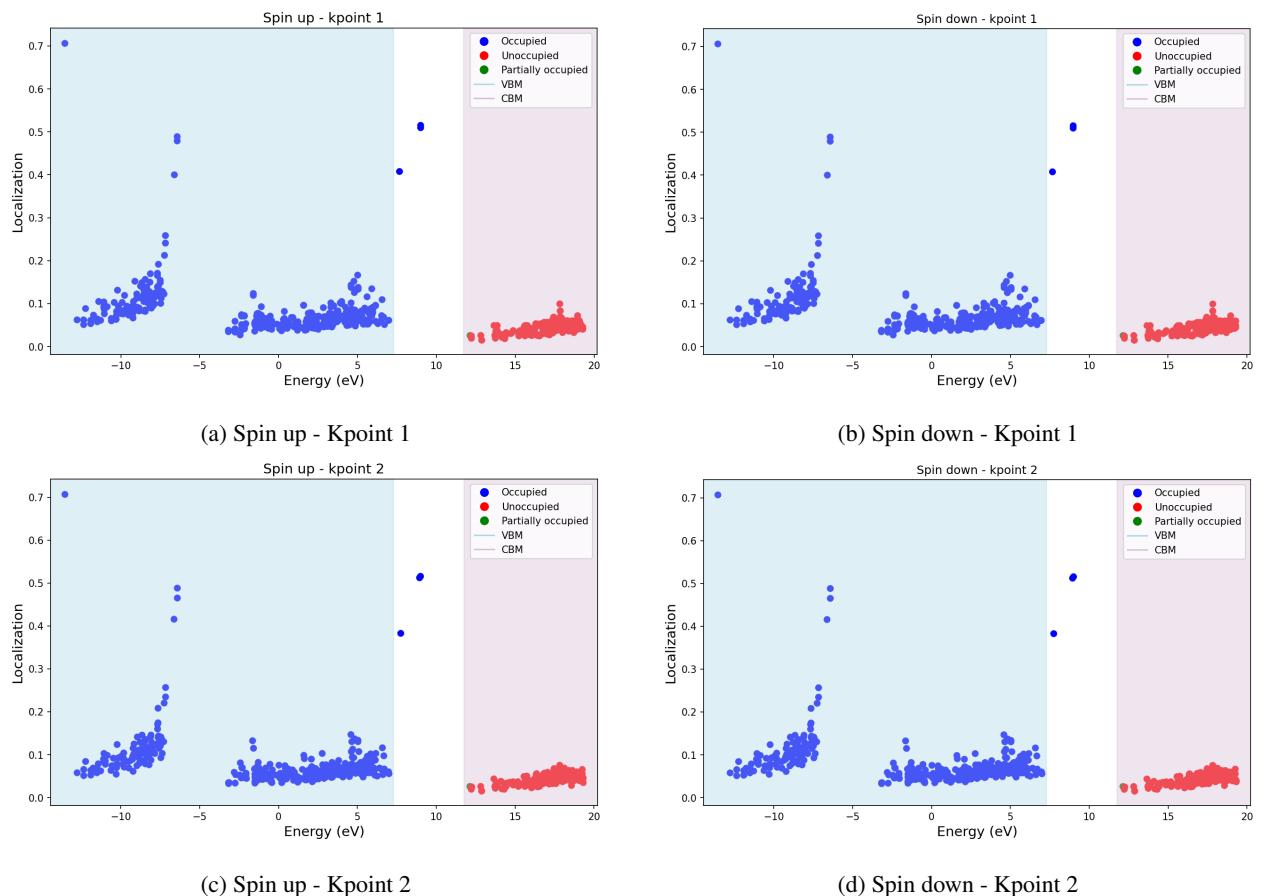


Figure 243: Localization factor using projected orbitals (s, p, and d).

6.118 Complex: $(V_B - Si_B)^0$

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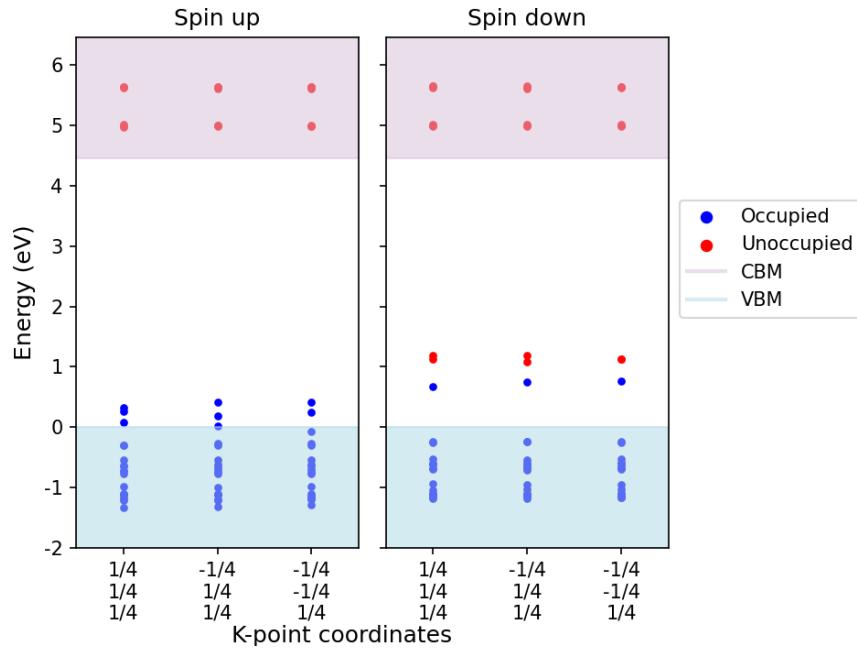


Figure 244: Kohn-Sham states.

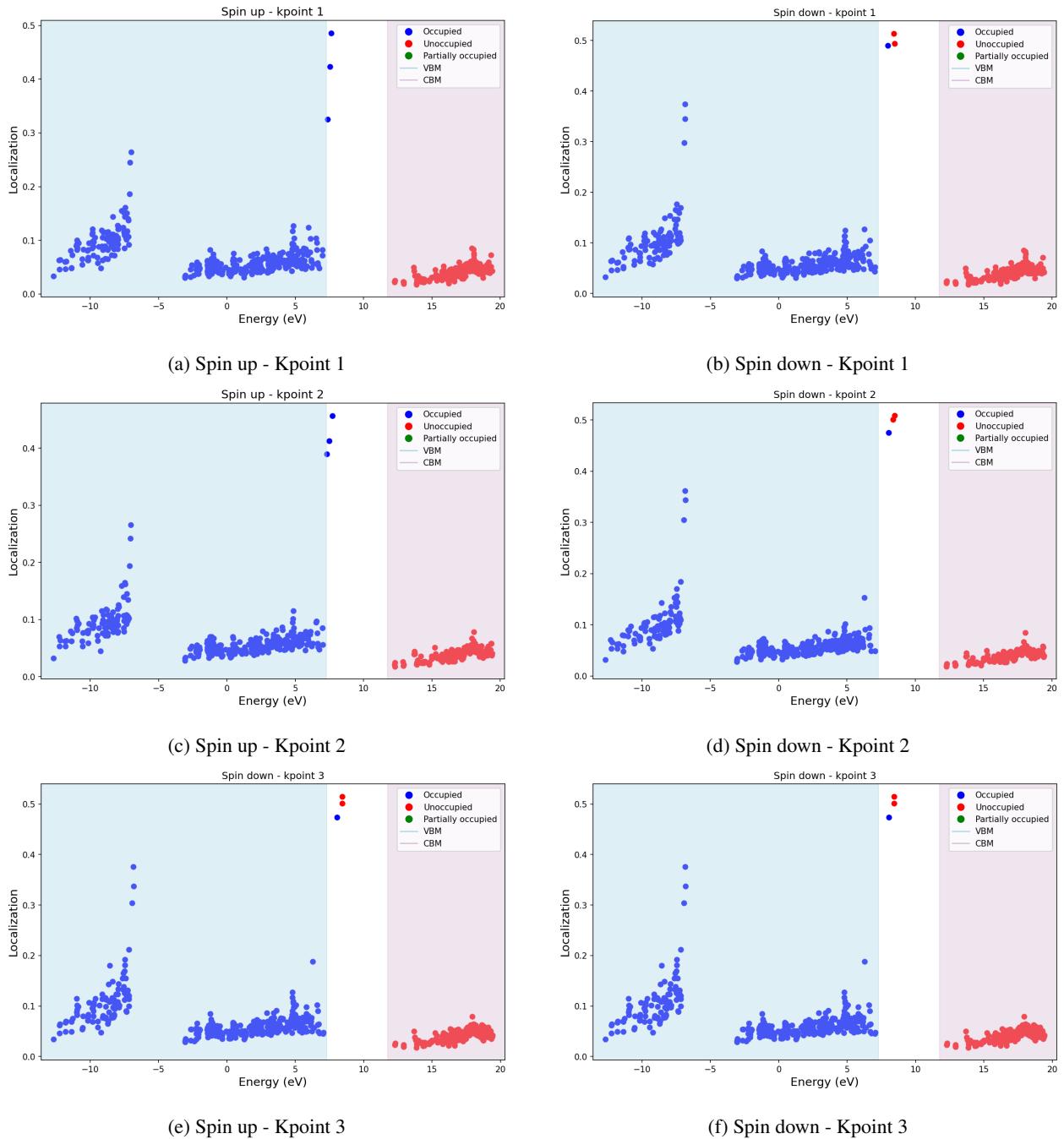


Figure 245: Localization factor using projected orbitals (s, p, and d).

6.119 Complex: $(V_B - Si_B)^{+1}$

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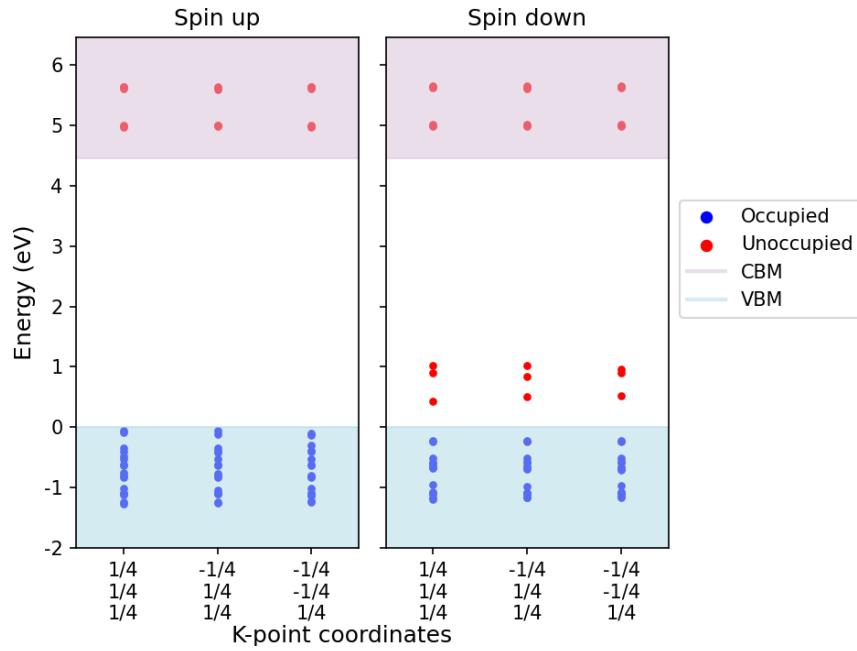


Figure 246: Kohn-Sham states.

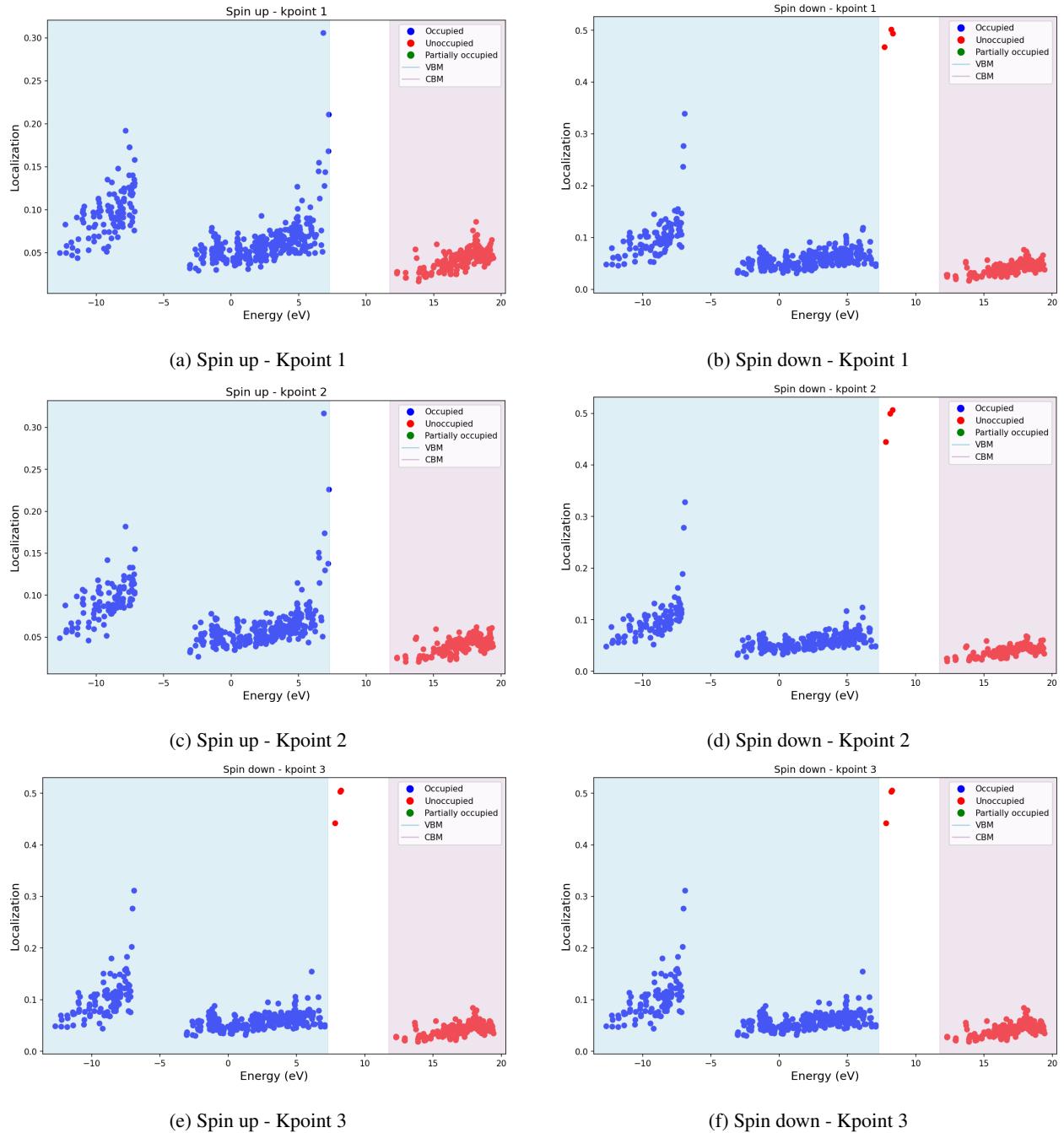


Figure 247: Localization factor using projected orbitals (s, p, and d).

6.120 Complex: $(V_B - Si_B)^{+2}$

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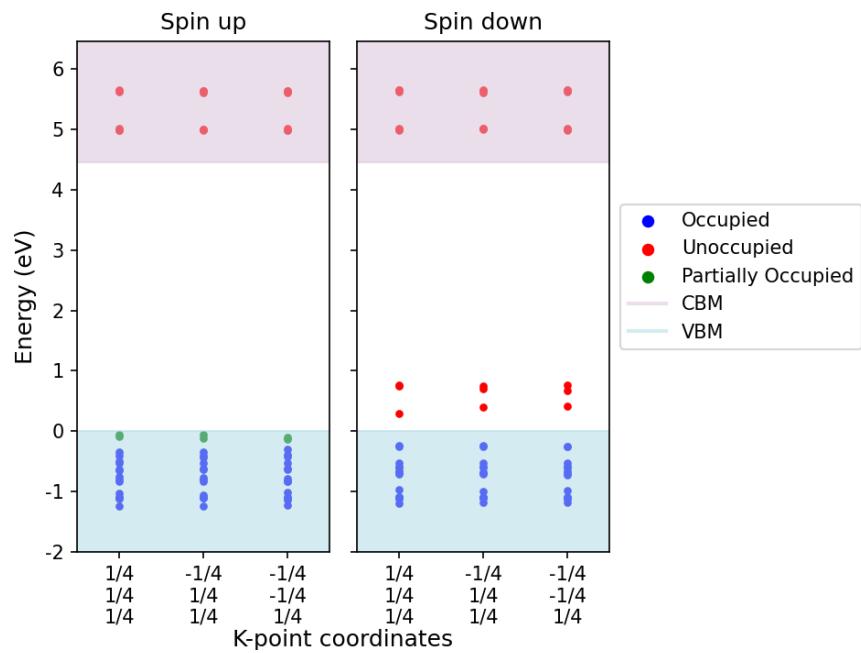


Figure 248: Kohn-Sham states.

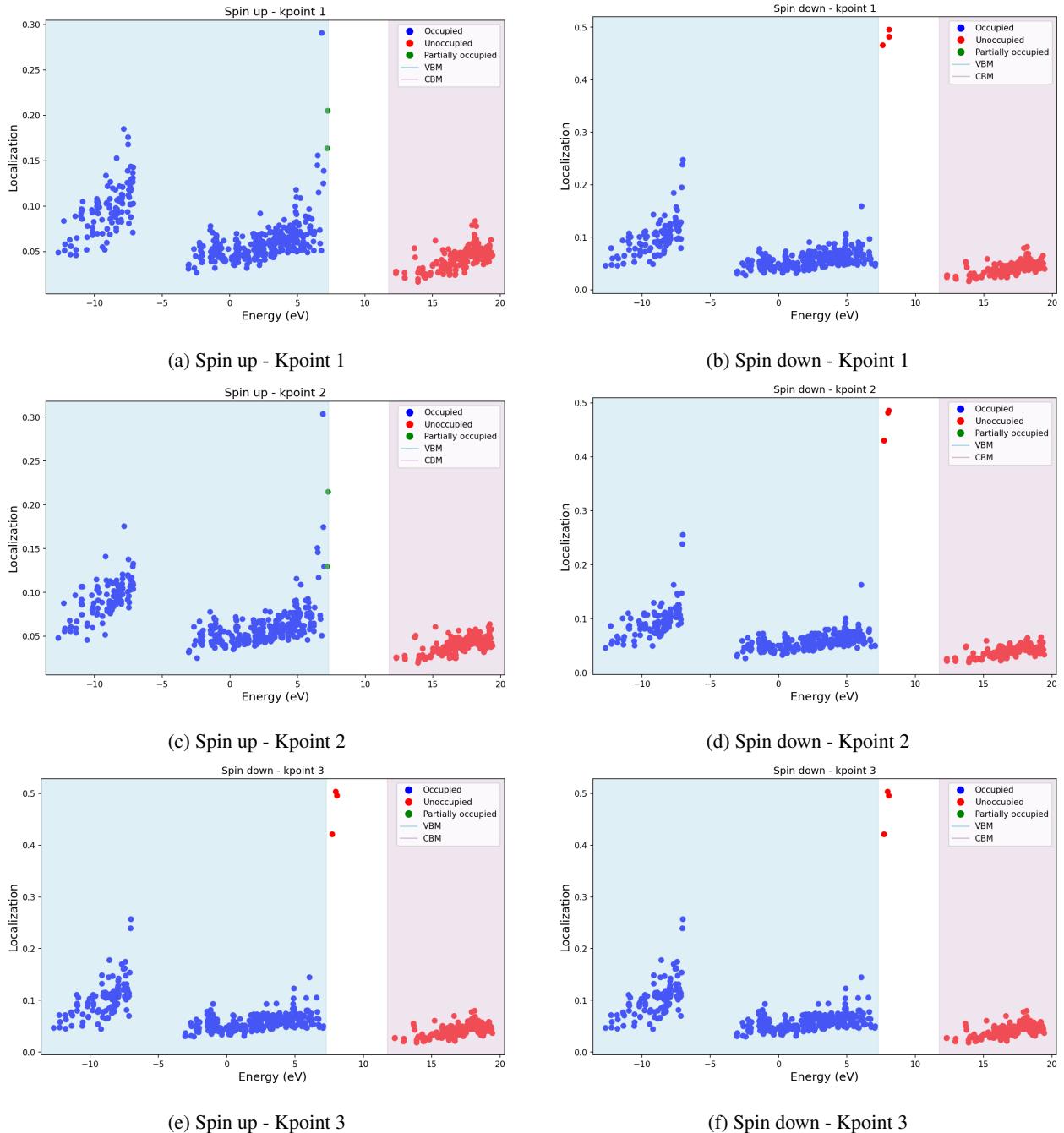


Figure 249: Localization factor using projected orbitals (s, p, and d).

6.121 Complex: $(V_B - Si_B)^{-1}$

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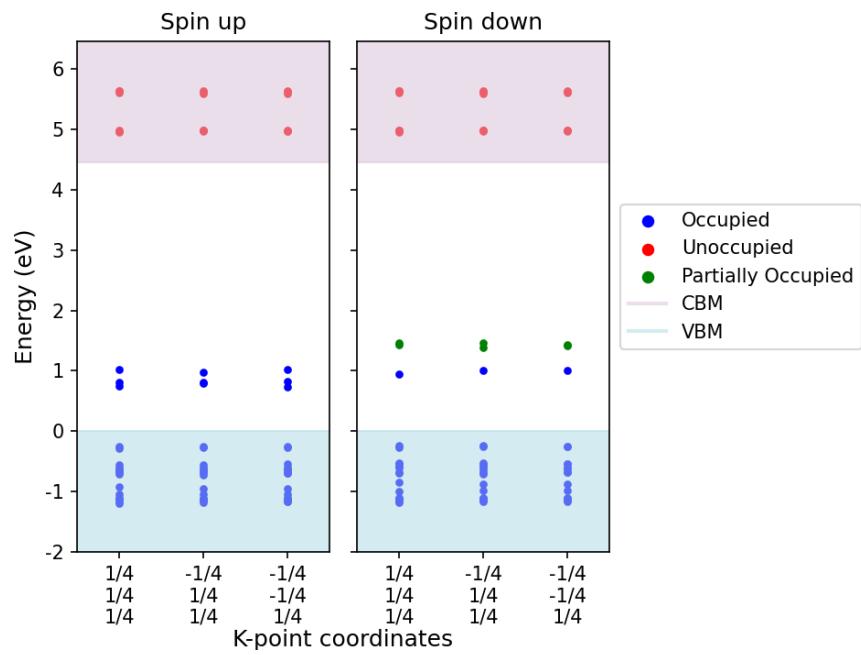


Figure 250: Kohn-Sham states.

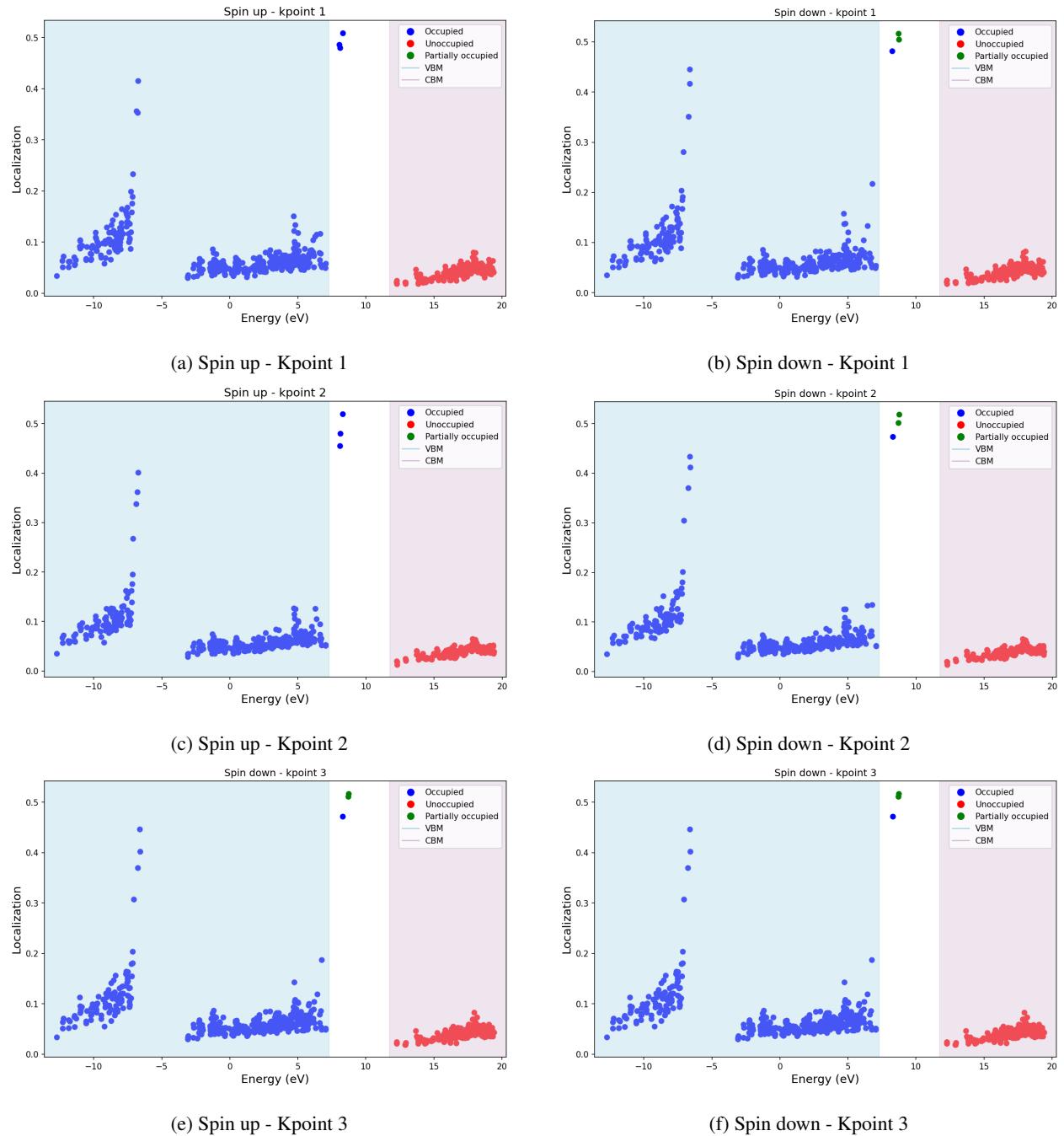


Figure 251: Localization factor using projected orbitals (s, p, and d).

6.122 Complex: $(V_B - Si_B)^{-2}$

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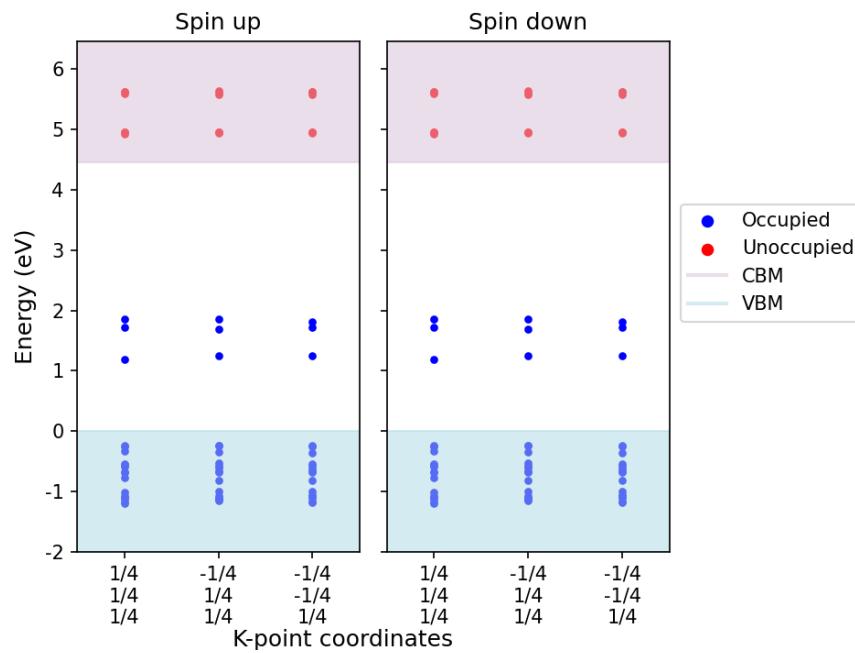


Figure 252: Kohn-Sham states.

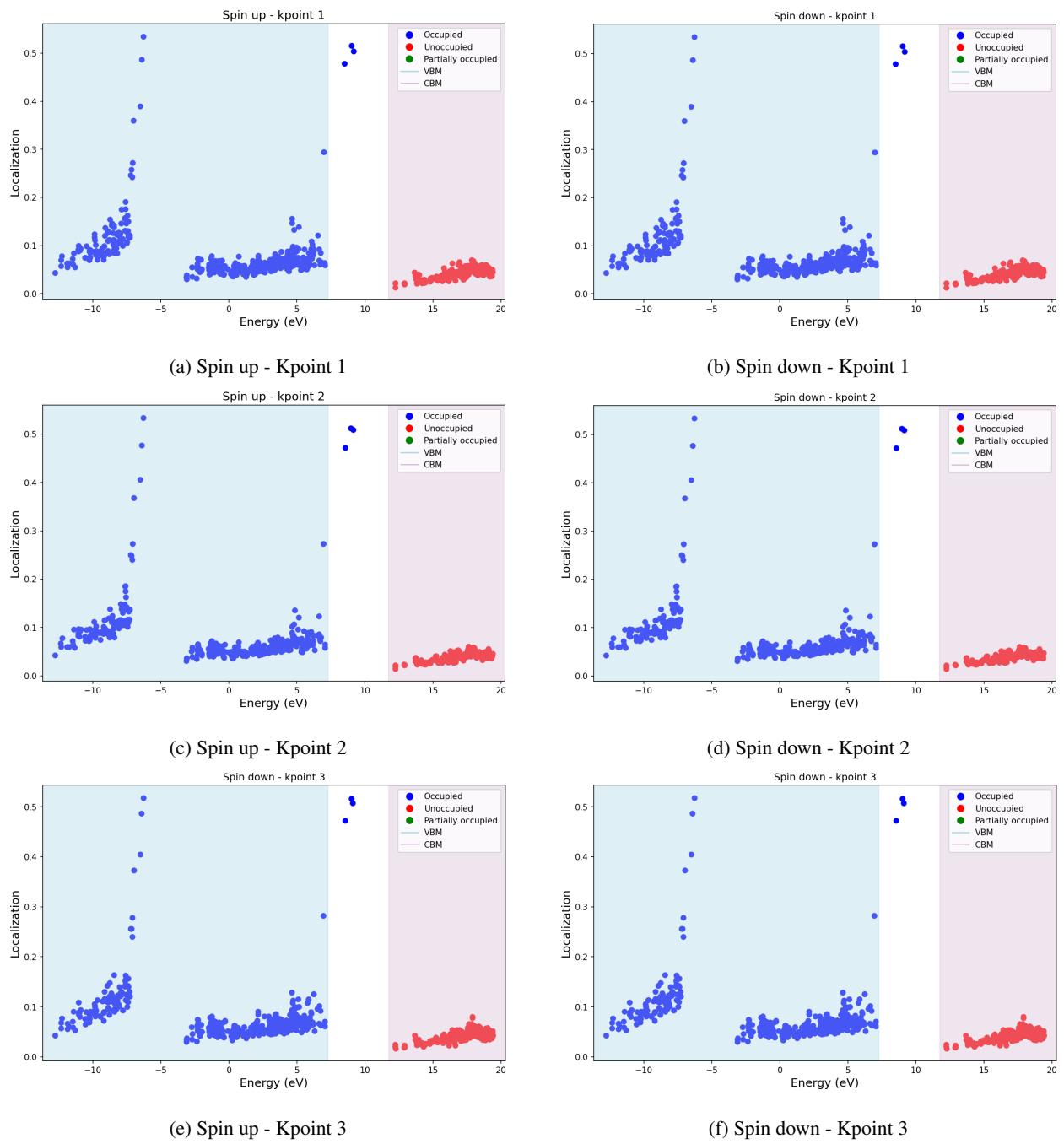


Figure 253: Localization factor using projected orbitals (s, p, and d).

6.123 Complex: $(V_B - Si_B)^{-3}$

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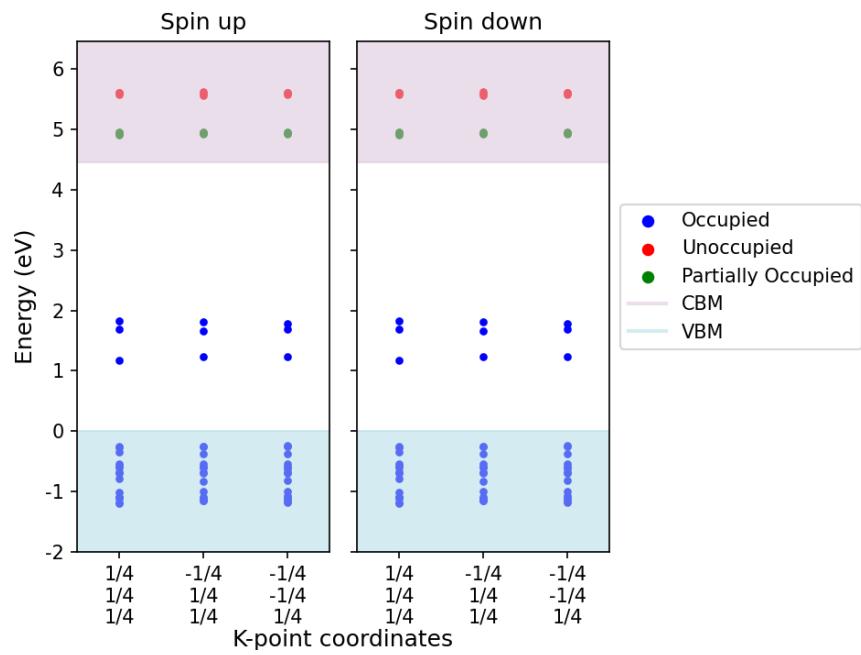


Figure 254: Kohn-Sham states.

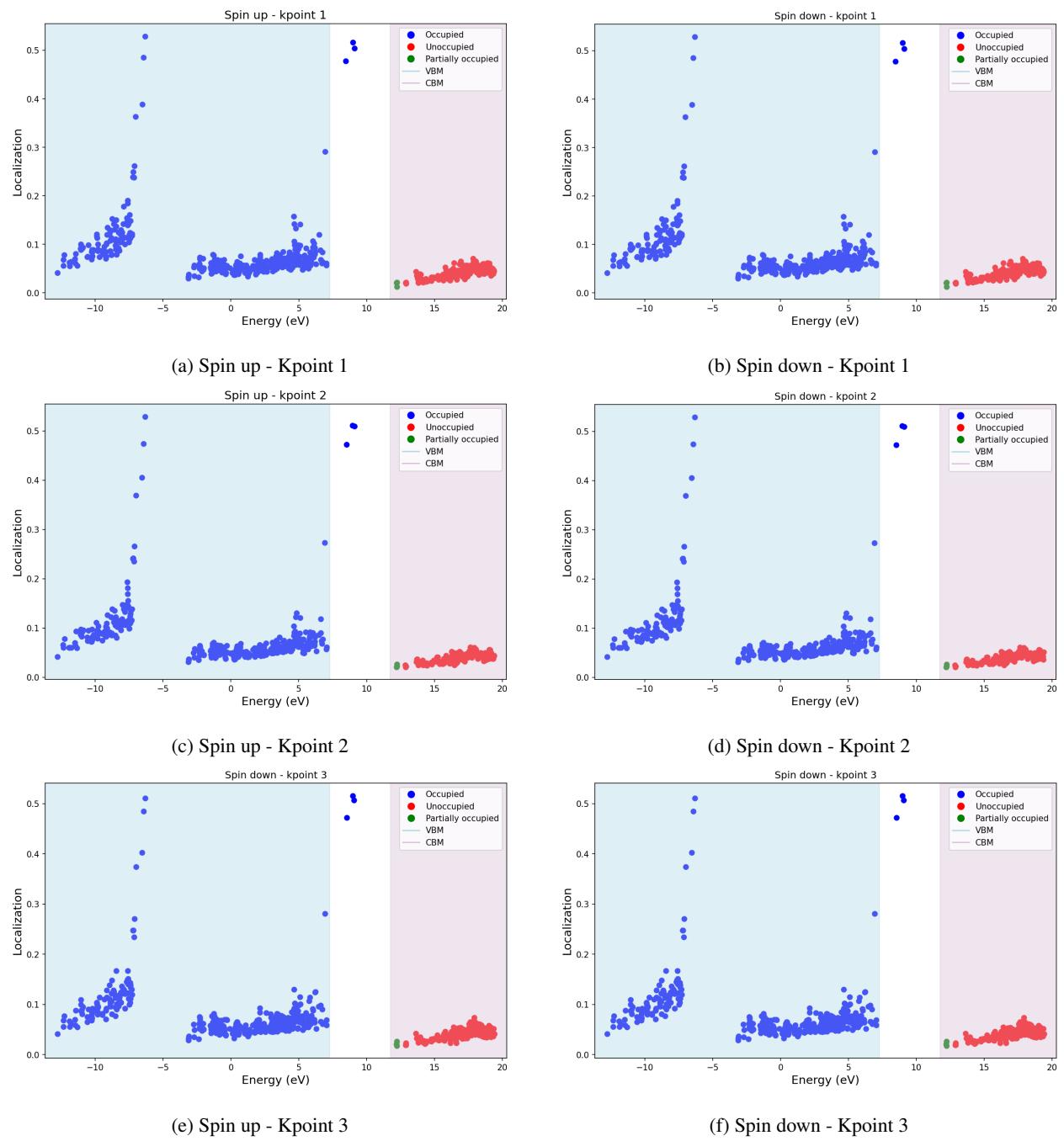


Figure 255: Localization factor using projected orbitals (s, p, and d).

7 Formation energy diagrams

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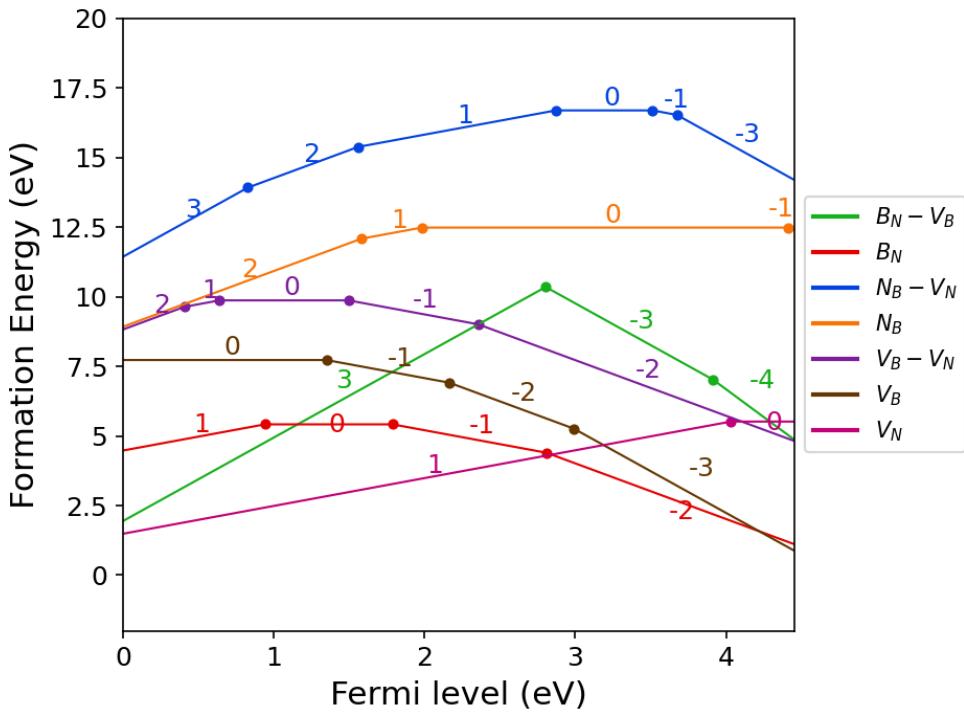


Figure 256: Boron rich condition. Also includes correction energies.

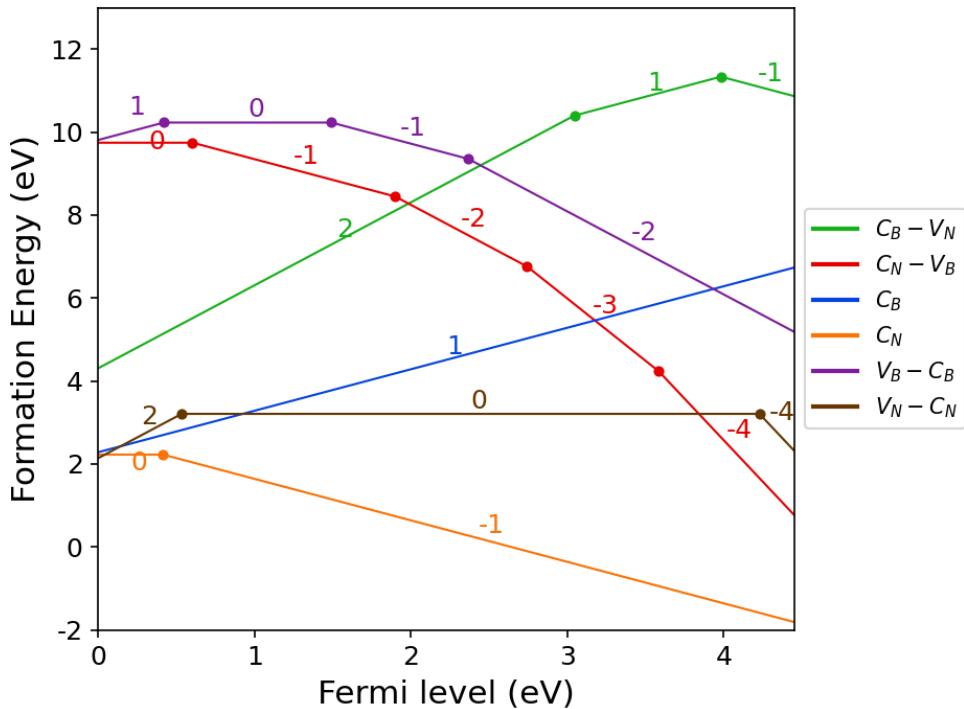


Figure 257: Boron rich condition. Also includes correction energies.

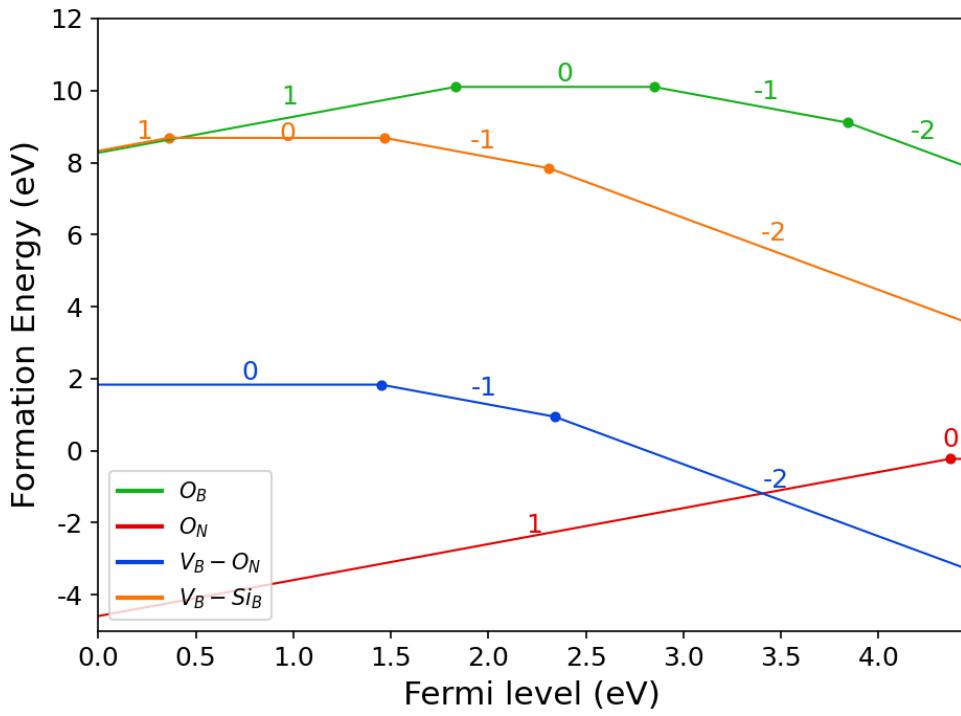


Figure 258: Boron rich condition. Also includes correction energies.