

## 1 Post-analysis - PBE functional

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

Table 1: Boron and nitrogen vacancies.

Defect	Charge	Magnetization ( $\mu_B$ )	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 2: Antisite vacancies.

Defect	Charge	Magnetization ( $\mu_B$ )	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 3: complex

Defect	Charge	Magnetization ( $\mu_B$ )	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 4: di-vac

Defect	Charge	Magnetization ( $\mu_B$ )	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 5: di-vacancy

Defect	Charge	Magnetization ( $\mu_B$ )	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 6: Fig-4

Defect	Charge	Magnetization ( $\mu_B$ )	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 7: Fig-5

Defect	Charge	Magnetization ( $\mu_B$ )	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 8: C-dimer

Defect	Charge	Magnetization ( $\mu_B$ )	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 9: 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

[Go to the Formation energy diagrams](#)

[Go to the selected defects in Table 54](#)

## 1.1 Vacancy: $V_B^0$

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Table 10:  $V_B^0$

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

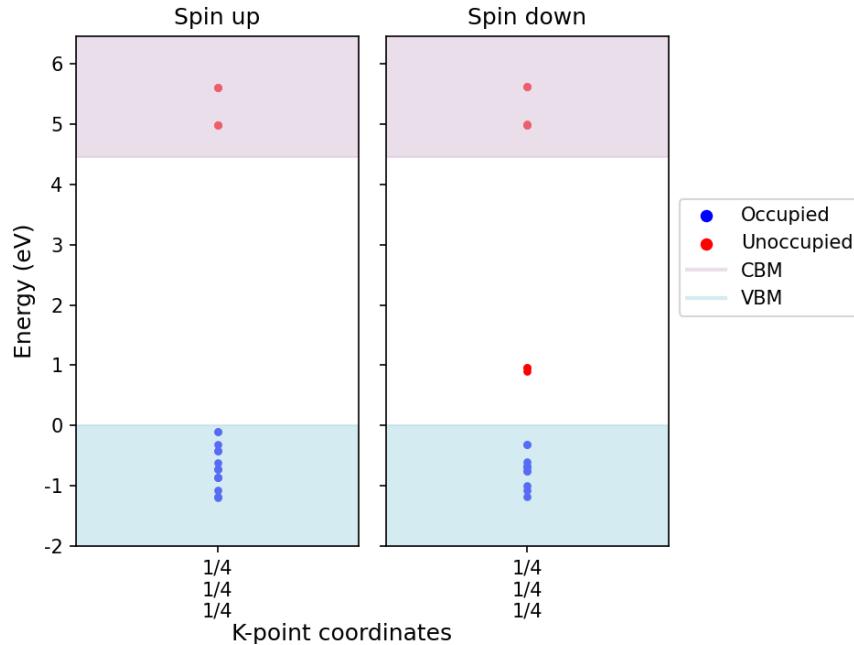


Figure 1: Kohn-Sham states.

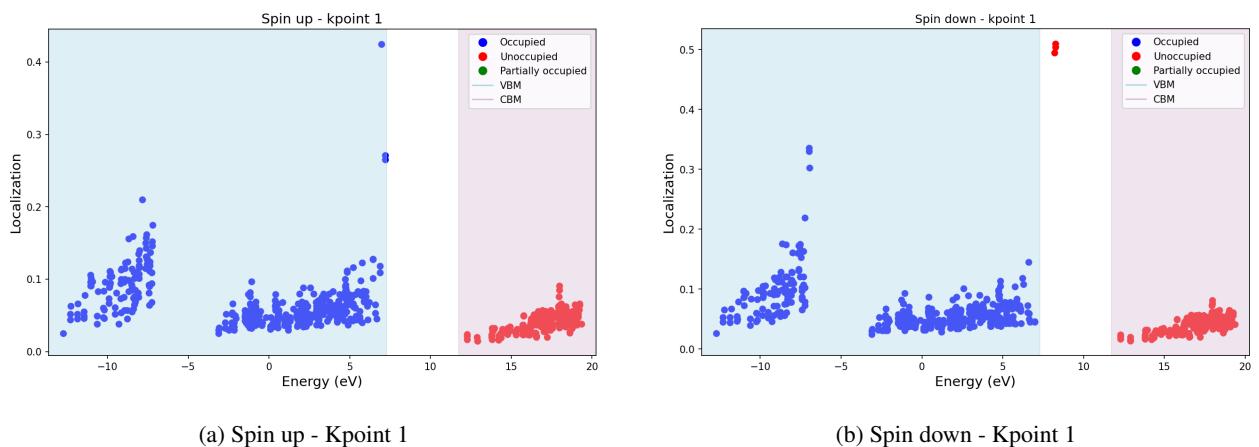


Figure 2: Localization factor using projected orbitals (s, p and d).

## 1.2 Vacancy: $V_B^{+1}$

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Table 11:  $V_B^{+1}$

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

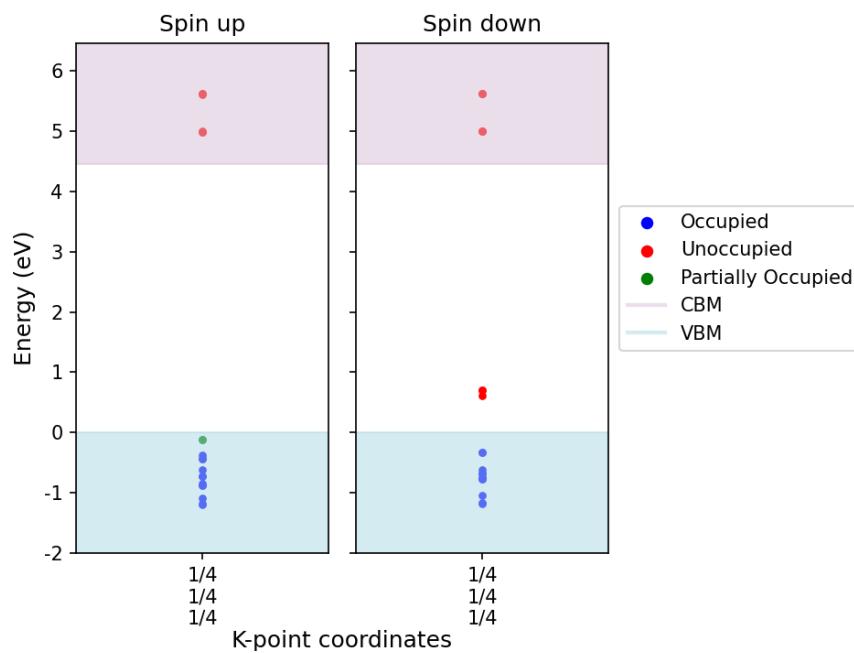


Figure 3: Kohn-Sham states.

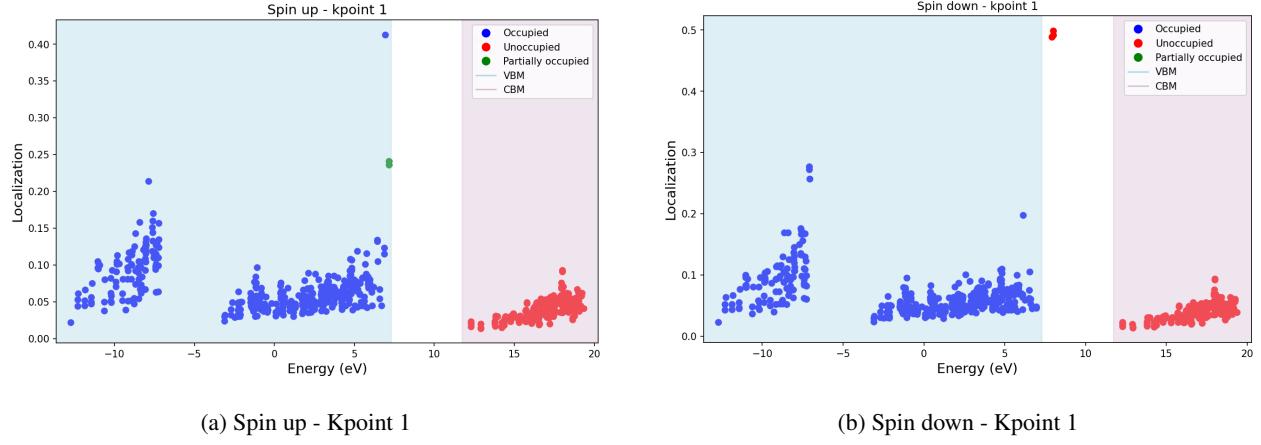


Figure 4: Localization factor using projected orbitals (s, p and d).

### 1.3 Vacancy: $V_B^{+2}$

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Table 12:  $V_B^{+2}$

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

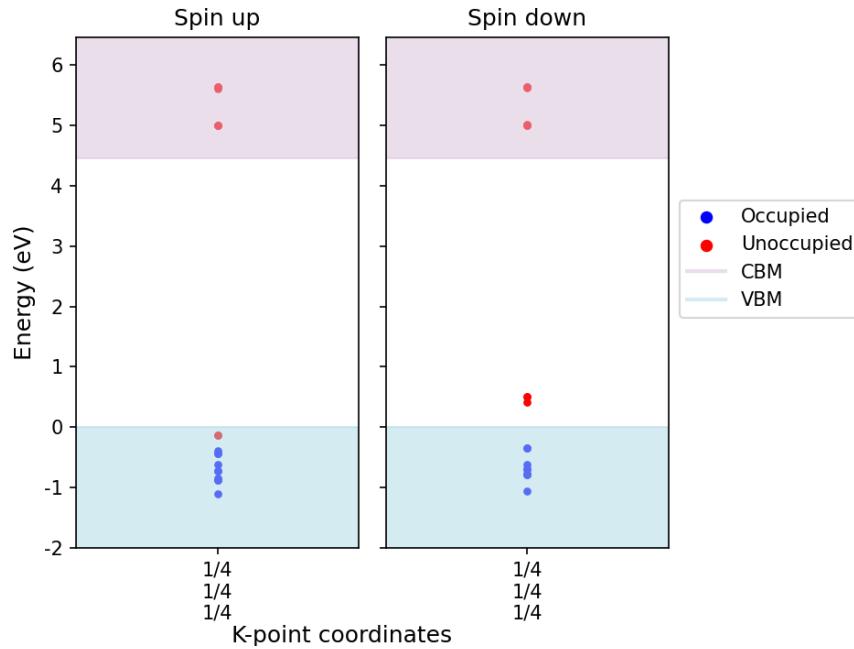


Figure 5: Kohn-Sham states.

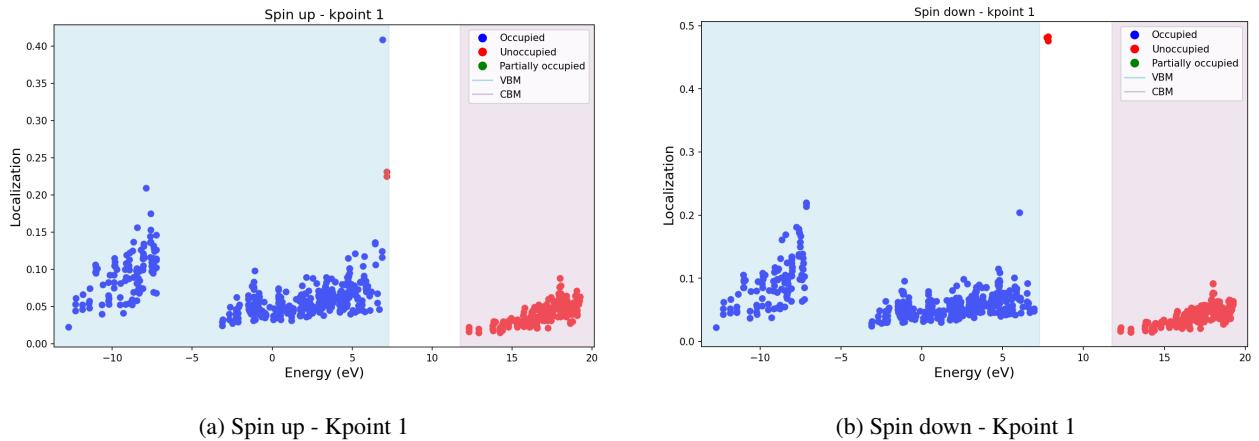


Figure 6: Localization factor using projected orbitals (s, p and d).

## 1.4 Vacancy: $V_B^{-1}$

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Table 13:  $V_B^{-1}$

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

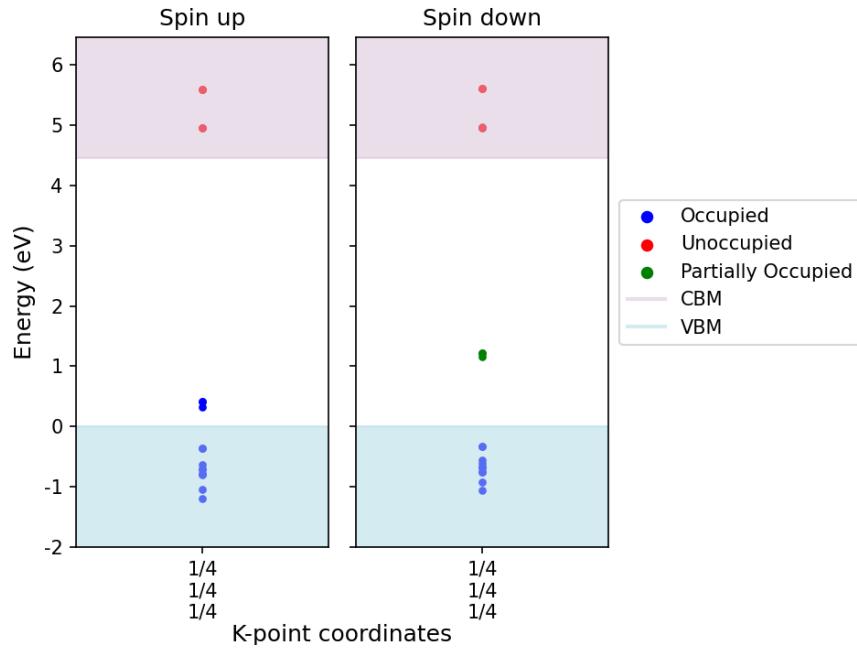


Figure 7: Kohn-Sham states.

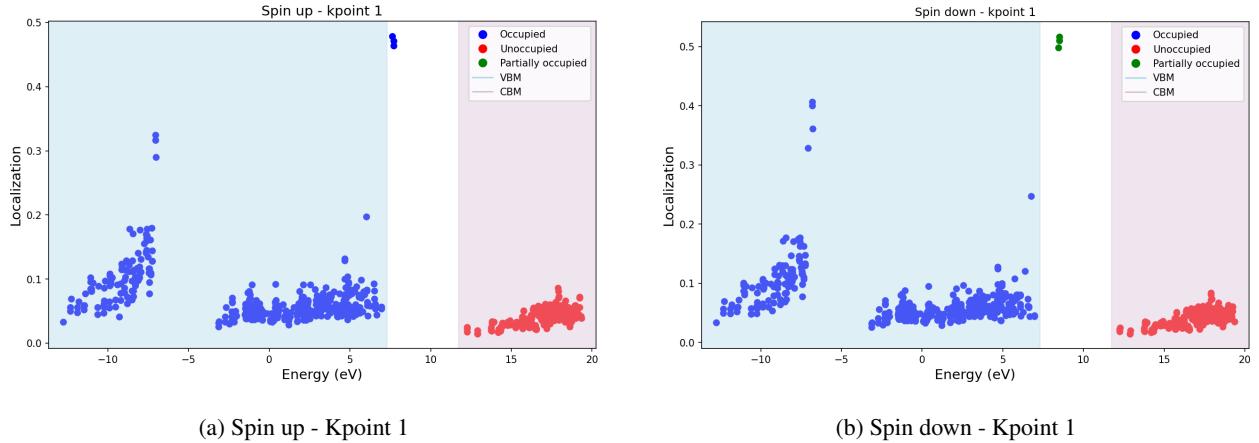


Figure 8: Localization factor using projected orbitals (s, p and d).

## 1.5 Vacancy: $V_B^{-2}$

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Table 14:  $V_B^{-2}$

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

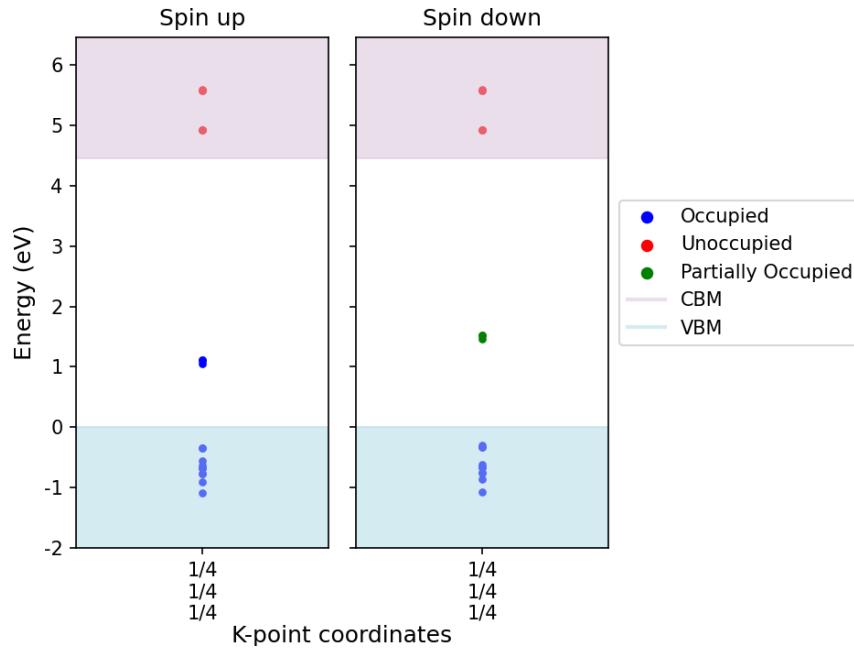


Figure 9: Kohn-Sham states.

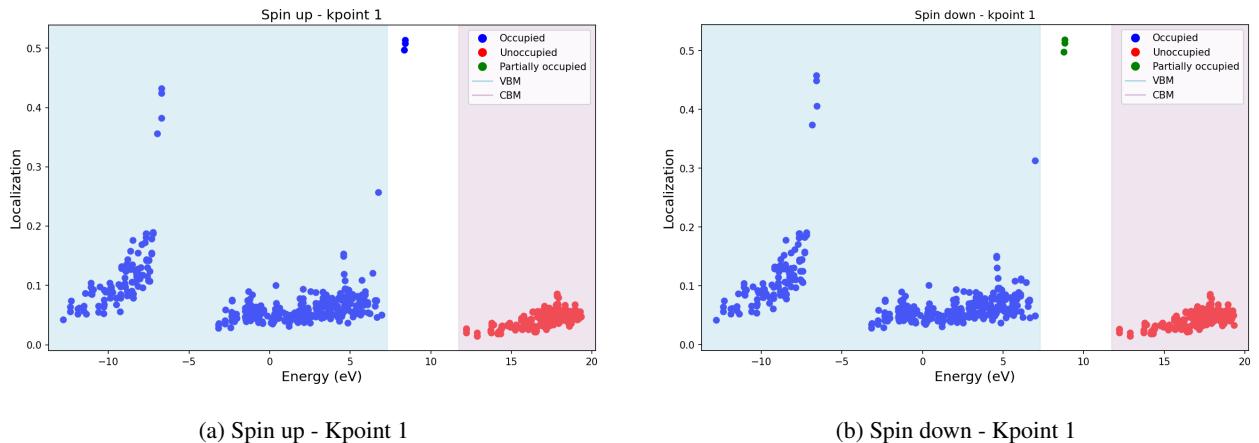


Figure 10: Localization factor using projected orbitals (s, p and d).

## 1.6 Vacancy: $V_B^{-3}$

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Table 15:  $V_B^{-3}$

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

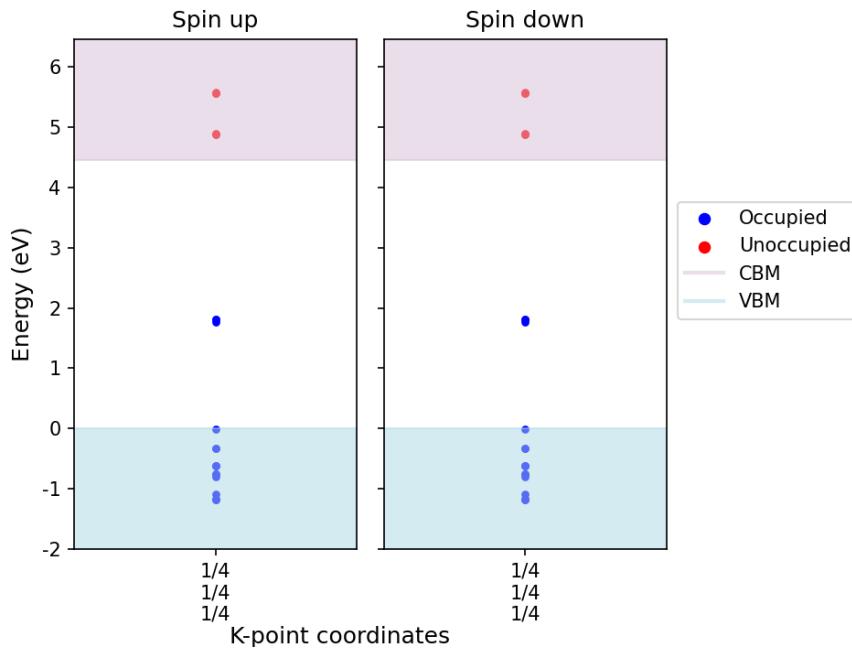


Figure 11: Kohn-Sham states.

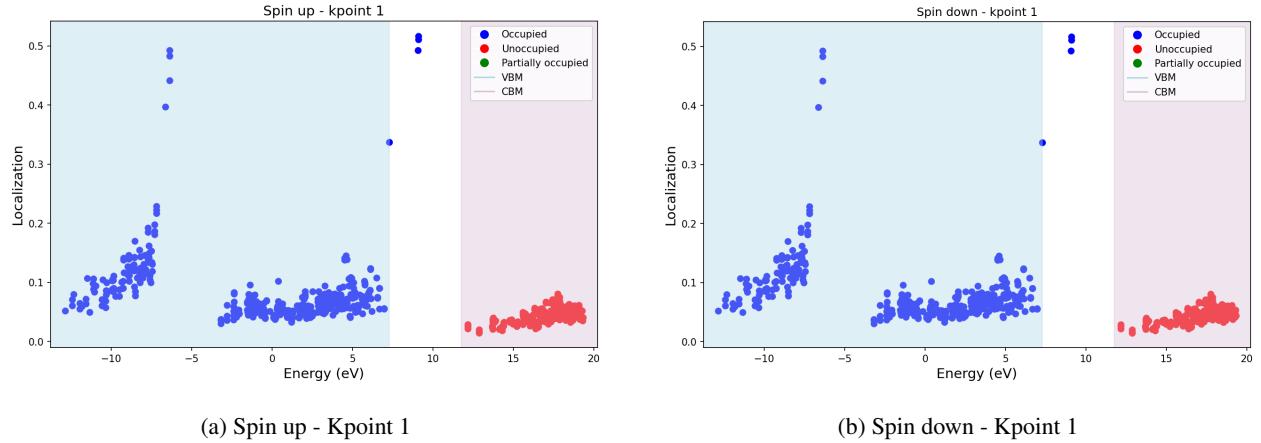


Figure 12: Localization factor using projected orbitals (s, p and d).

## 1.7 Vacancy: $V_B^{-4}$

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Table 16:  $V_B^{-4}$

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

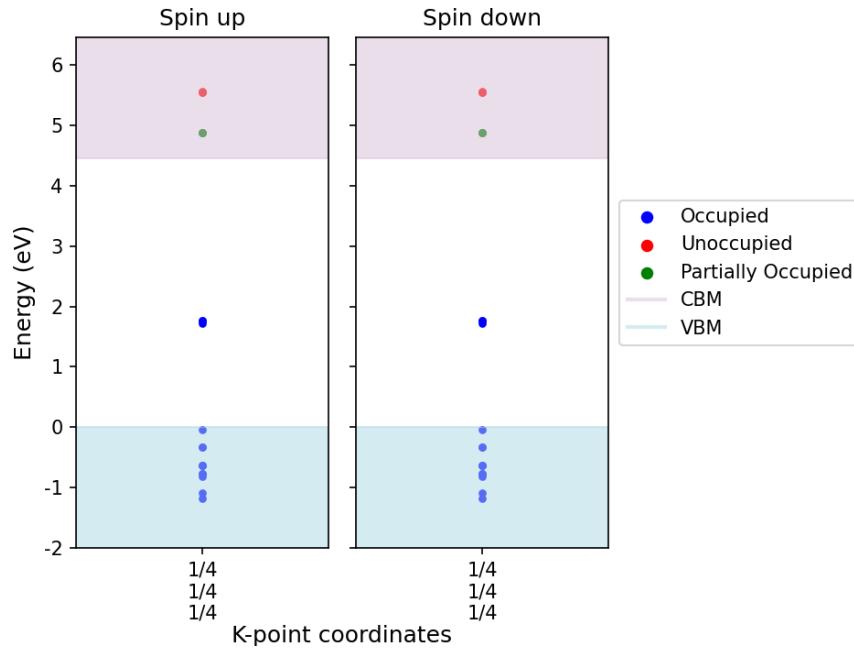


Figure 13: Kohn-Sham states.

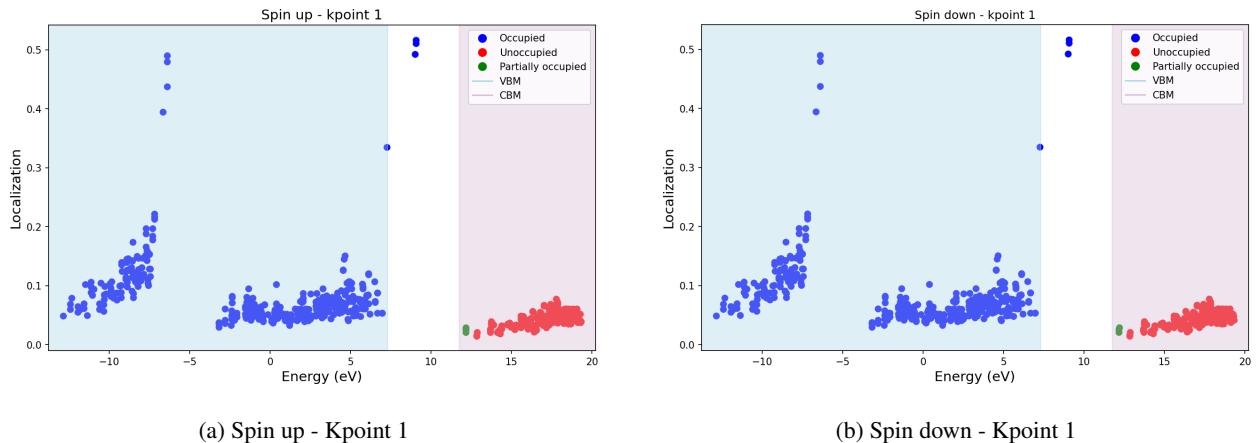


Figure 14: Localization factor using projected orbitals (s, p and d).

## 1.8 Vacancy: $V_N^0$

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Table 17:  $V_N^0$

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	-

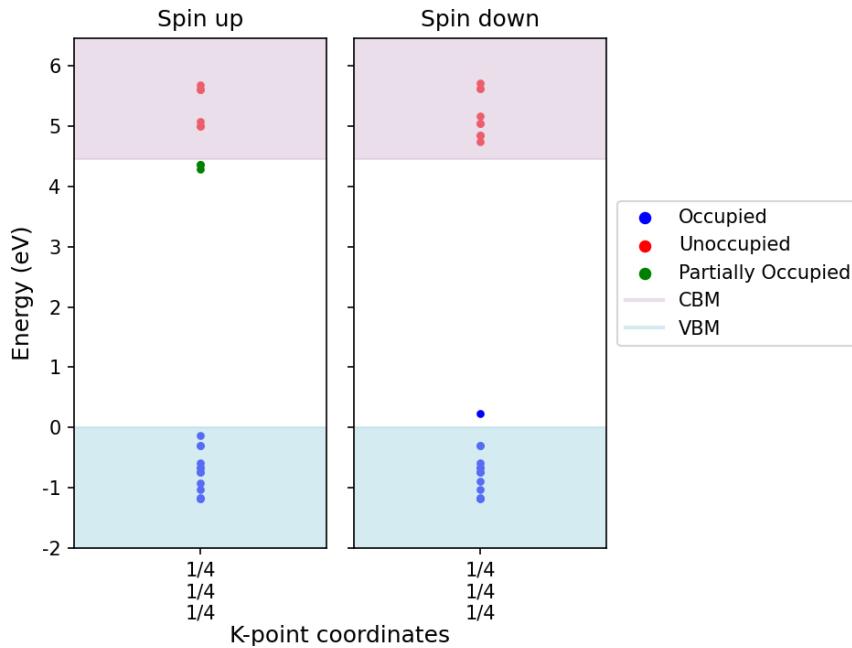


Figure 15: Kohn-Sham states.

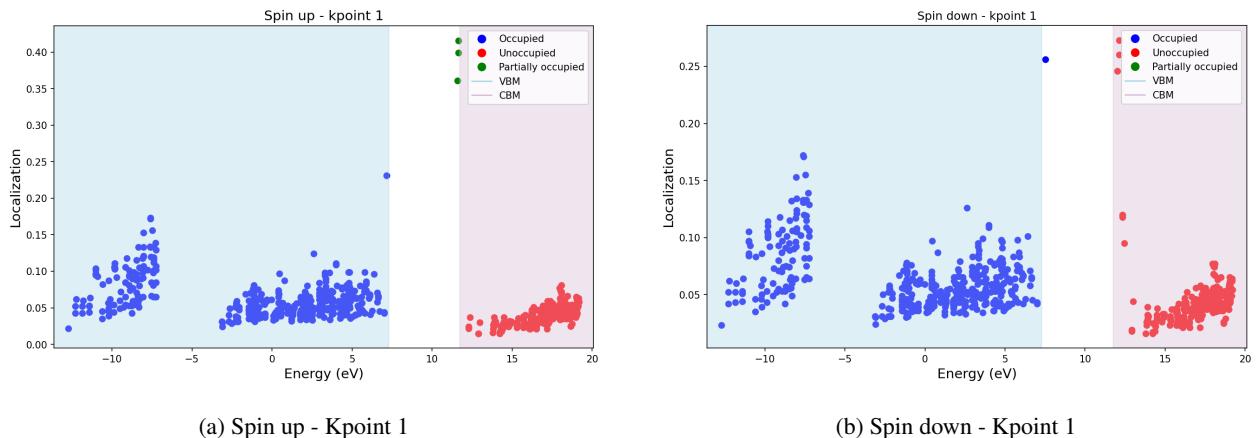


Figure 16: Localization factor using projected orbitals (s, p and d).

## 1.9 Vacancy: $V_N^{+1}$

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Table 18:  $V_N^{+1}$

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

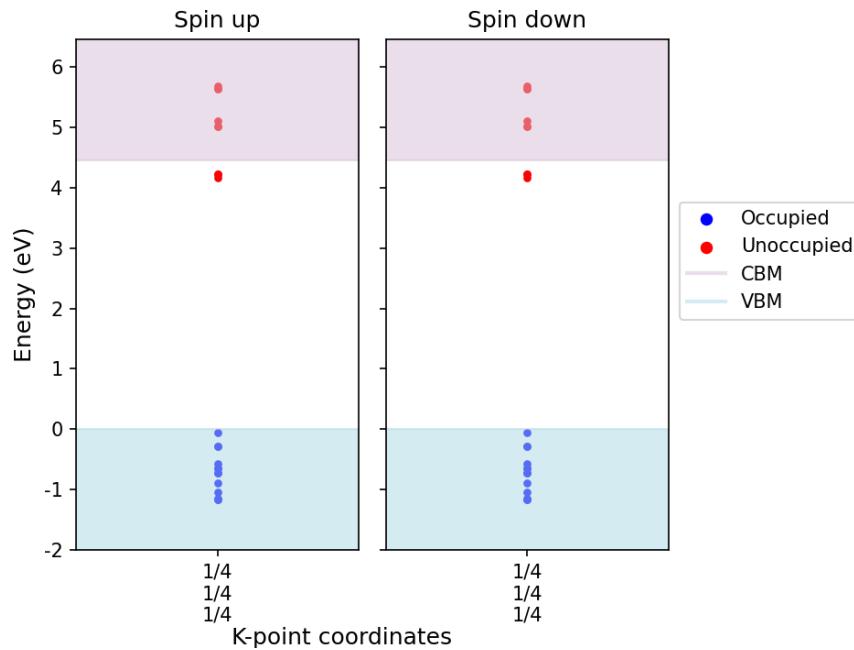


Figure 17: Kohn-Sham states.

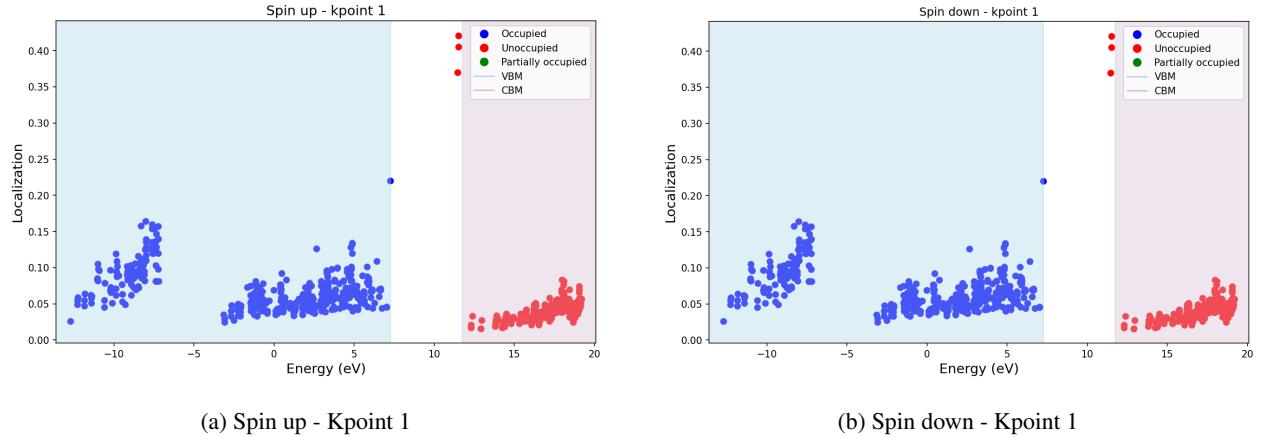


Figure 18: Localization factor using projected orbitals (s, p and d).

### 1.10 Vacancy: $V_N^{+2}$

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Table 19:  $V_N^{+2}$

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

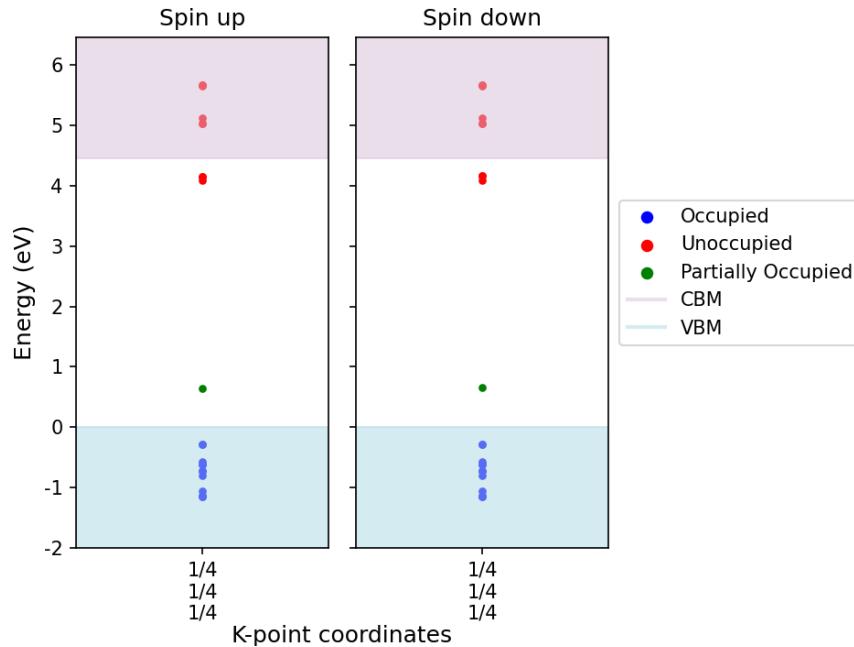


Figure 19: Kohn-Sham states.

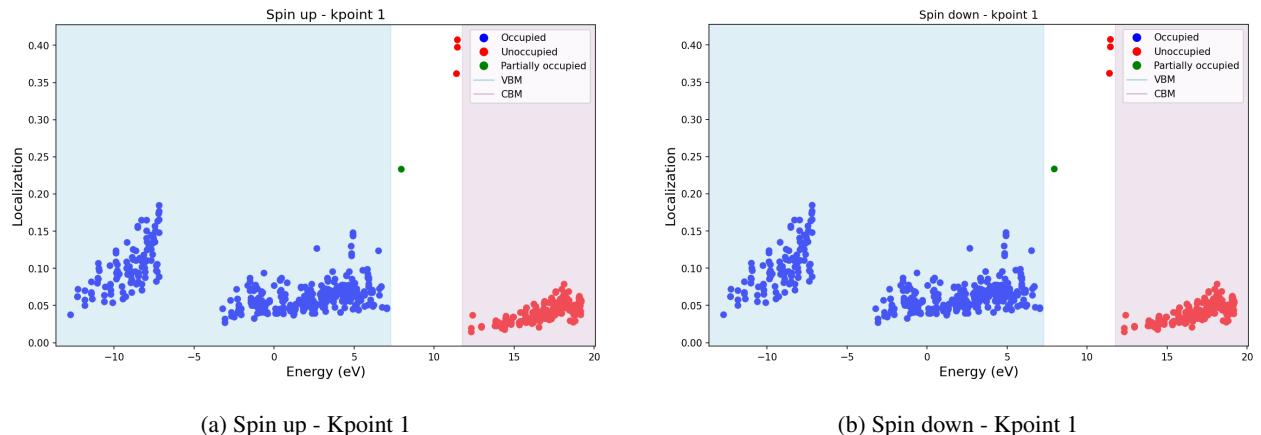


Figure 20: Localization factor using projected orbitals (s, p and d).

## 1.11 Vacancy: $V_N^{+3}$

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Table 20:  $V_N^{+3}$ 

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

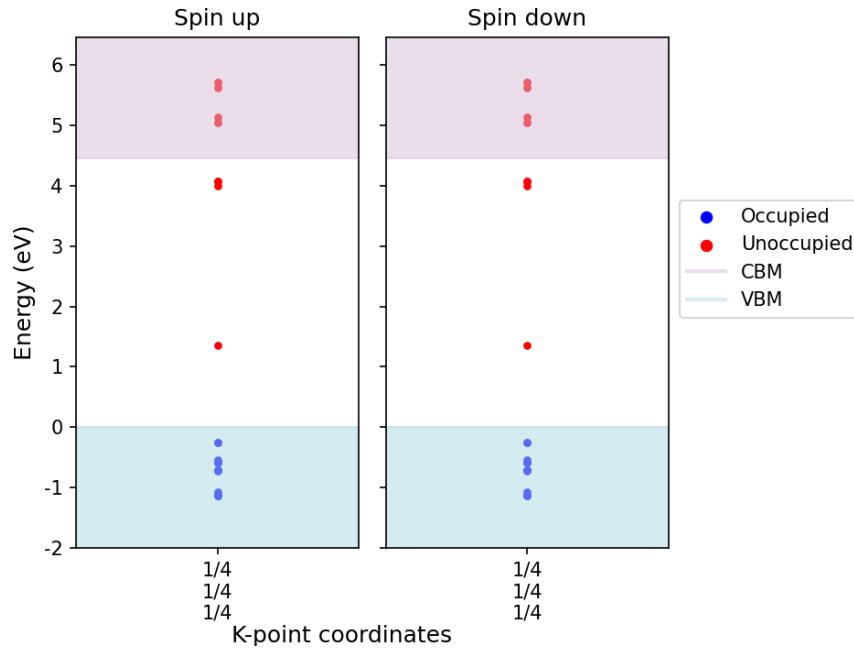
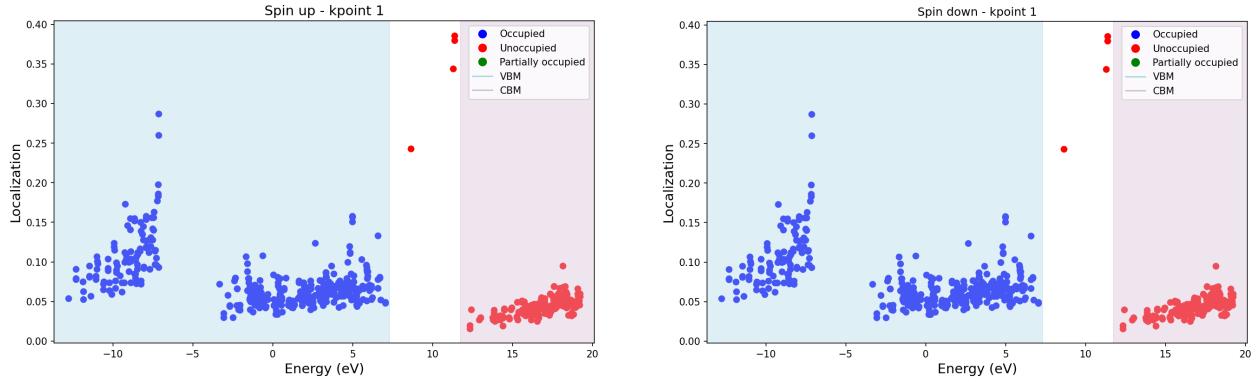


Figure 21: Kohn-Sham states.



(a) Spin up - Kpoint 1

(b) Spin down - Kpoint 1

Figure 22: Localization factor using projected orbitals (s, p and d).

## 1.12 Vacancy: $V_N^{+4}$

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Table 21:  $V_N^{+4}$ 

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

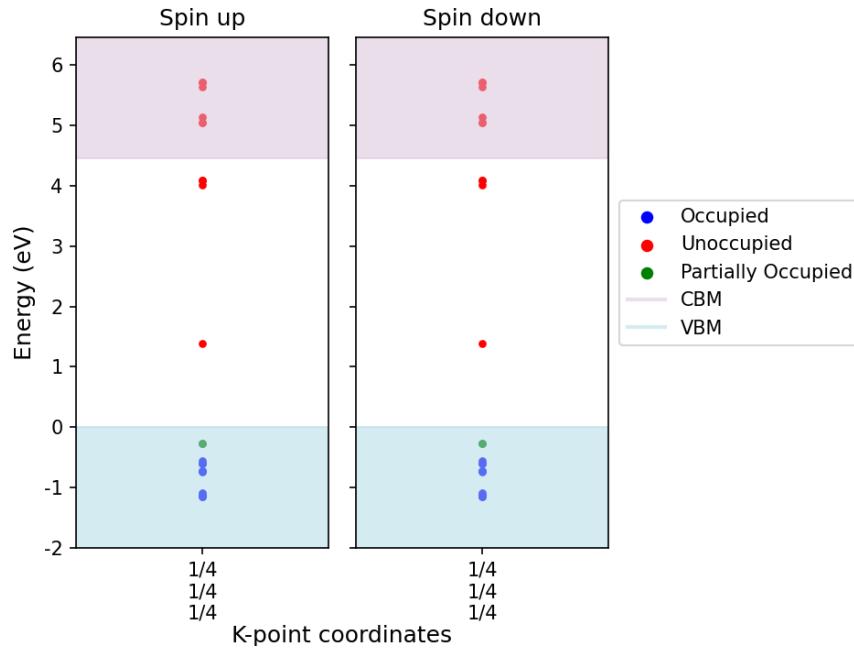


Figure 23: Kohn-Sham states.

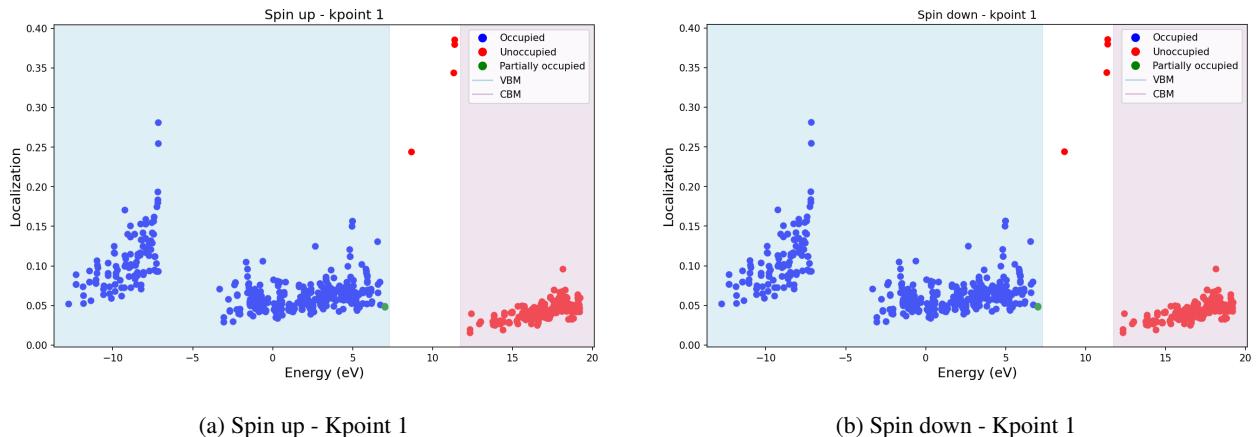


Figure 24: Localization factor using projected orbitals (s, p and d).

### 1.13 Vacancy: $V_N^{-1}$

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Table 22:  $V_N^{-1}$

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

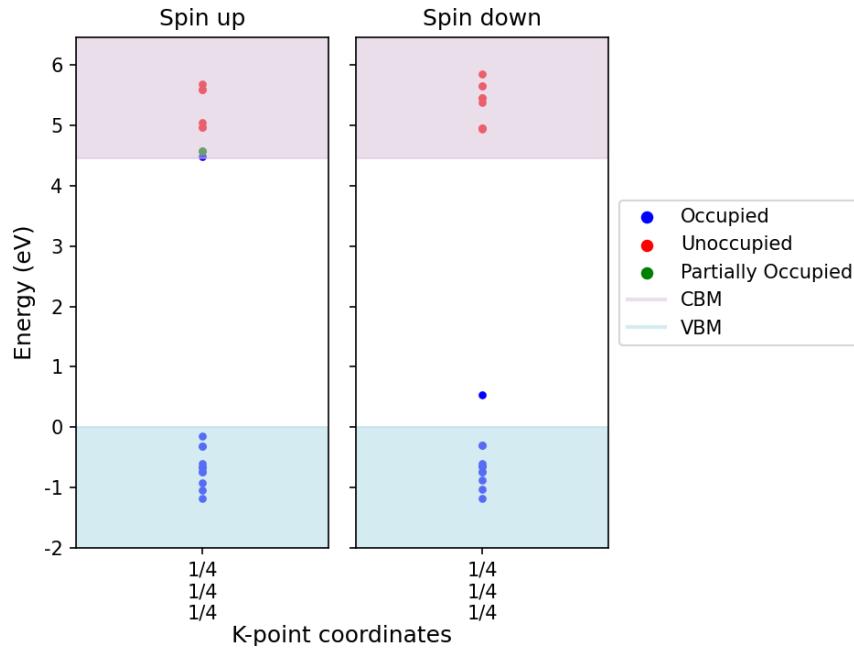


Figure 25: Kohn-Sham states.

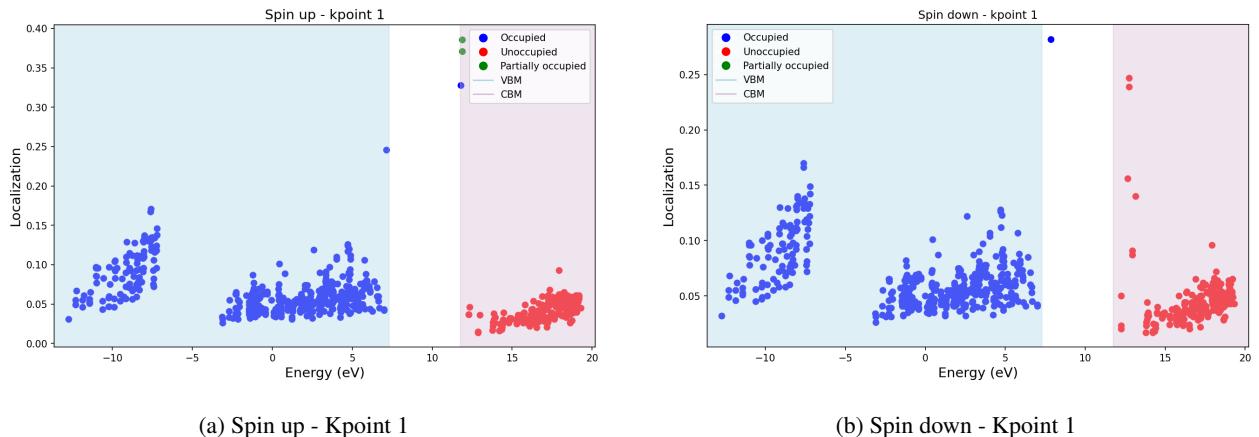


Figure 26: Localization factor using projected orbitals (s, p and d).

## 1.14 Antisite: $B_N^0$

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Table 23:  $B_N^0$

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*

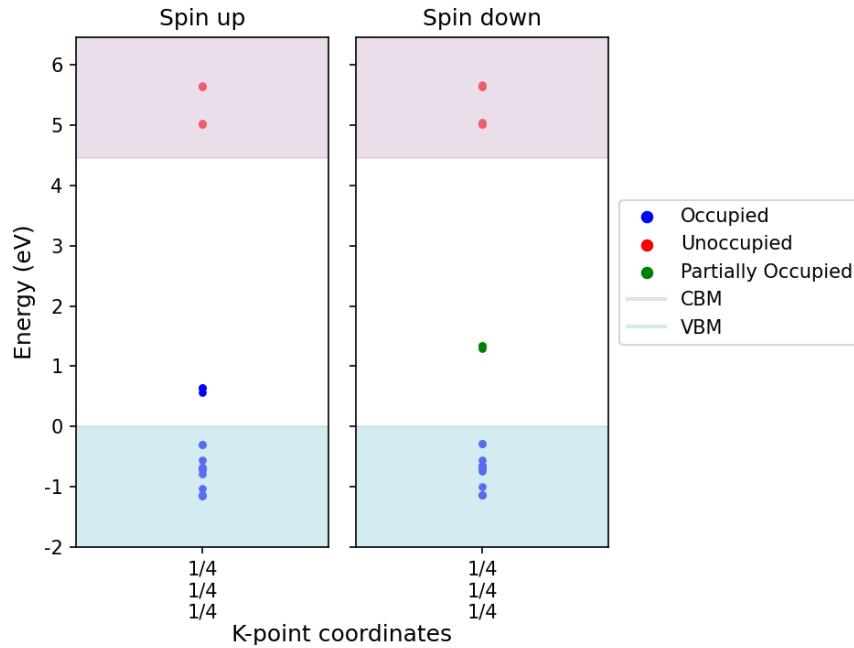


Figure 27: Kohn-Sham states.

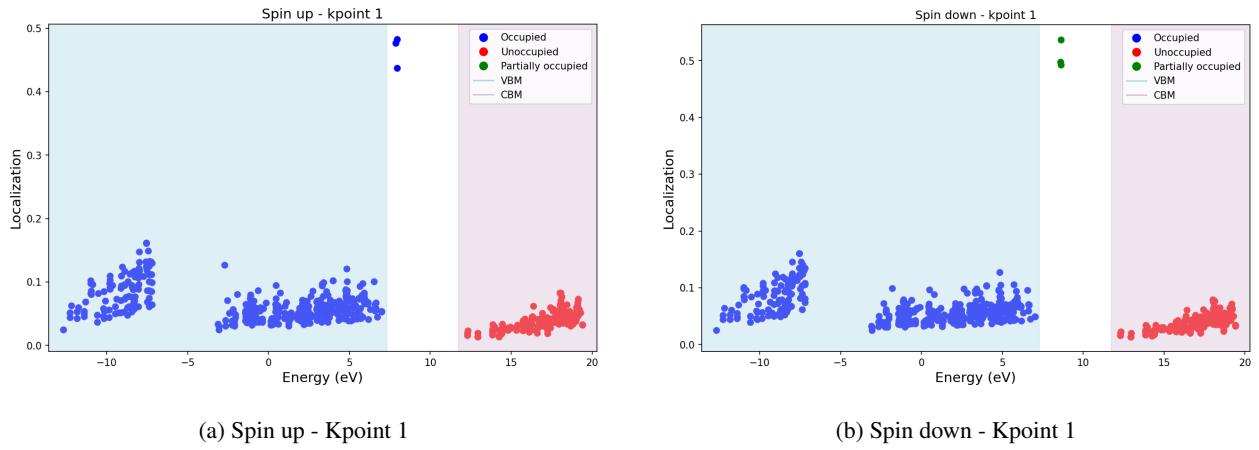


Figure 28: Localization factor using projected orbitals (s, p and d).

### 1.15 Antisite: $B_N^{+1}$

## **Go back to the Table 9**

Table 24:  $B_N^{+1}$

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*

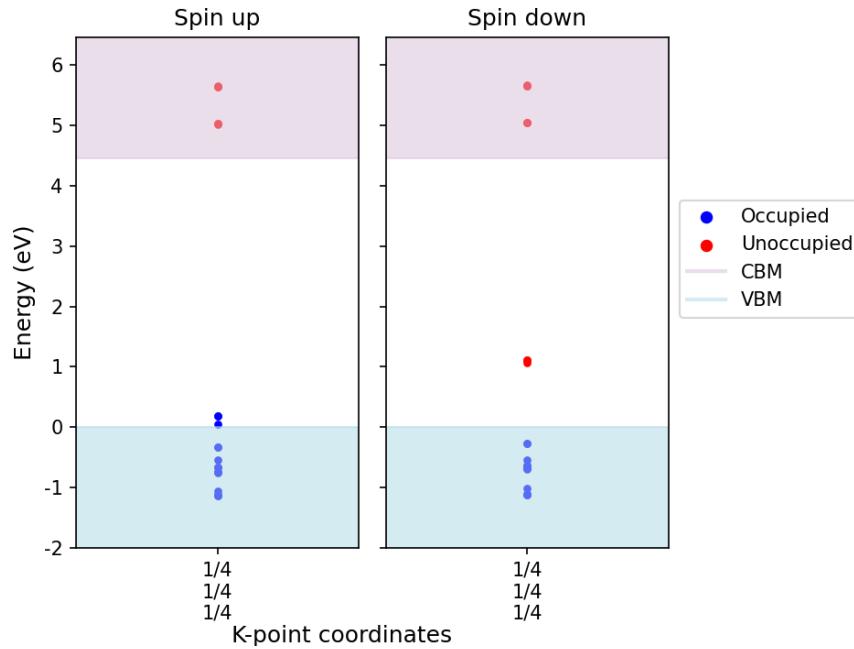


Figure 29: Kohn-Sham states.

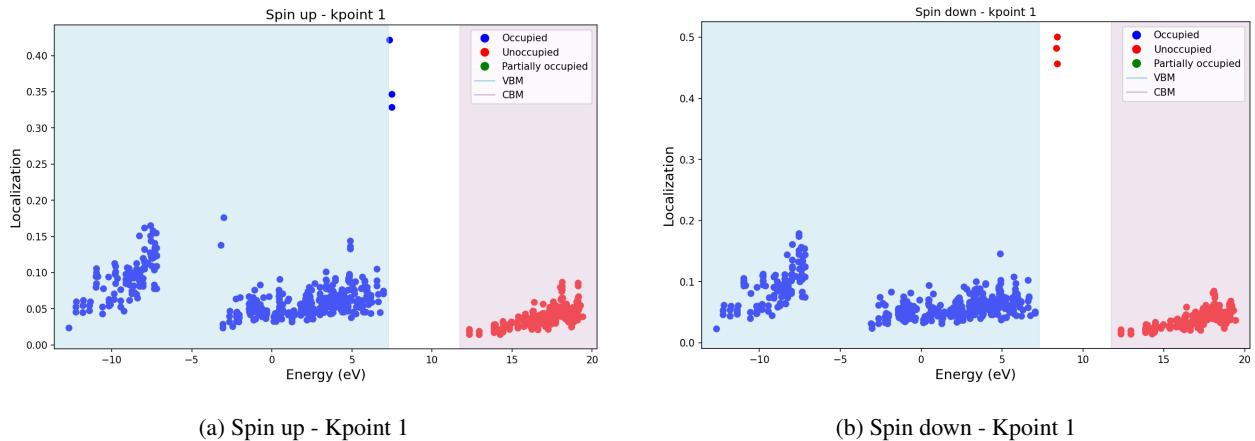


Figure 30: Localization factor using projected orbitals (s, p and d).

## 1.16 Antisite: $B_N^{+2}$

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Table 25:  $B_N^{+2}$

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*

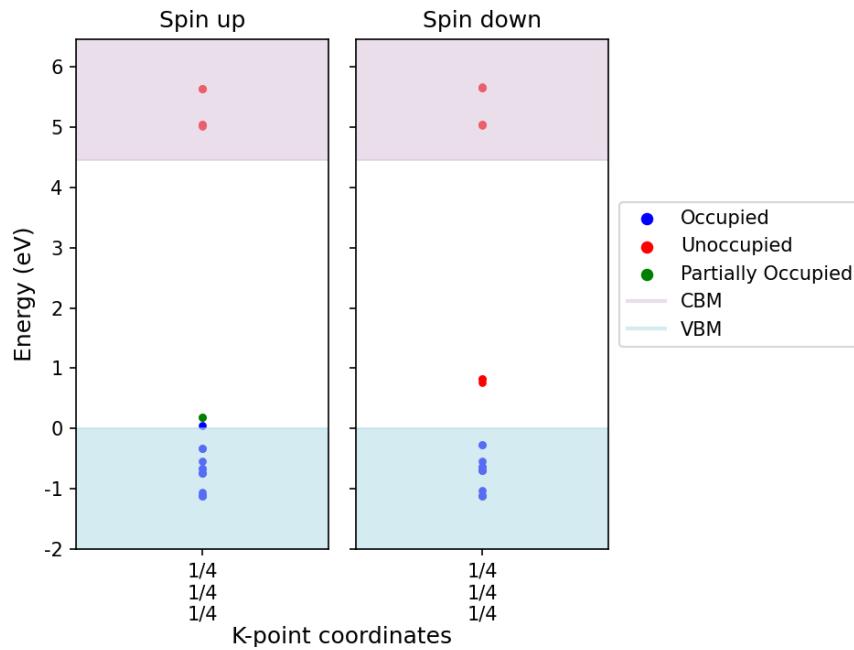


Figure 31: Kohn-Sham states.

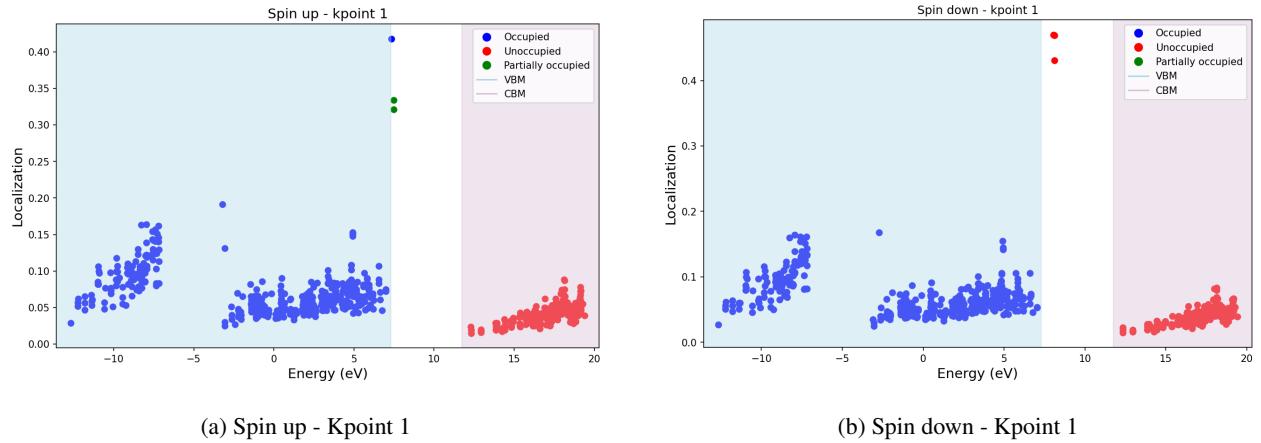


Figure 32: Localization factor using projected orbitals (s, p and d).

### 1.17 Antisite: $B_N^{+3}$

[Go back to the Table 9](#)

Table 26:  $B_N^{+3}$

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*

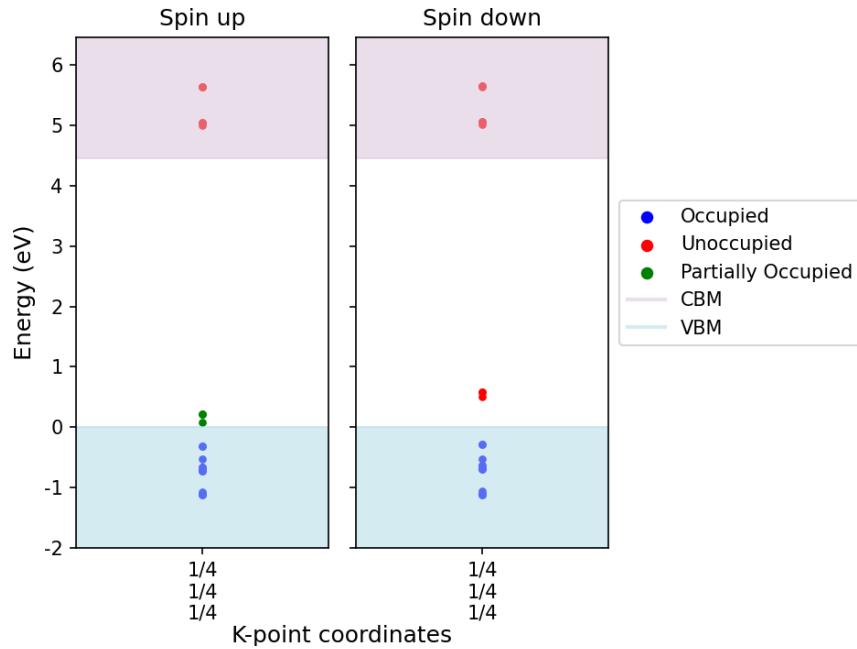


Figure 33: Kohn-Sham states.

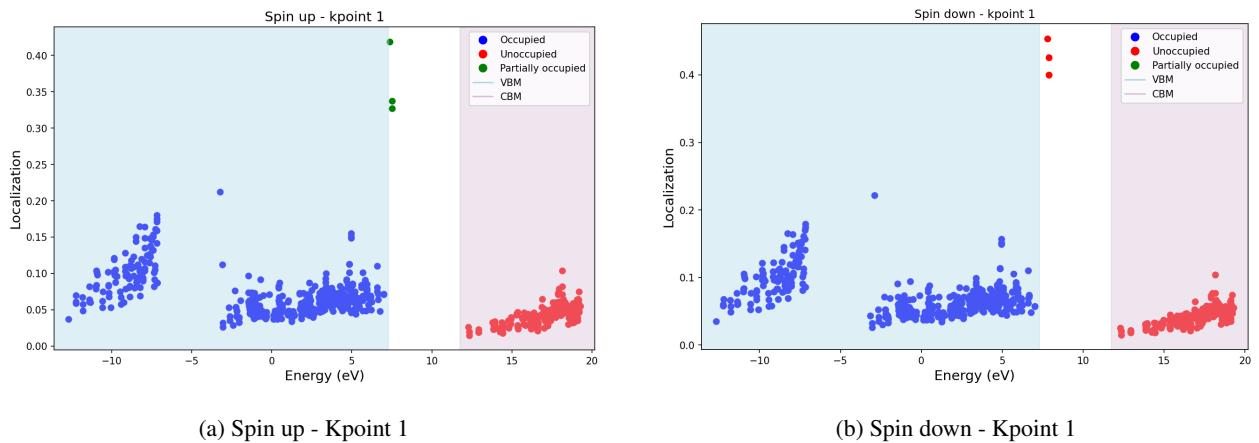


Figure 34: Localization factor using projected orbitals (s, p and d).

## 1.18 Antisite: $B_N^{+4}$

[Go back to the Table 9](#)

Table 27:  $B_N^{+4}$

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*

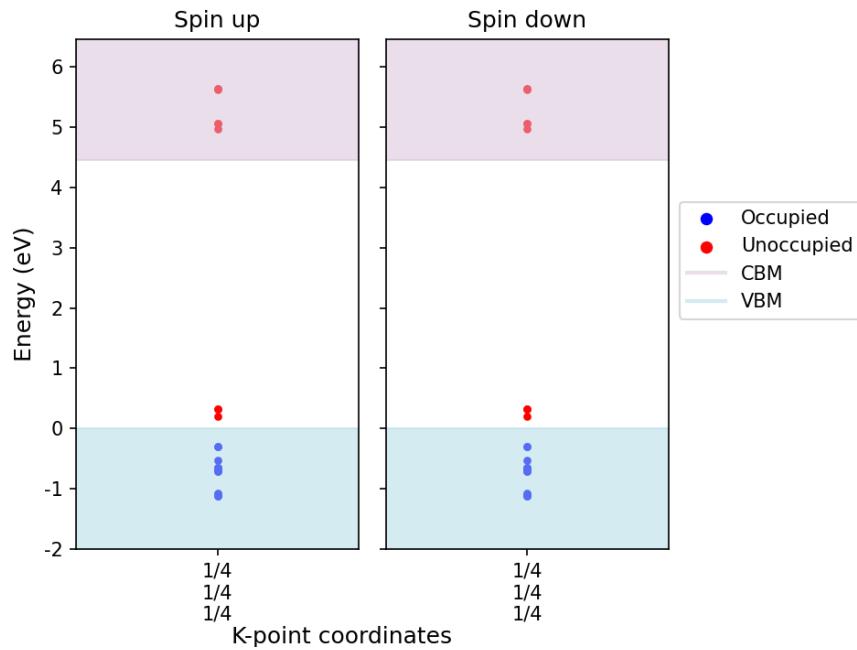


Figure 35: Kohn-Sham states.

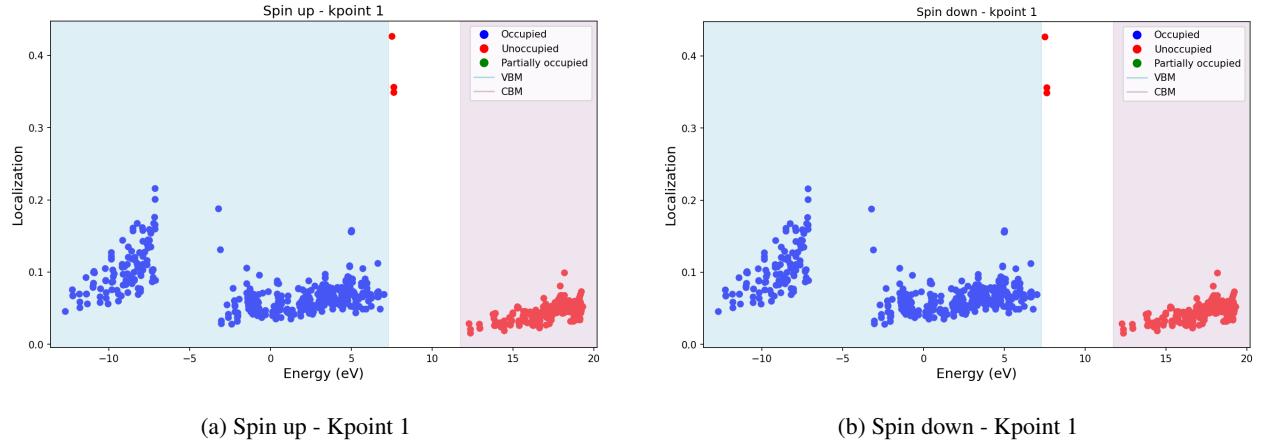


Figure 36: Localization factor using projected orbitals (s, p and d).

### 1.19 Antisite: $B_N^{-1}$

[Go back to the Table 9](#)

Table 28:  $B_N^{-1}$

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*

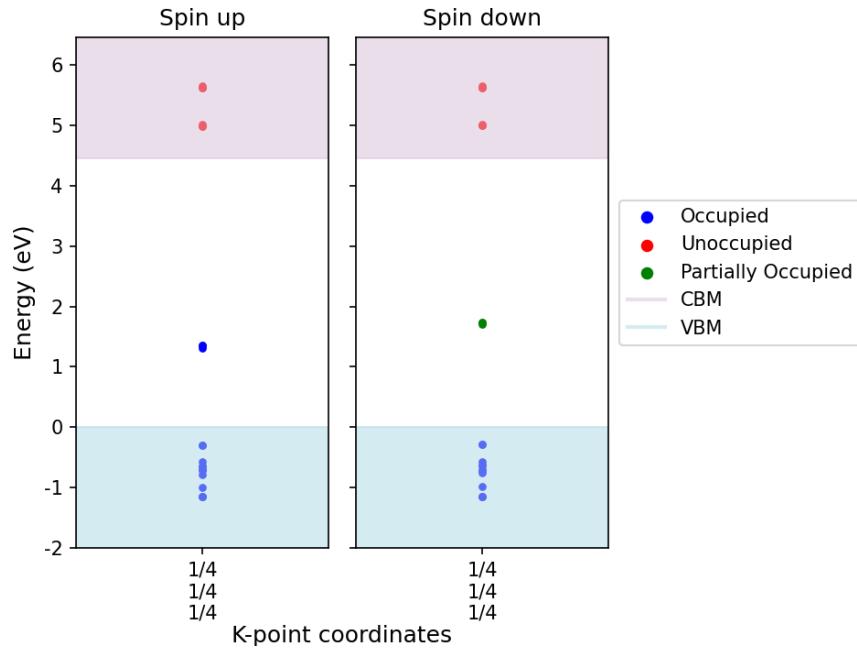


Figure 37: Kohn-Sham states.

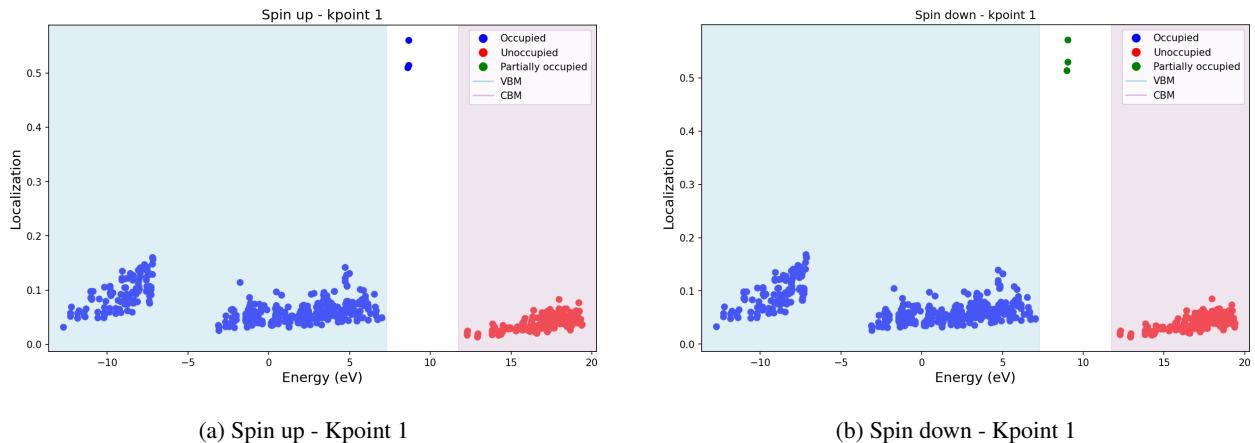


Figure 38: Localization factor using projected orbitals (s, p and d).

## 1.20 Antisite: $B_N^{-2}$

[Go back to the Table 9](#)

Table 29:  $B_N^{-2}$

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*

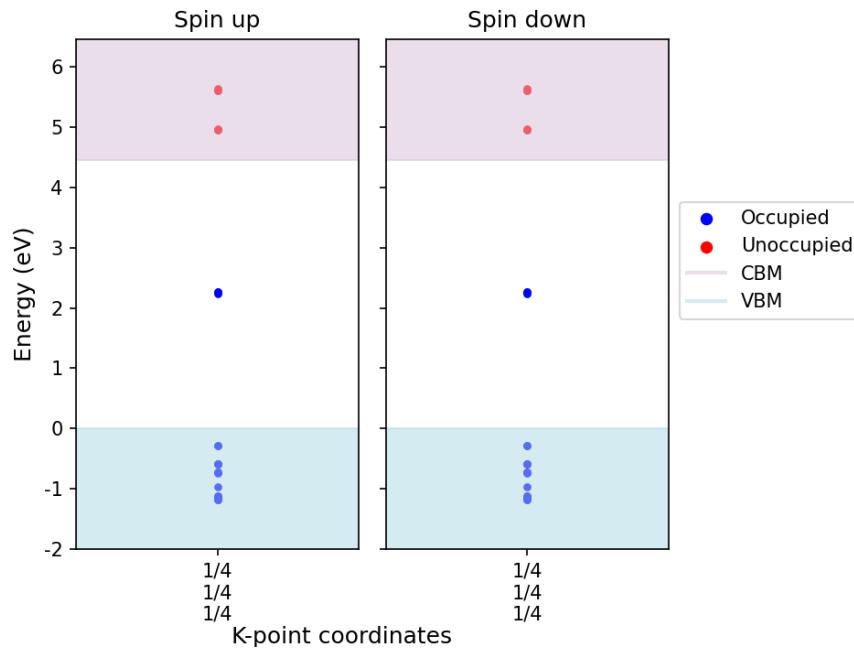


Figure 39: Kohn-Sham states.

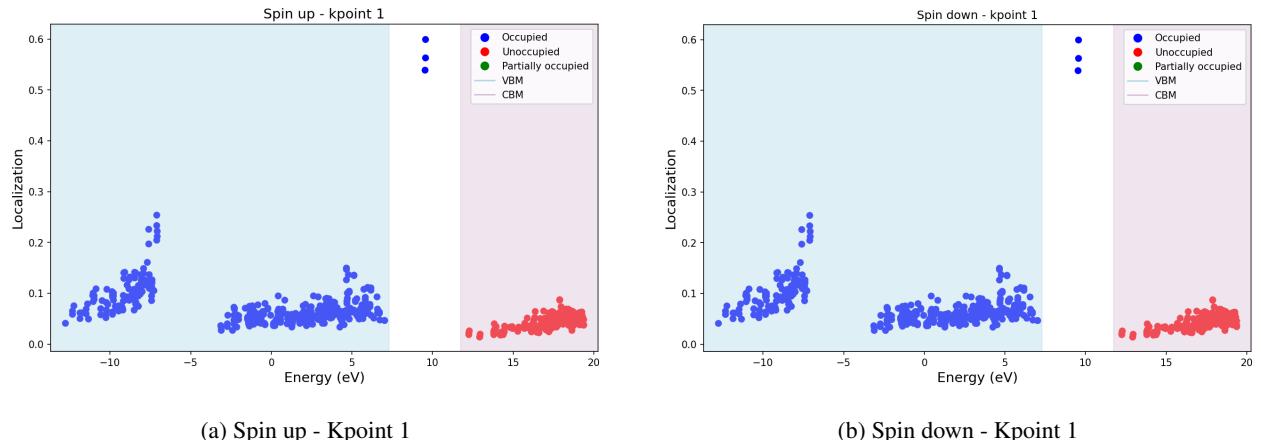


Figure 40: Localization factor using projected orbitals (s, p and d).

## 1.21 Antisite: $B_N^{-3}$

[Go back to the Table 9](#)

Table 30:  $B_N^{-3}$

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*

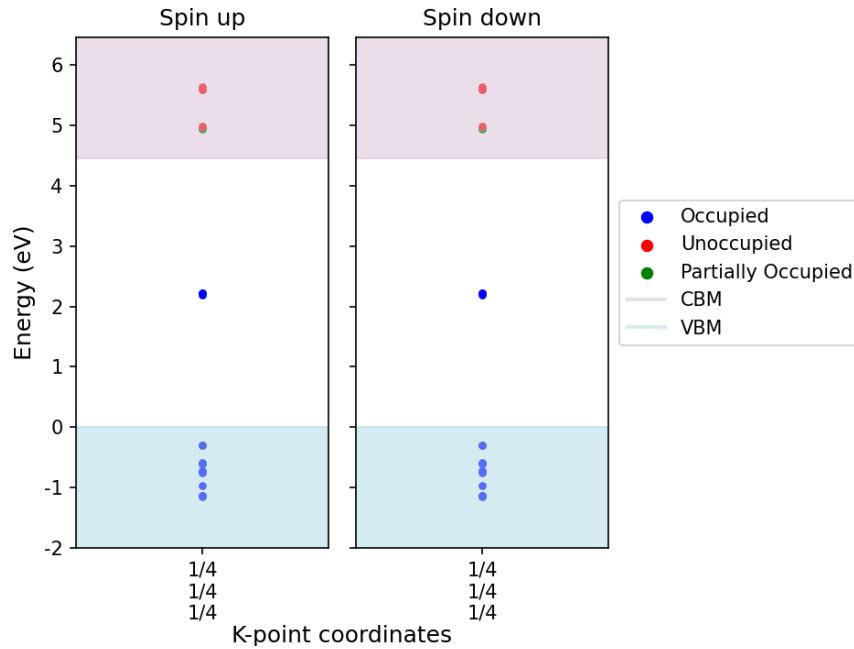


Figure 41: Kohn-Sham states.

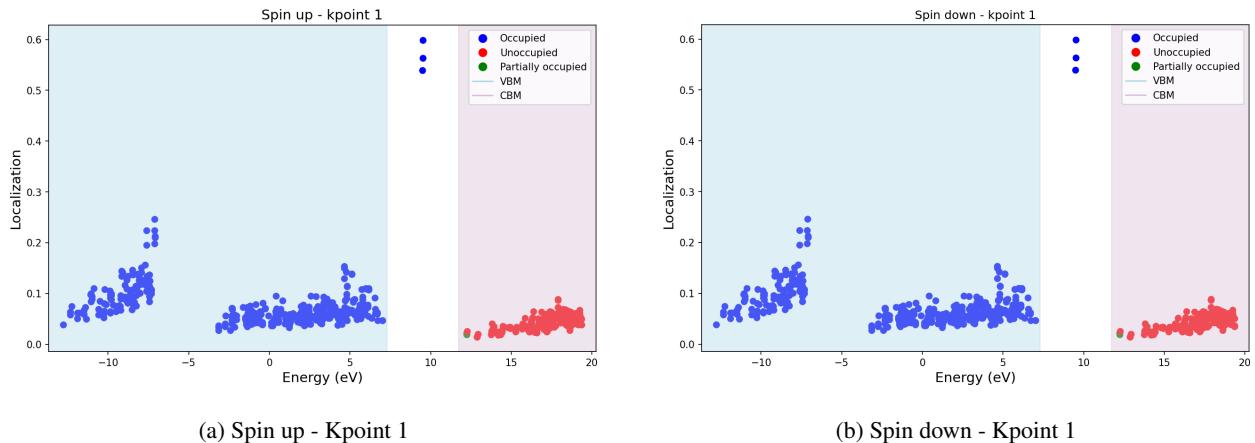


Figure 42: Localization factor using projected orbitals (s, p and d).

## 1.22 Antisite: $B_N^{-4}$

[Go back to the Table 9](#)

Table 31:  $B_N^{-4}$

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*

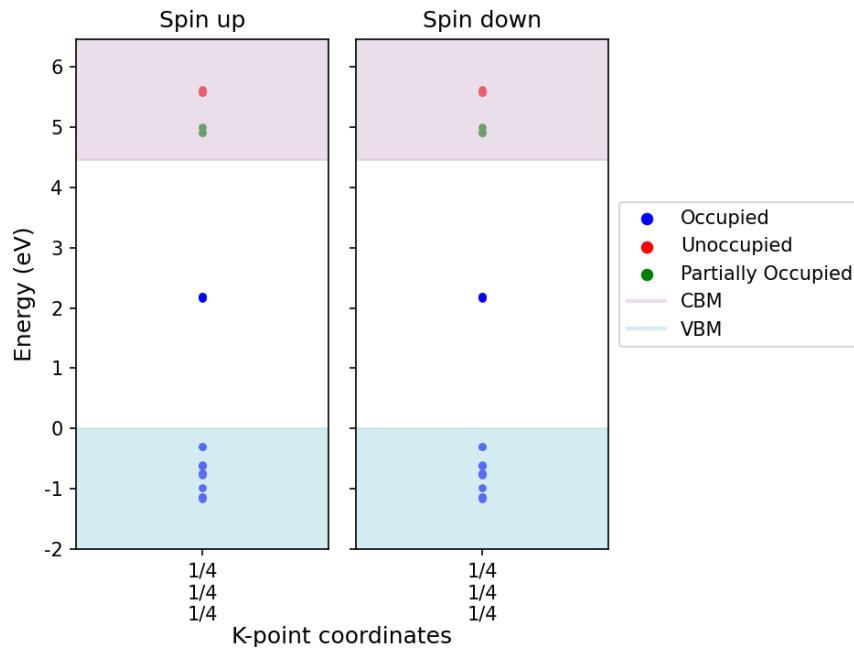


Figure 43: Kohn-Sham states.

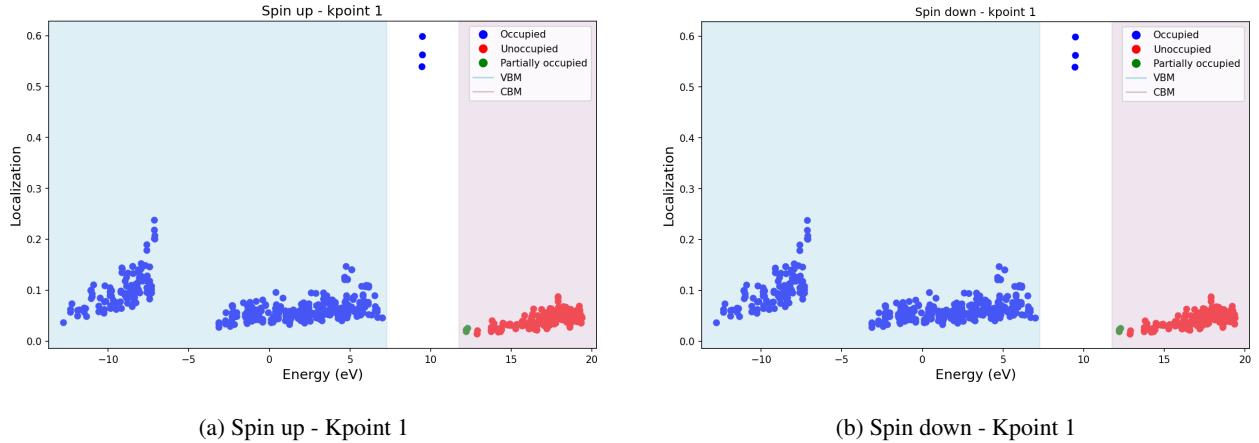


Figure 44: Localization factor using projected orbitals (s, p and d).

## 1.23 Antisite: $N_B^0$

[Go back to the Table 9](#)

Table 32:  $N_B^0$

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

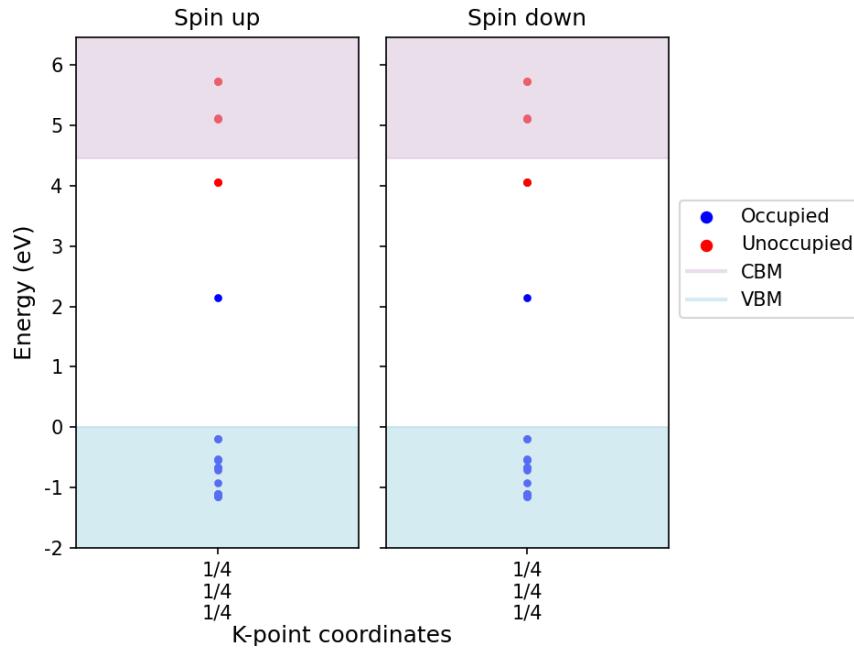


Figure 45: Kohn-Sham states.

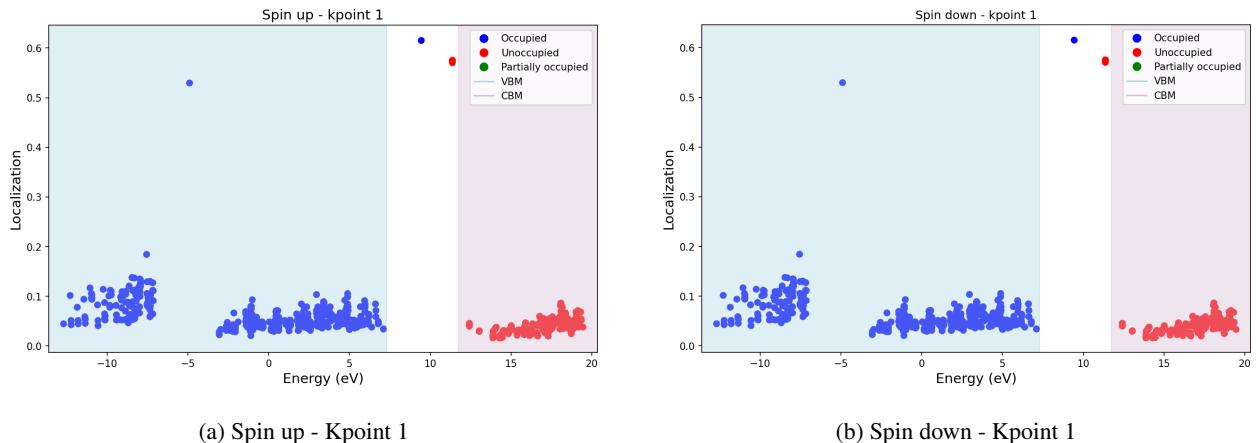


Figure 46: Localization factor using projected orbitals (s, p and d).

## 1.24 Antisite: $N_B^{+1}$

[Go back to the Table 9](#)

Table 33:  $N_B^{+1}$ 

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

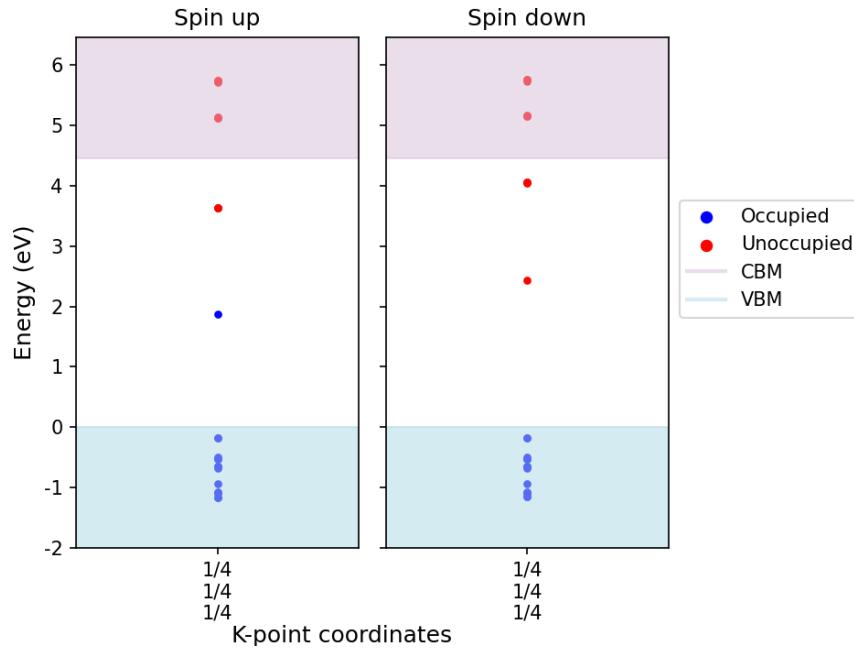


Figure 47: Kohn-Sham states.

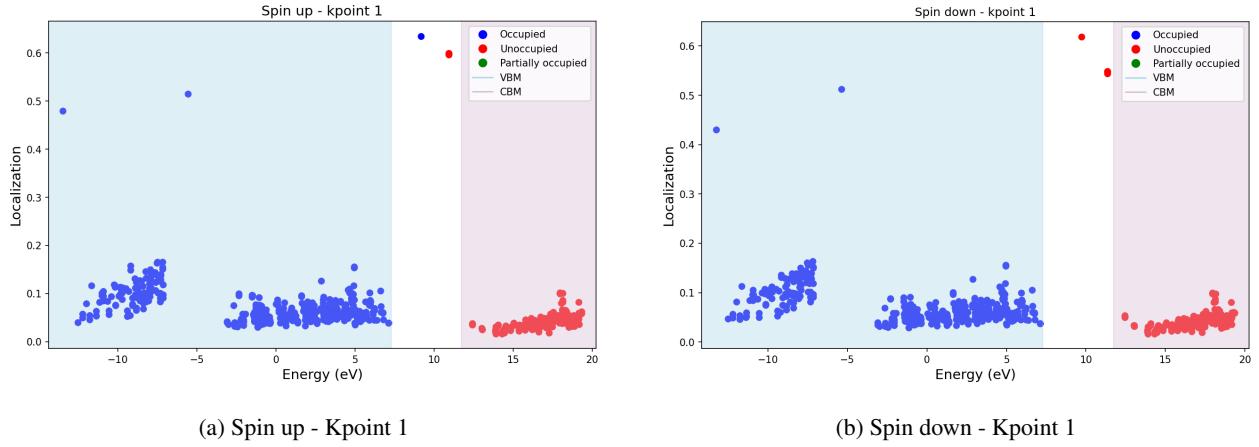


Figure 48: Localization factor using projected orbitals (s, p and d).

## 1.25 Antisite: $N_B^{+2}$

[Go back to the Table 9](#)

Table 34:  $N_B^{+2}$

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

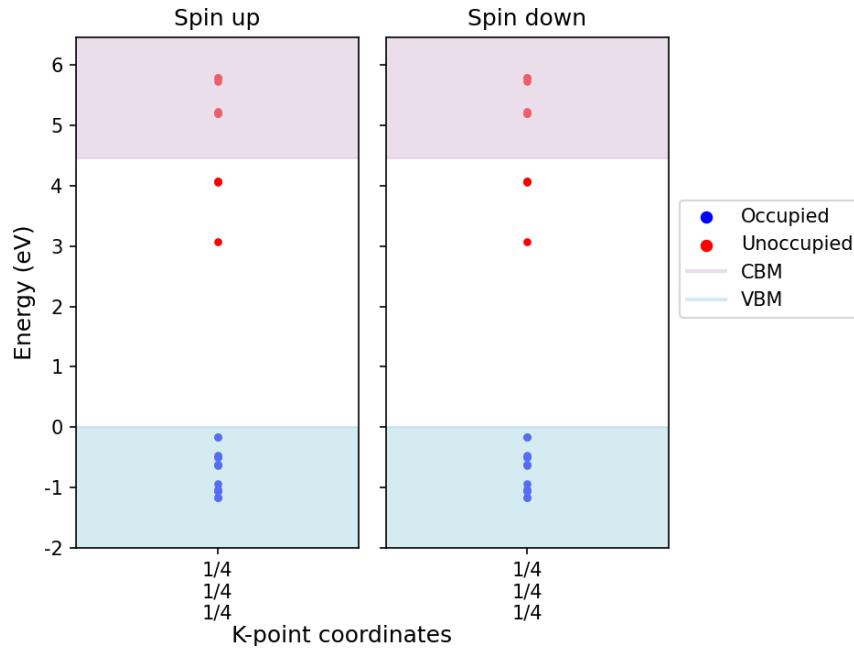


Figure 49: Kohn-Sham states.

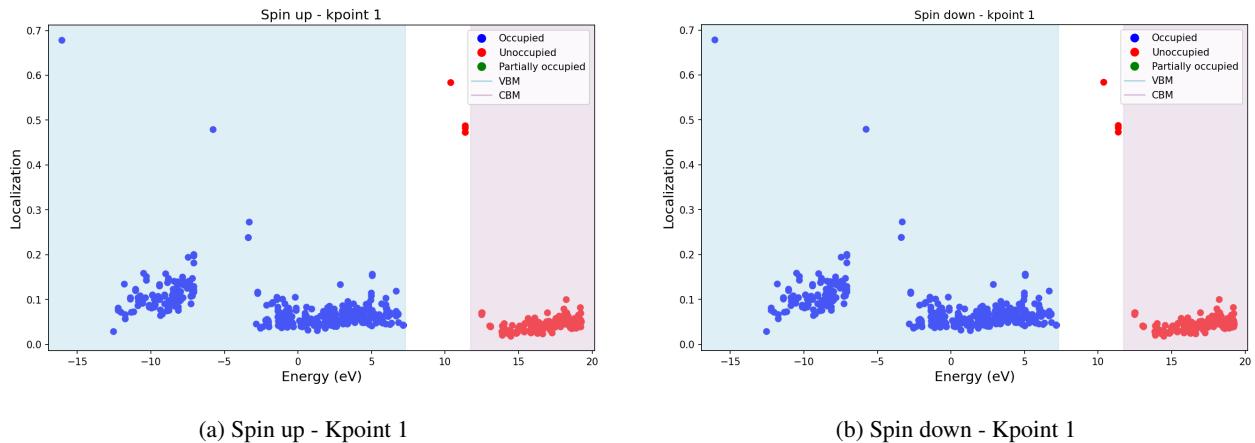


Figure 50: Localization factor using projected orbitals (s, p and d).

## 1.26 Antisite: $N_B^{+3}$

[Go back to the Table 9](#)

Table 35:  $N_B^{+3}$

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

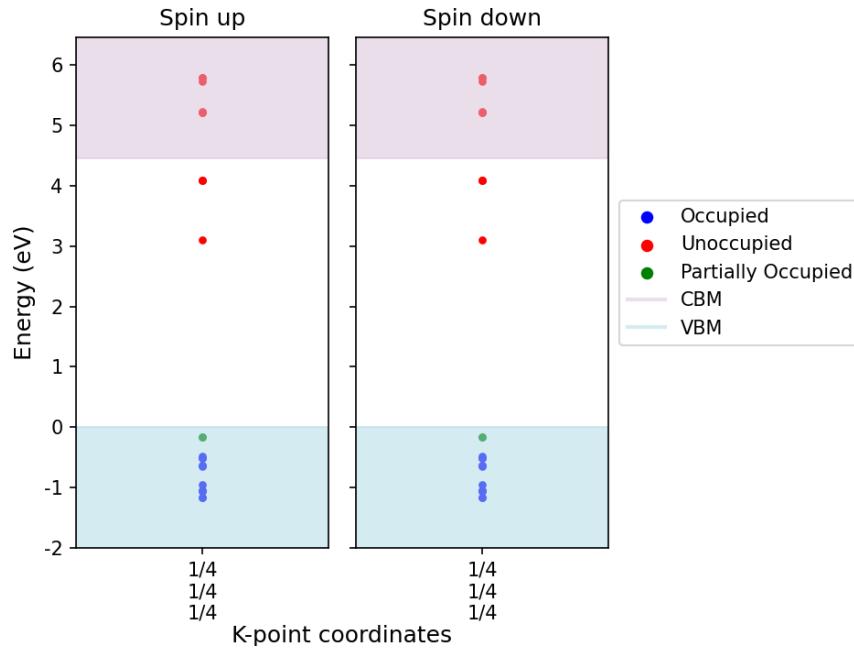


Figure 51: Kohn-Sham states.

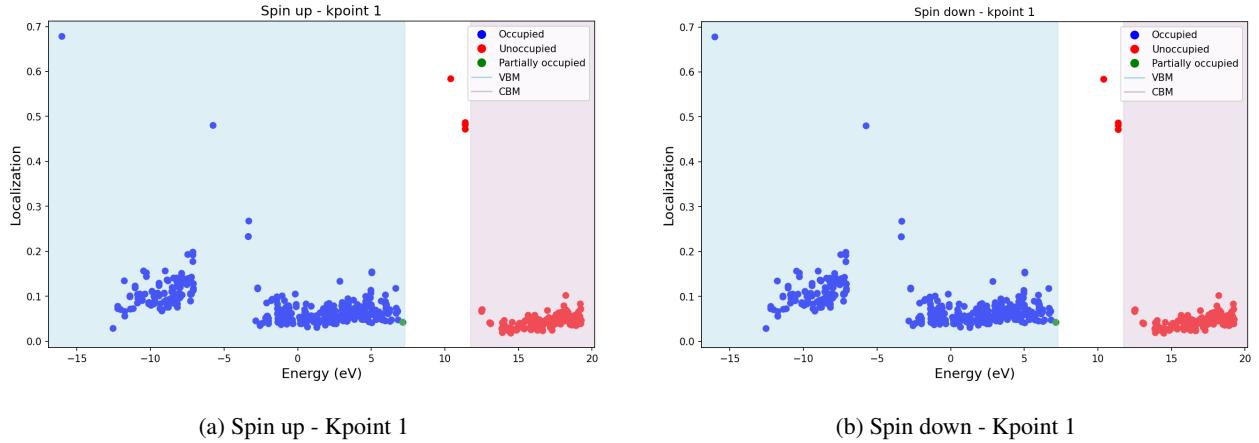


Figure 52: Localization factor using projected orbitals (s, p and d).

### 1.27 Antisite: $N_B^{+4}$

[Go back to the Table 9](#)

Table 36:  $N_B^{+4}$

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

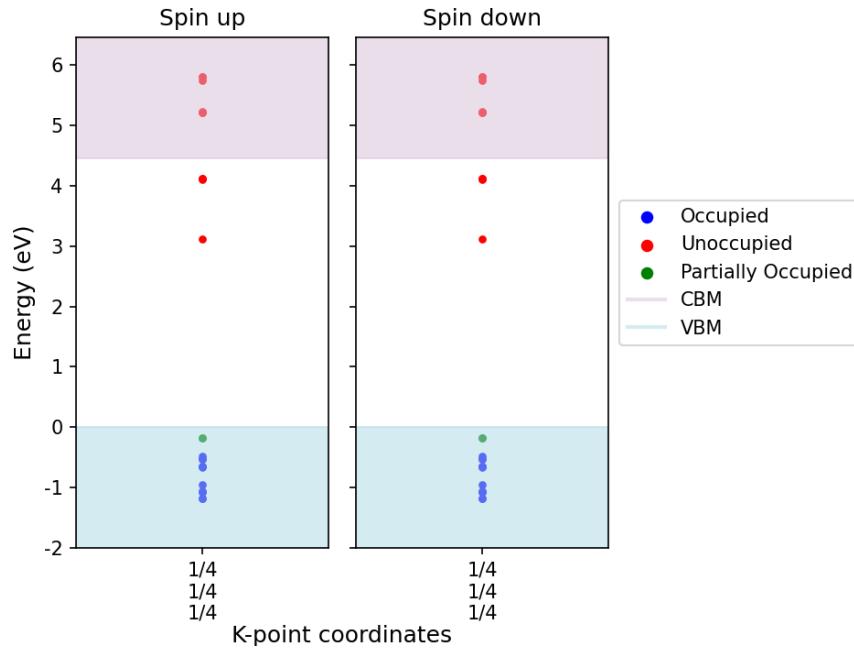


Figure 53: Kohn-Sham states.

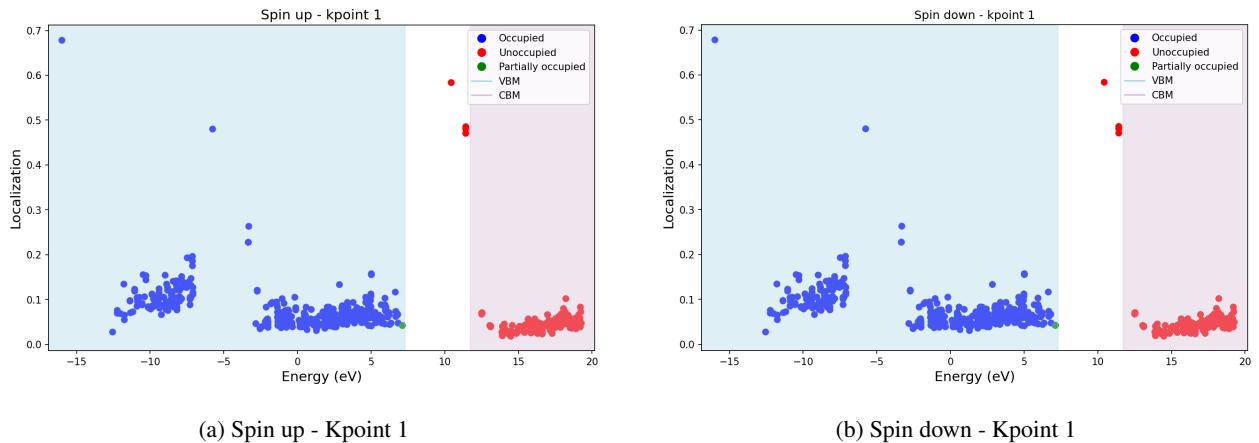


Figure 54: Localization factor using projected orbitals (s, p and d).

## 1.28 Antisite: $N_B^{-1}$

[Go back to the Table 9](#)

Table 37:  $N_B^{-1}$

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

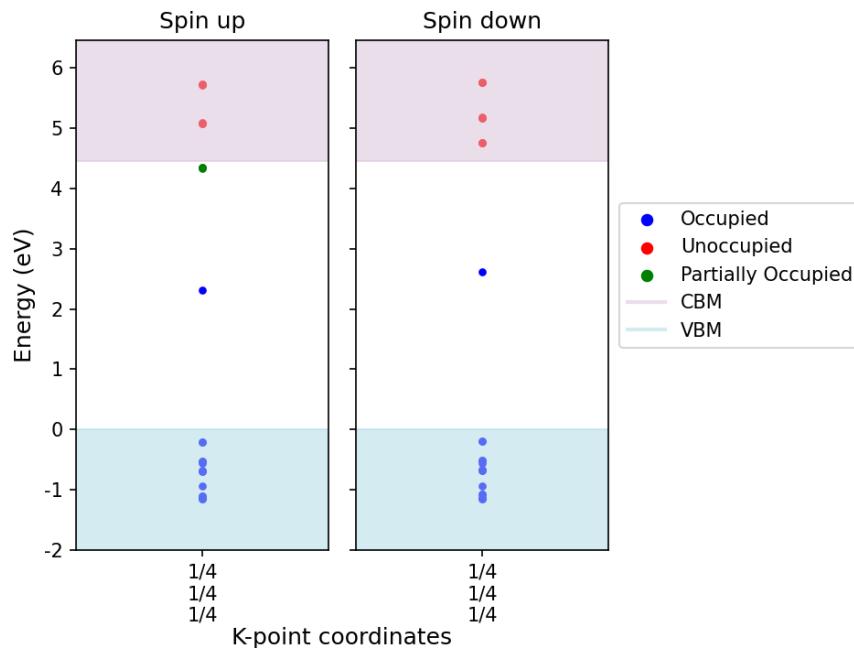


Figure 55: Kohn-Sham states.

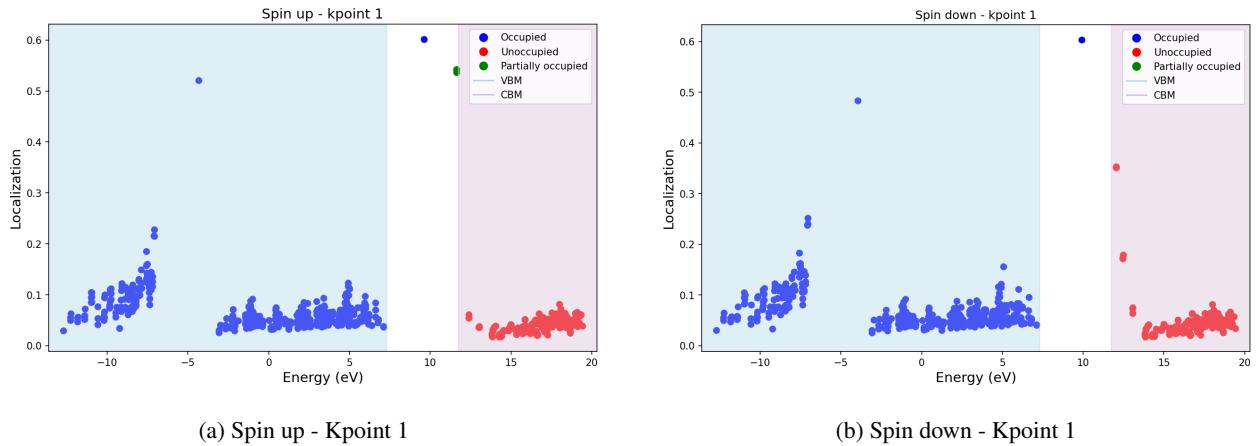


Figure 56: Localization factor using projected orbitals (s, p and d).

### 1.29 Antisite: $N_B^{-2}$

[Go back to the Table 9](#)

Table 38:  $N_B^{-2}$

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

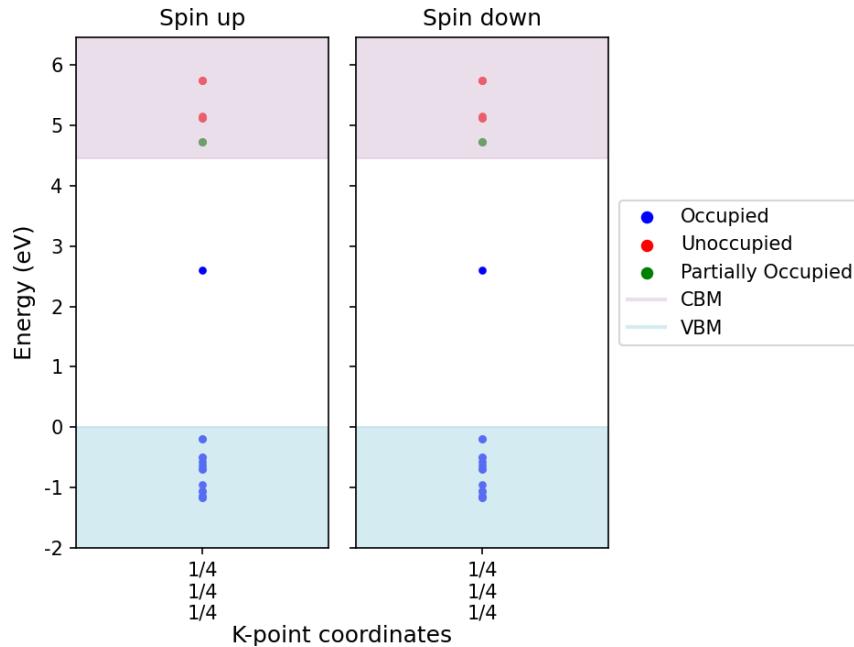


Figure 57: Kohn-Sham states.

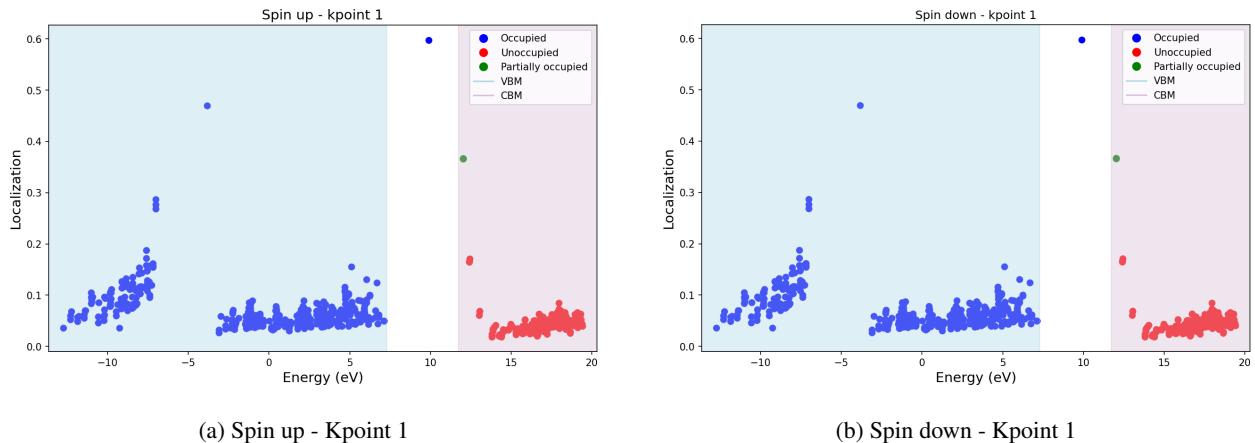


Figure 58: Localization factor using projected orbitals (s, p and d).

### 1.30 Antisite: $N_B^{-3}$

[Go back to the Table 9](#)

Table 39:  $N_B^{-3}$

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

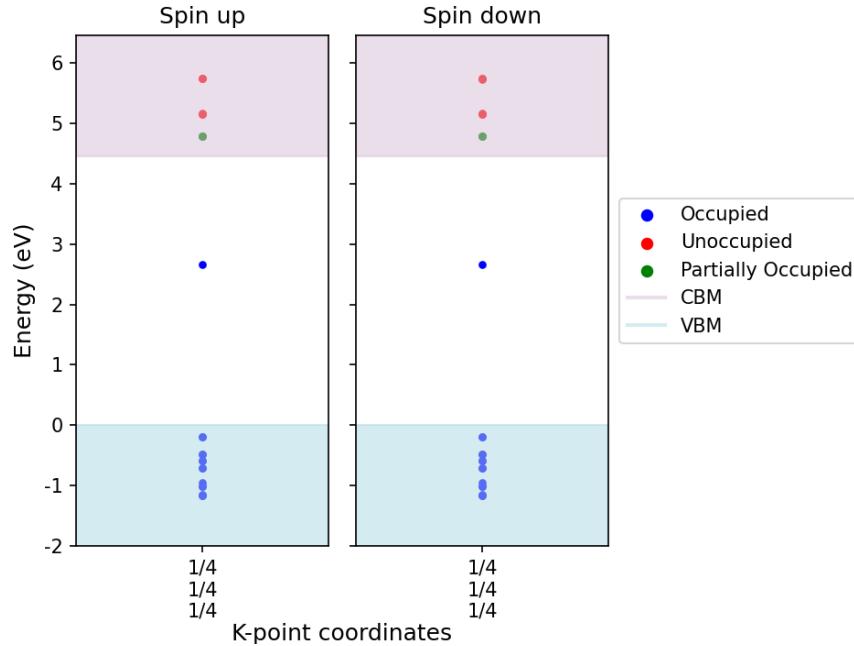


Figure 59: Kohn-Sham states.

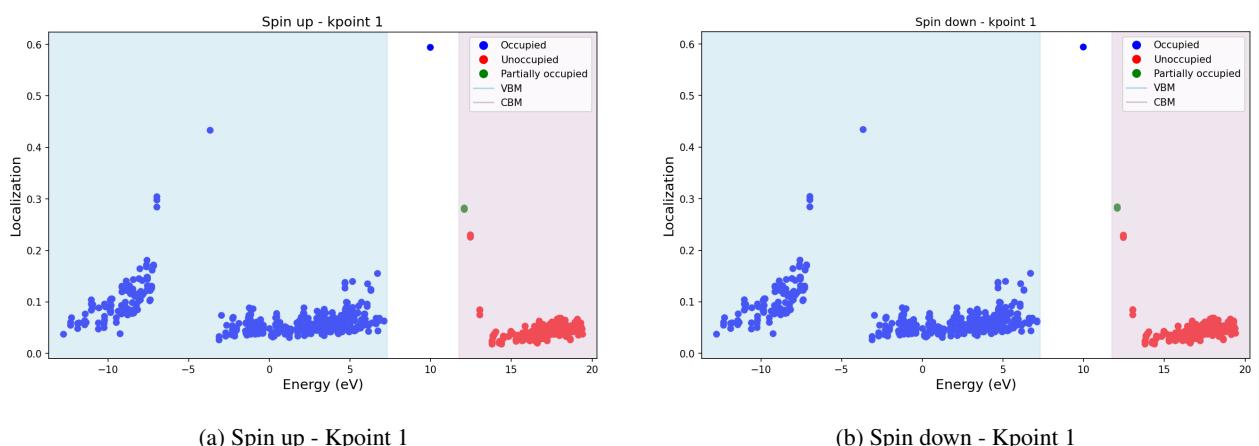


Figure 60: Localization factor using projected orbitals (s, p and d).

### 1.31 Antisite: $N_B^{-4}$

[Go back to the Table 9](#)

Table 40:  $N_B^{-4}$

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

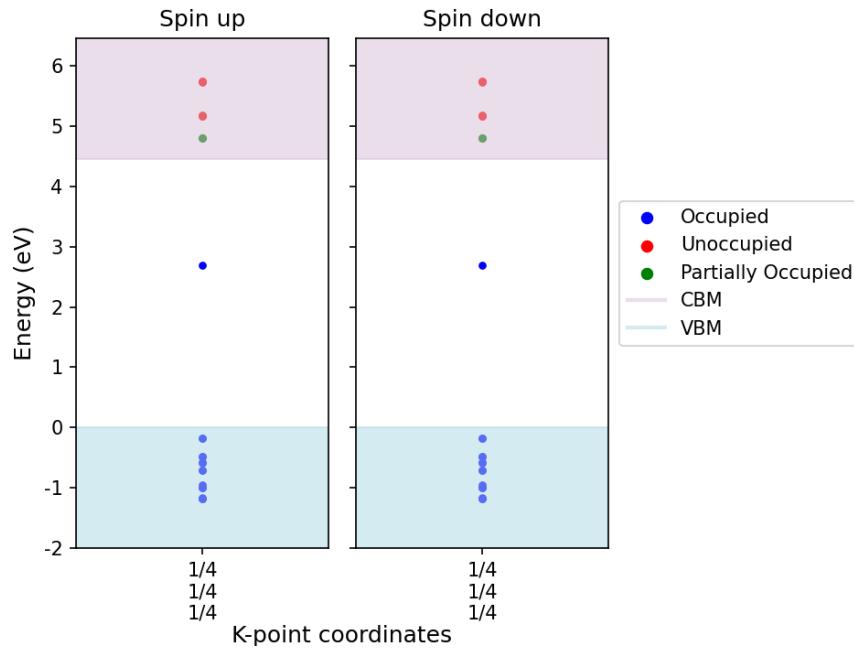


Figure 61: Kohn-Sham states.

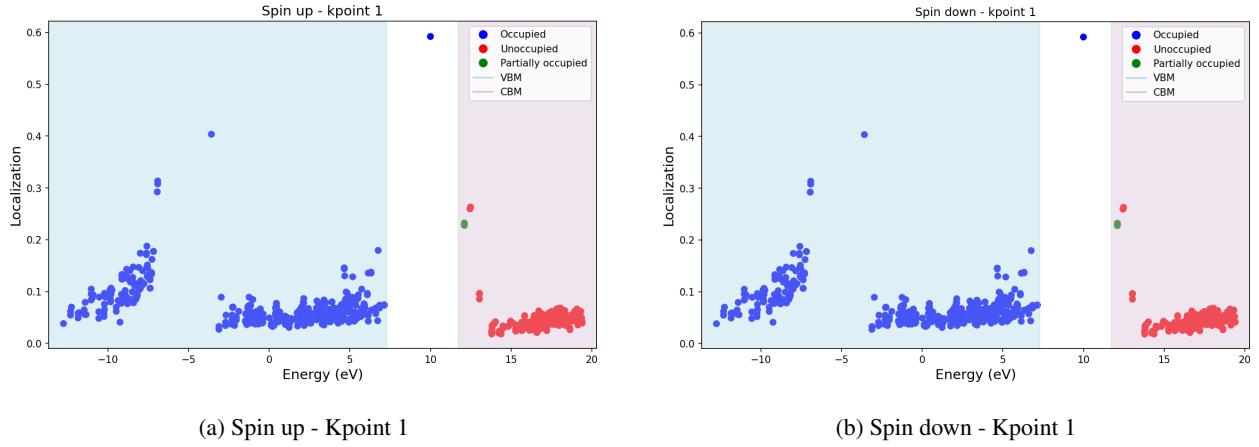


Figure 62: Localization factor using projected orbitals (s, p and d).

### 1.32 Complex: $(V_B - C_B)^0$

[Go back to the Table 9](#)

Table 41:  $(V_B - C_B)^0$

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

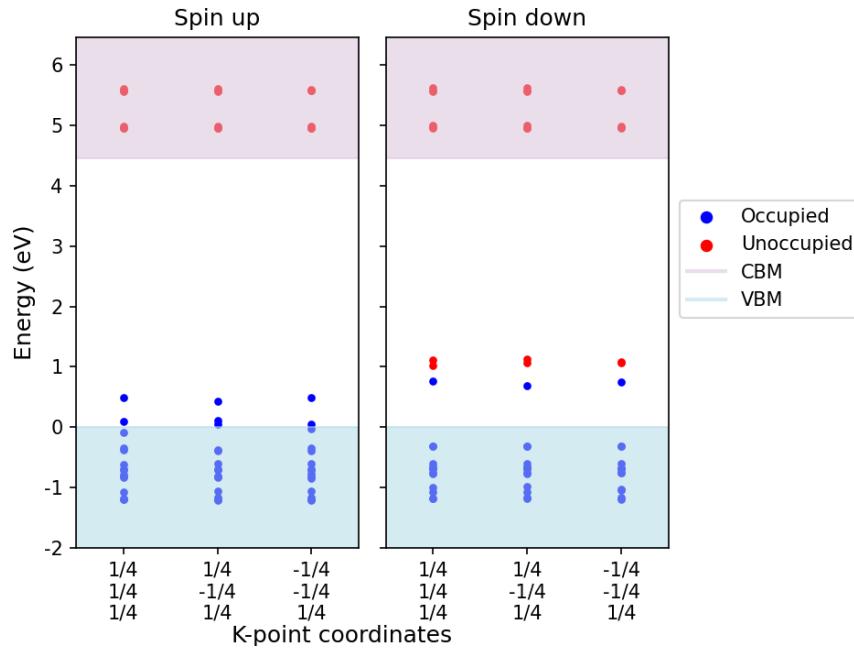


Figure 63: Kohn-Sham states.

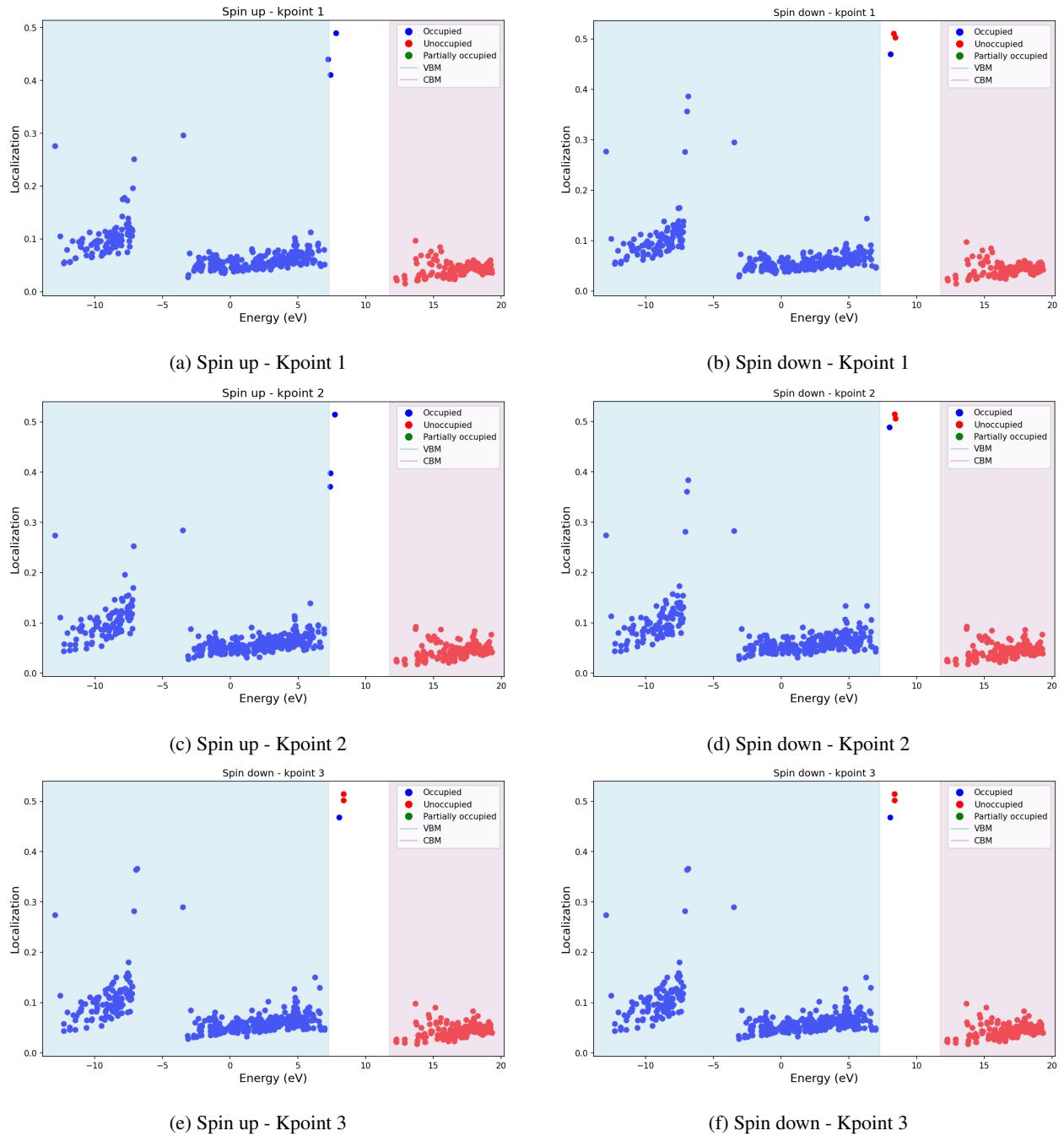


Figure 64: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

Table 42:  $(V_B - C_B)^{+1}$

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

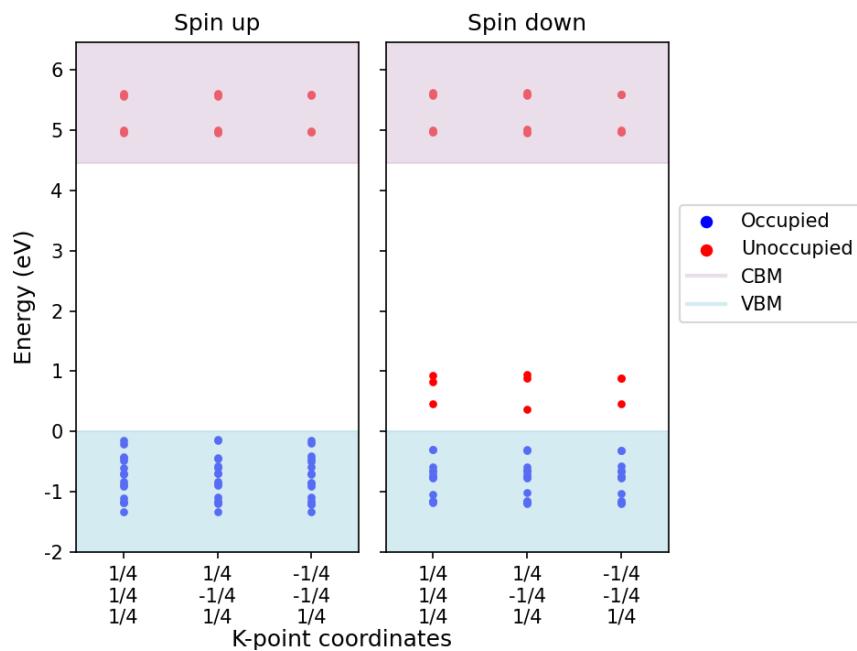


Figure 65: Kohn-Sham states.

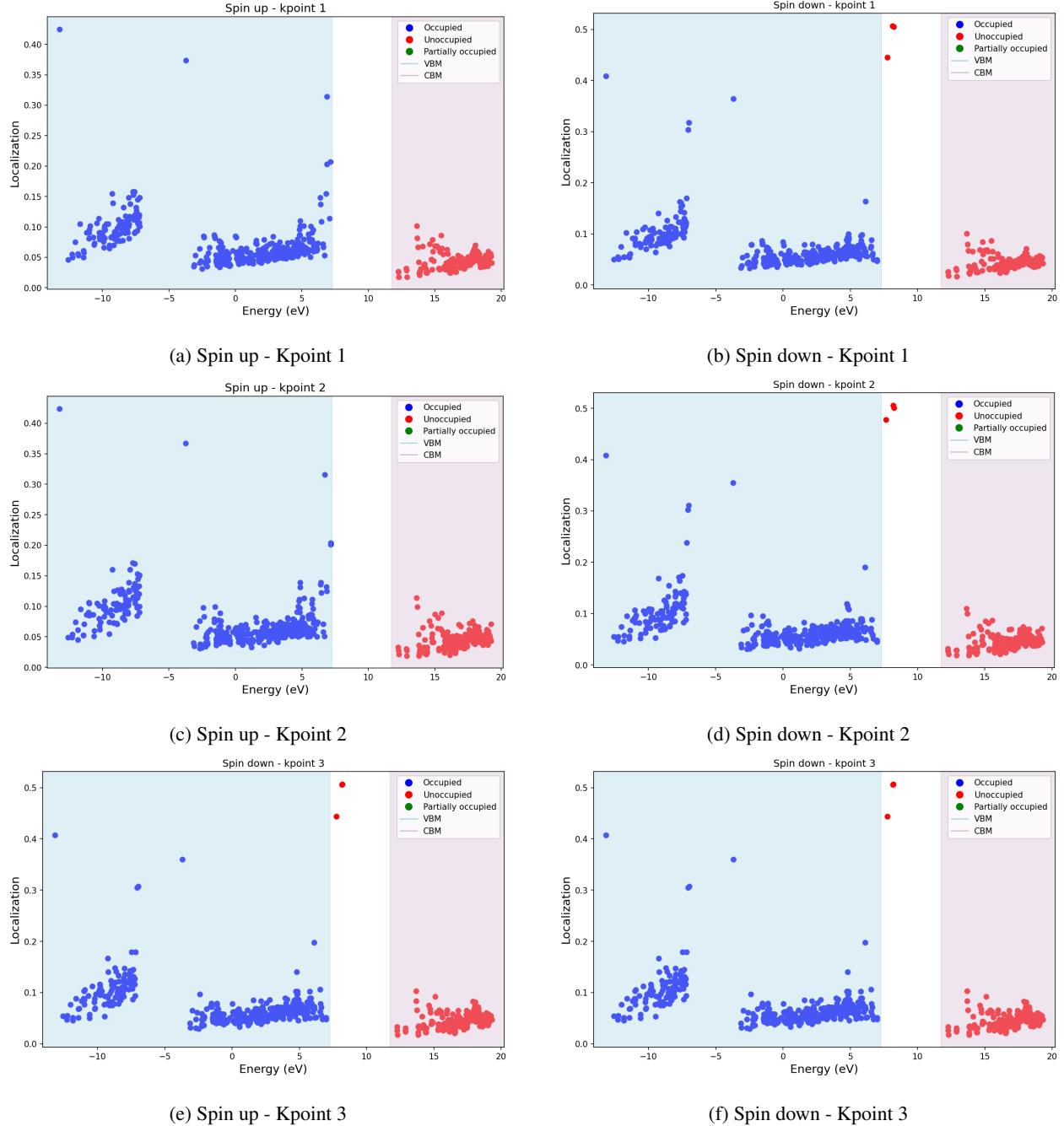


Figure 66: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

Table 43:  $(V_B - C_B)^{+2}$

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

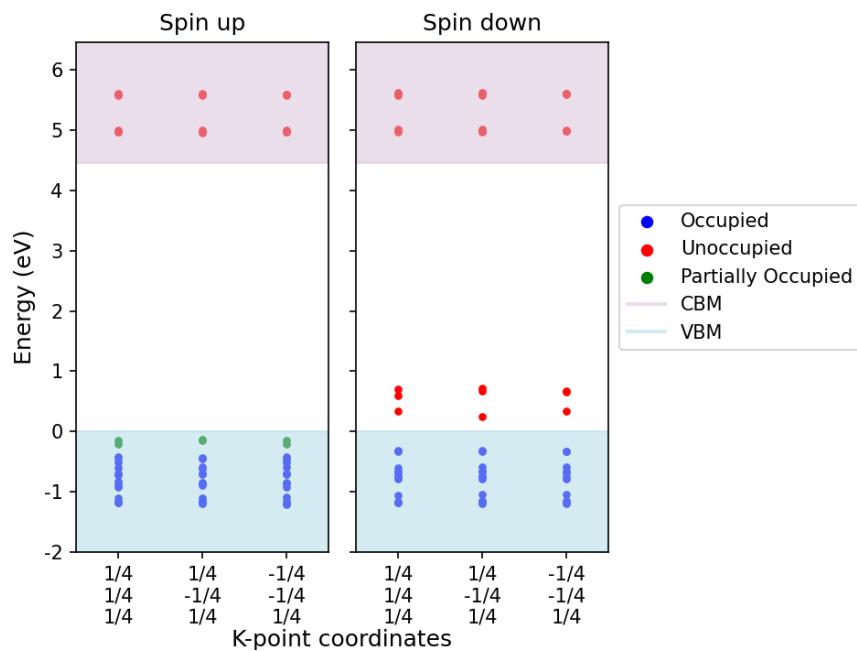


Figure 67: Kohn-Sham states.

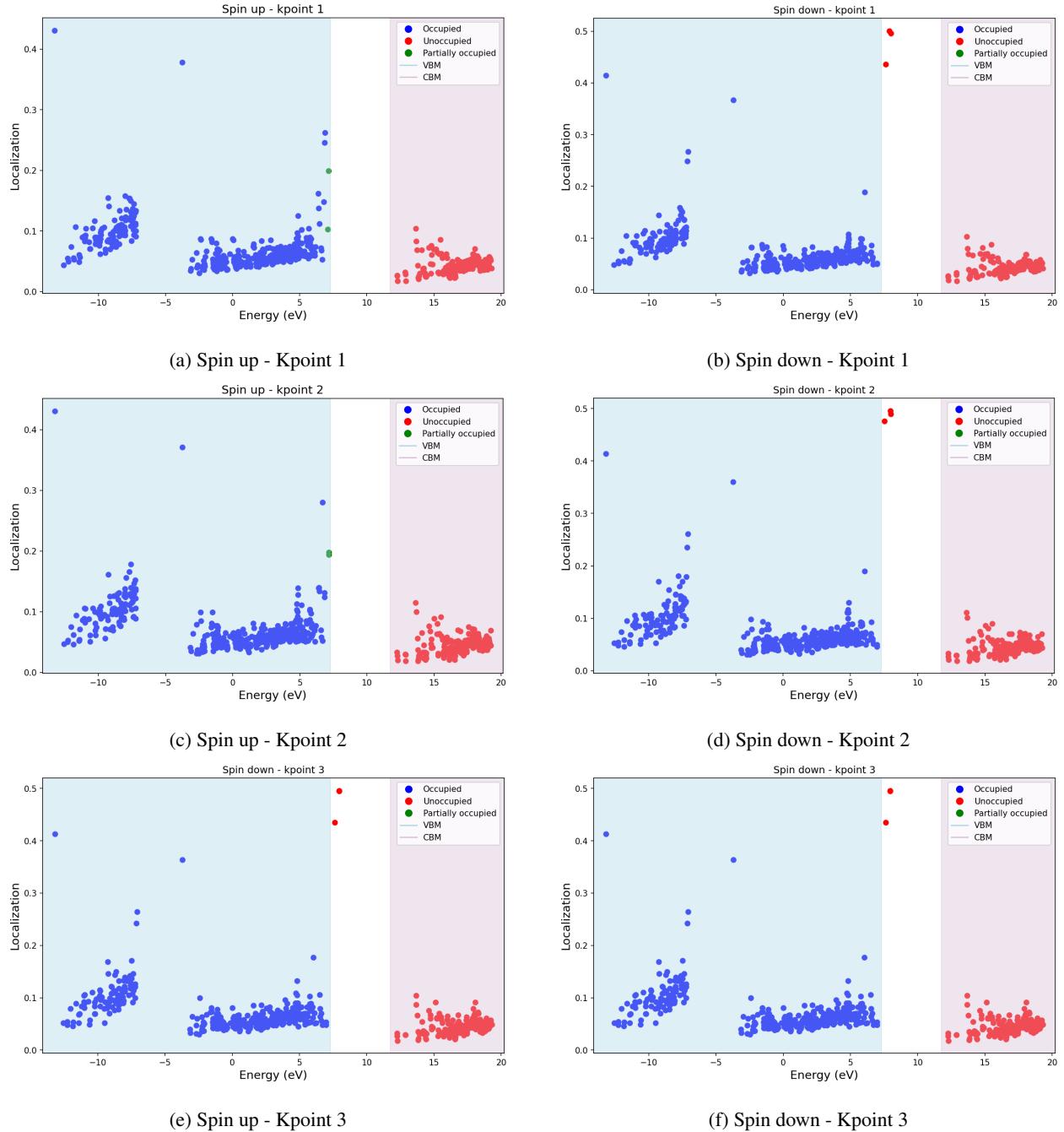


Figure 68: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

Table 44:  $(V_B - C_B)^{-1}$ 

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

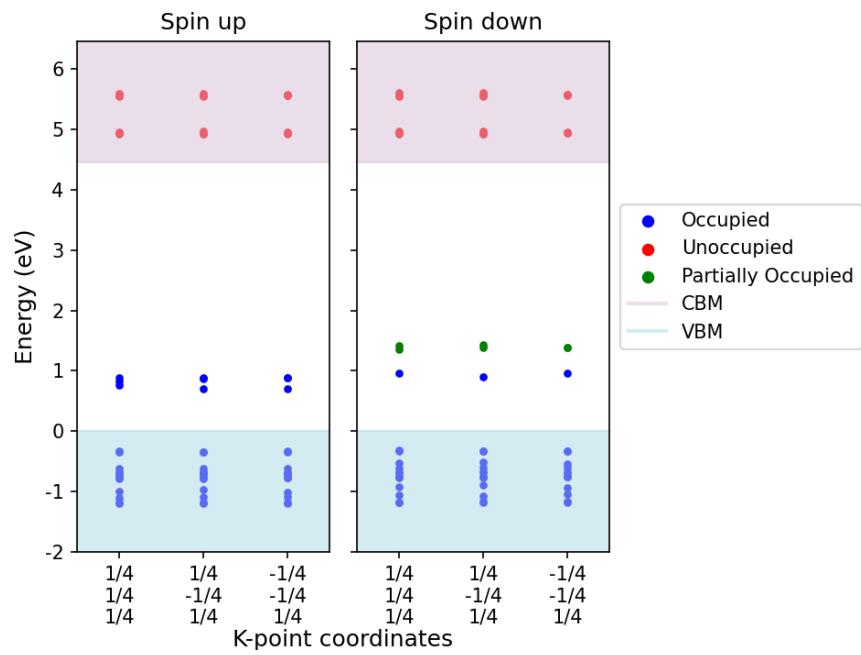


Figure 69: Kohn-Sham states.

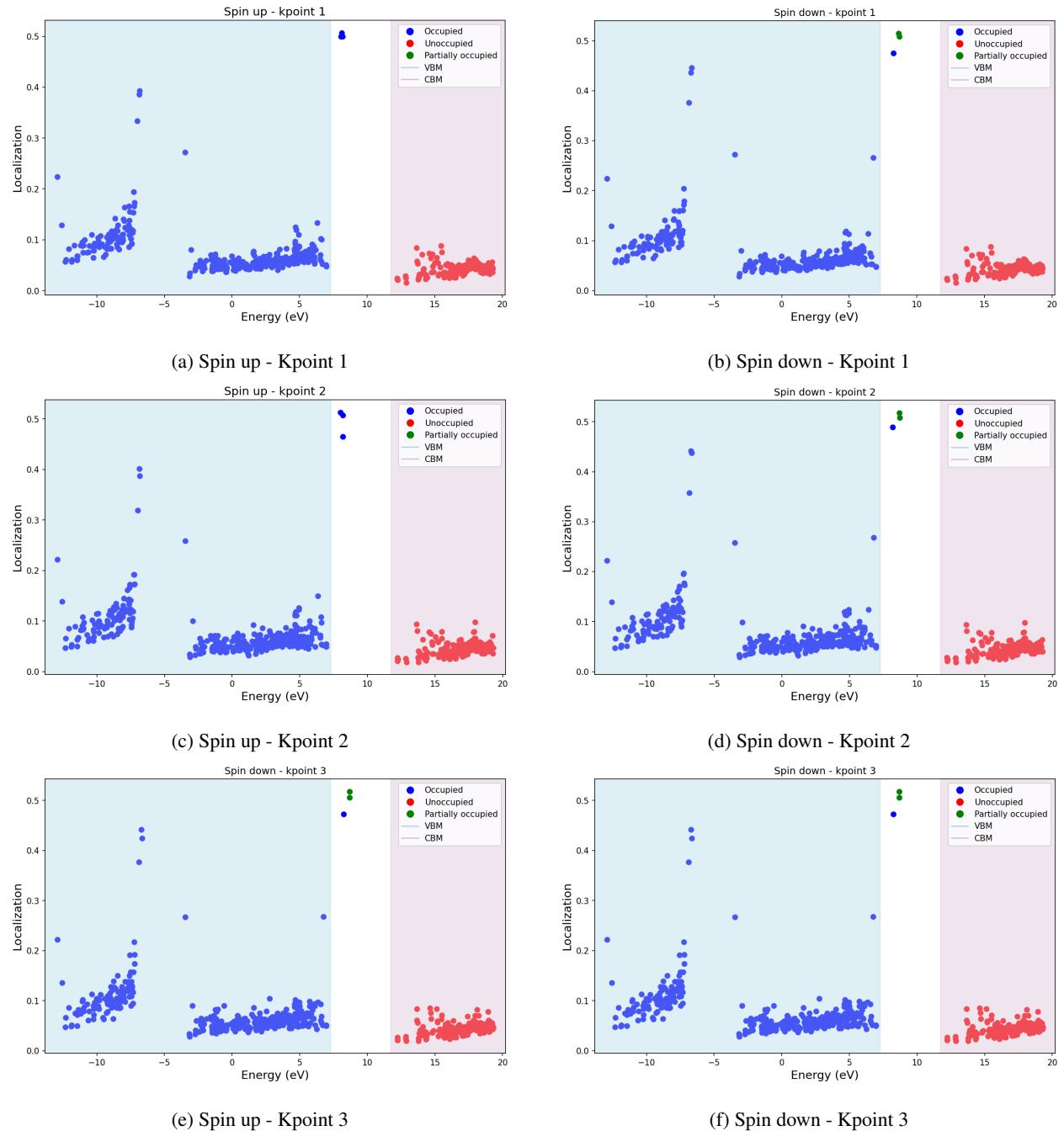


Figure 70: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

Table 45:  $(V_B - C_B)^{-2}$ 

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

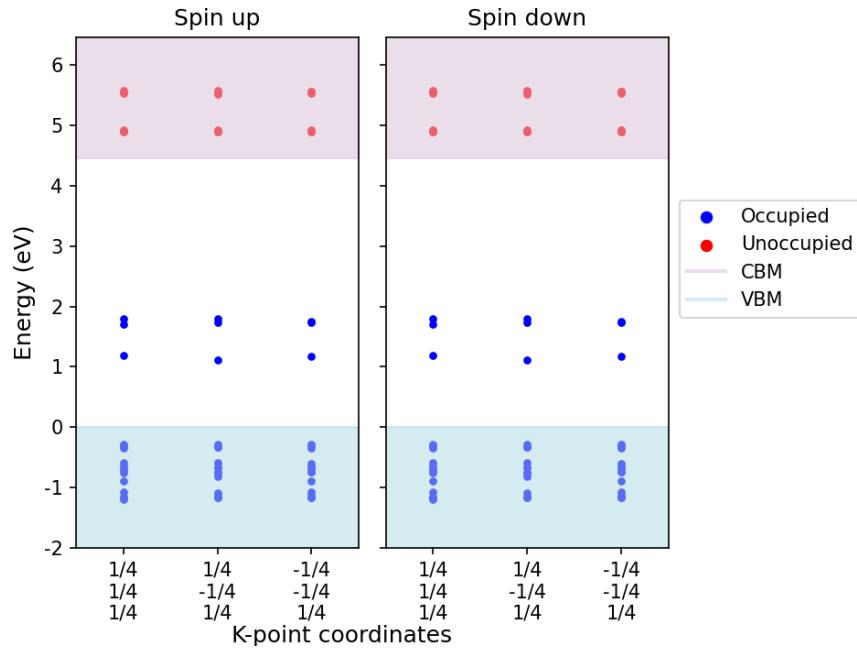


Figure 71: Kohn-Sham states.

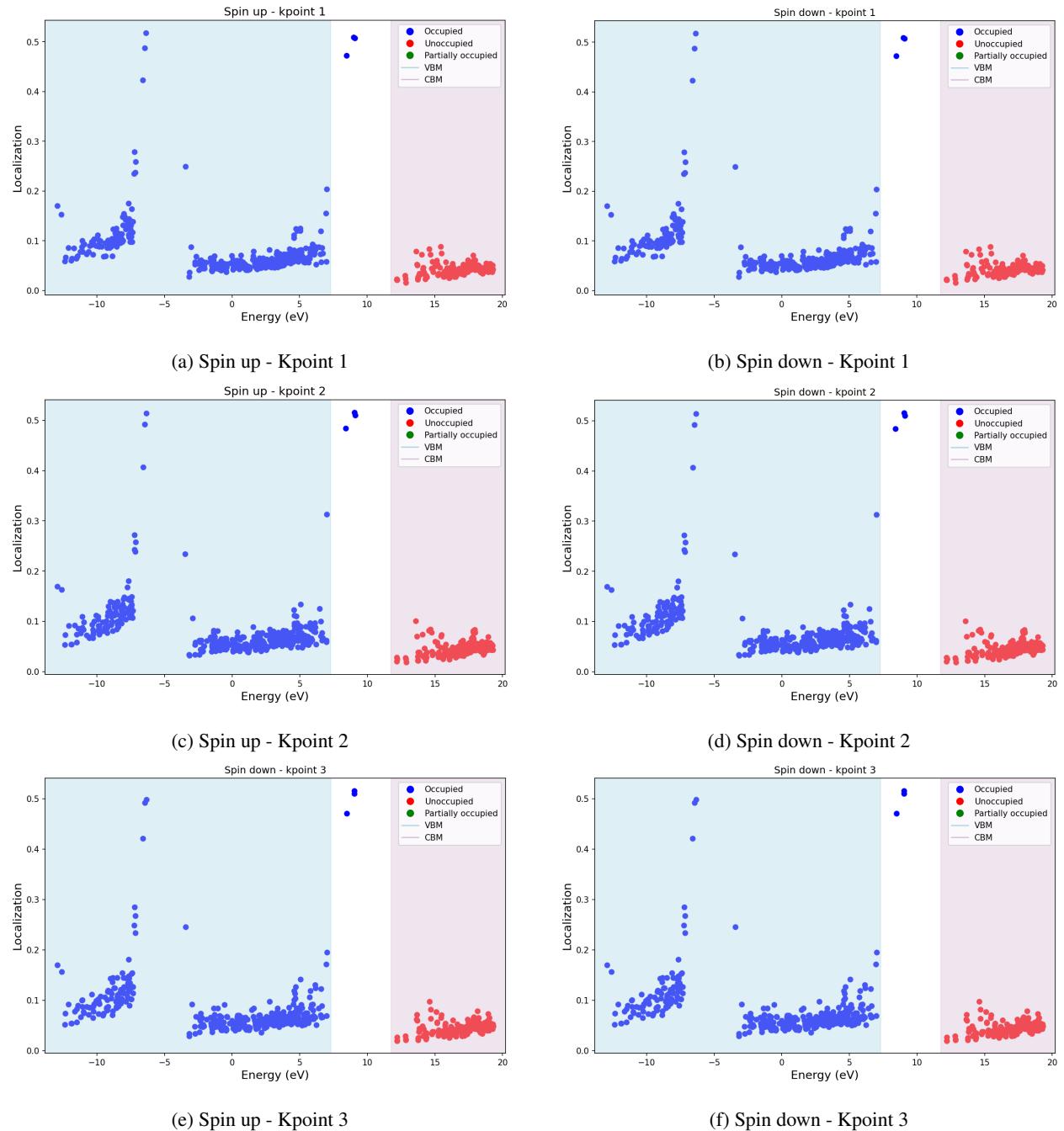


Figure 72: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

Table 46:  $(V_B - C_B)^{-3}$ 

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

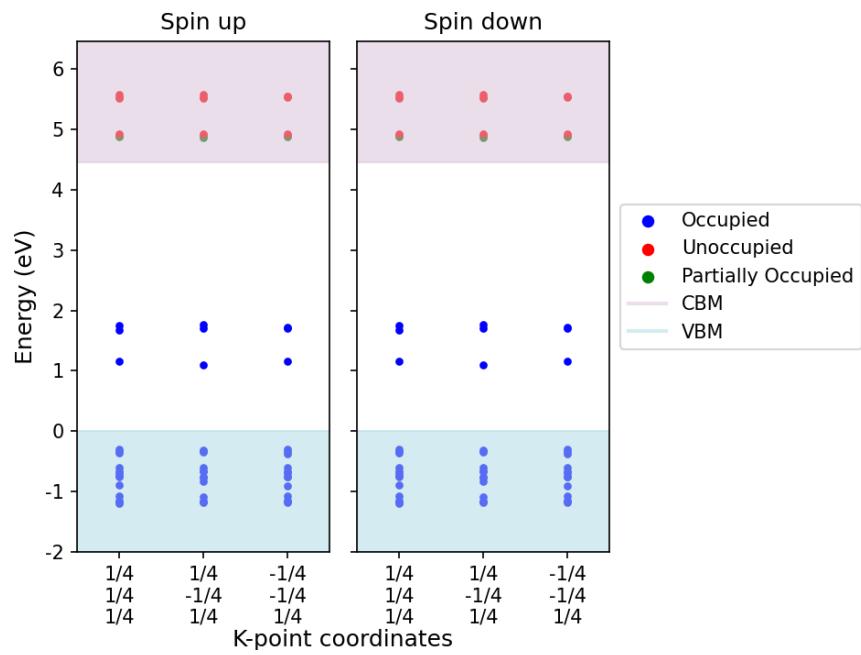


Figure 73: Kohn-Sham states.

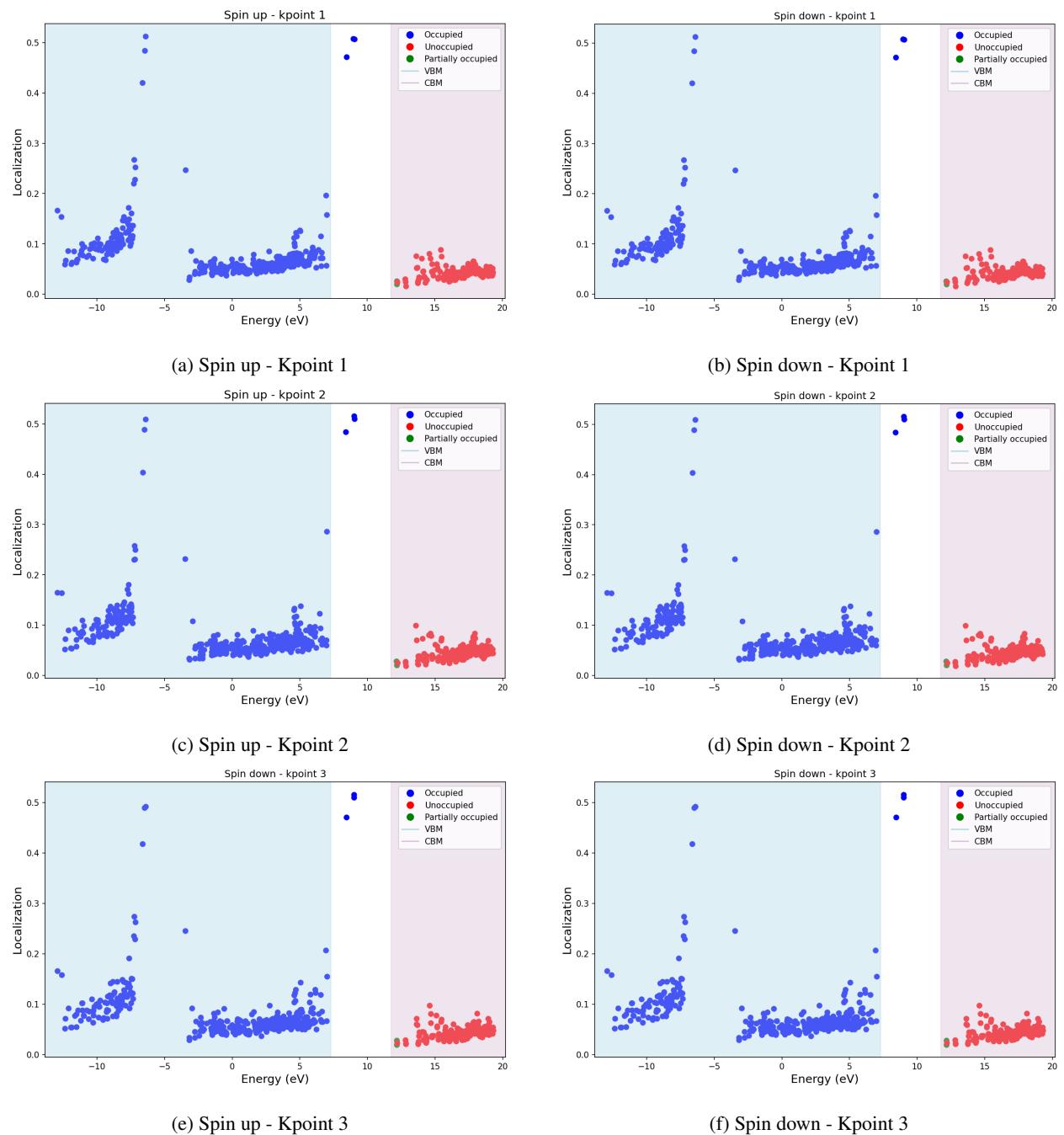


Figure 74: Localization factor using projected orbitals (s, p, and d).

### 1.38 Complex: $(V_N - C_N)^0$

[Go back to the Table 9](#)

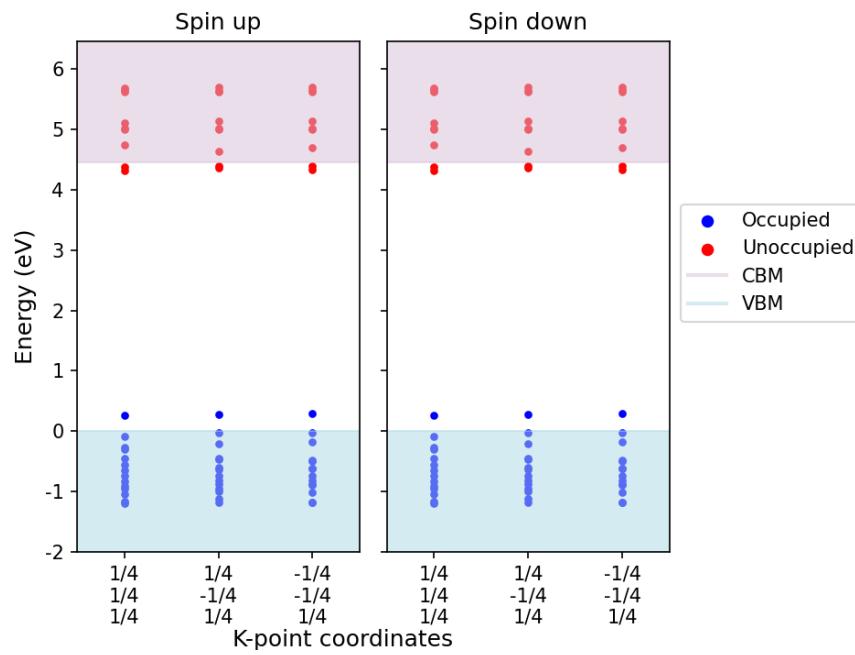


Figure 75: Kohn-Sham states.

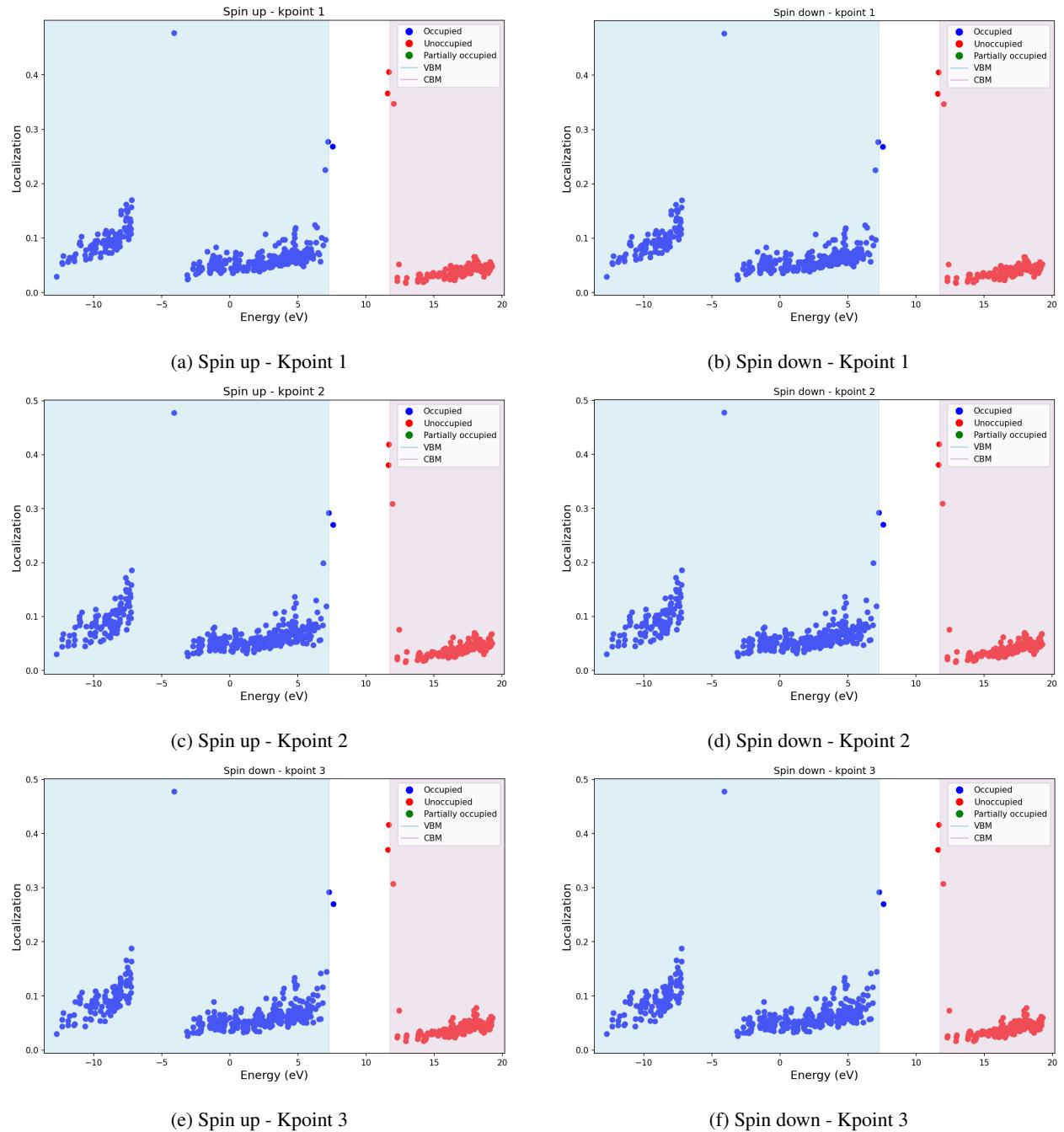


Figure 76: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

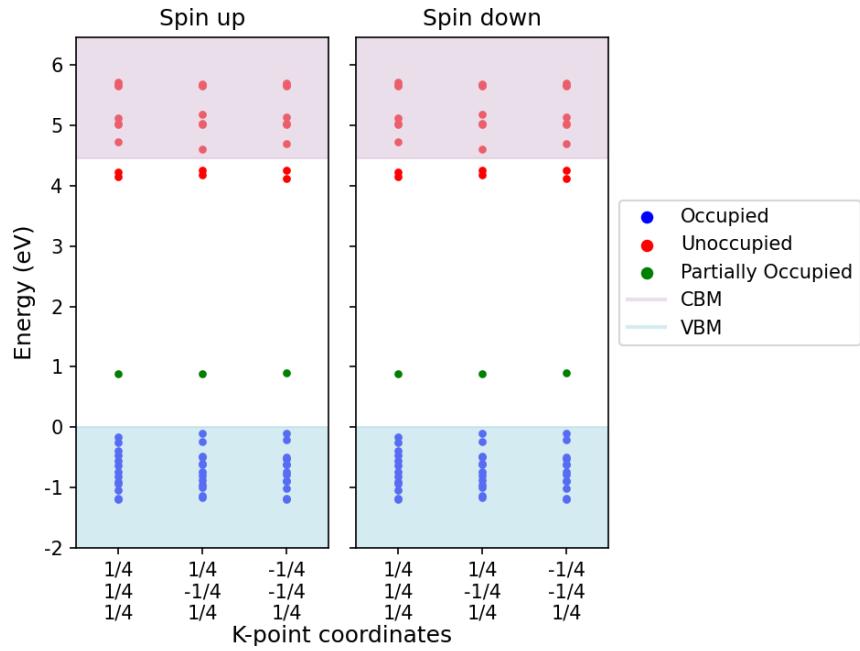


Figure 77: Kohn-Sham states.

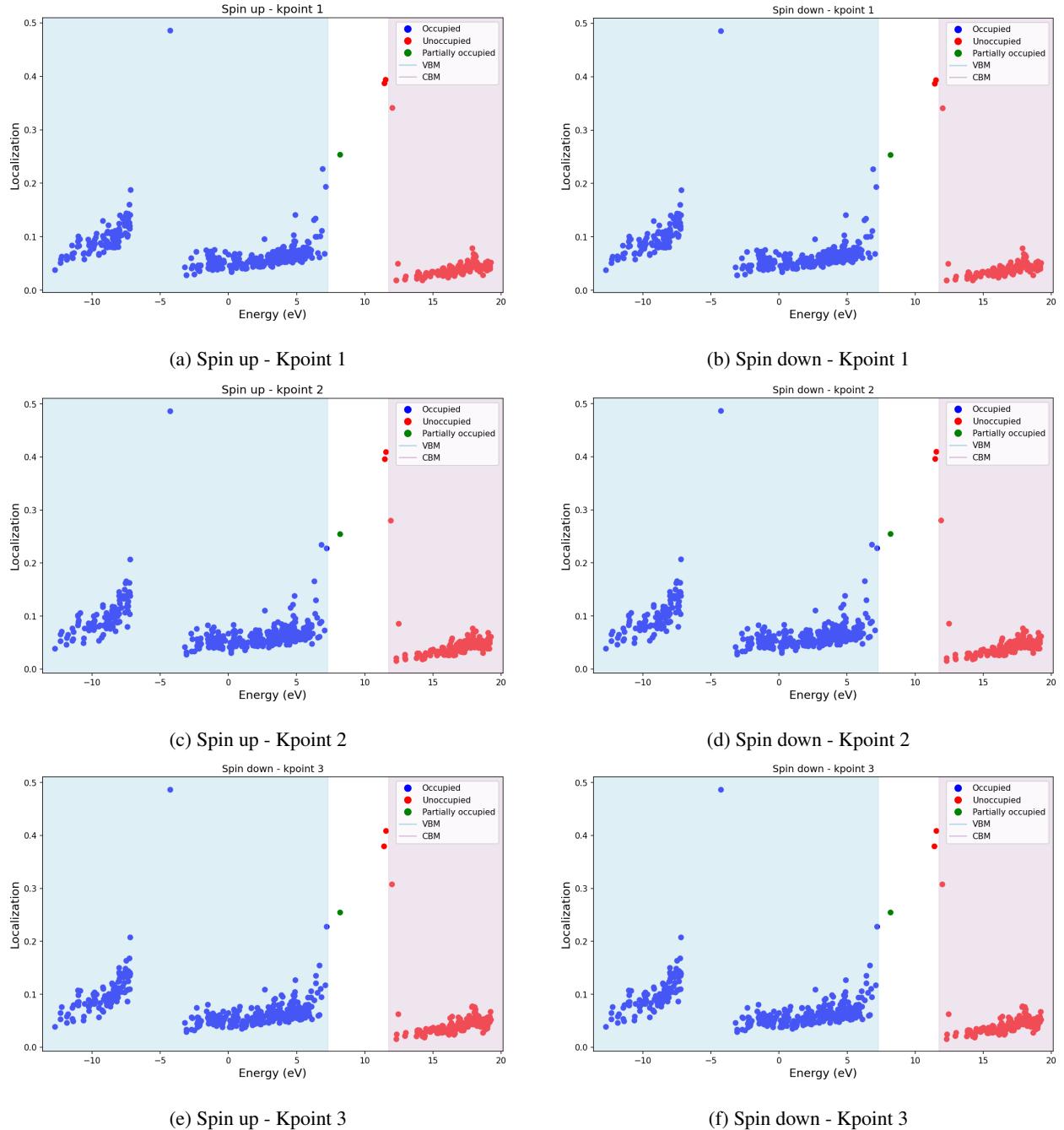


Figure 78: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

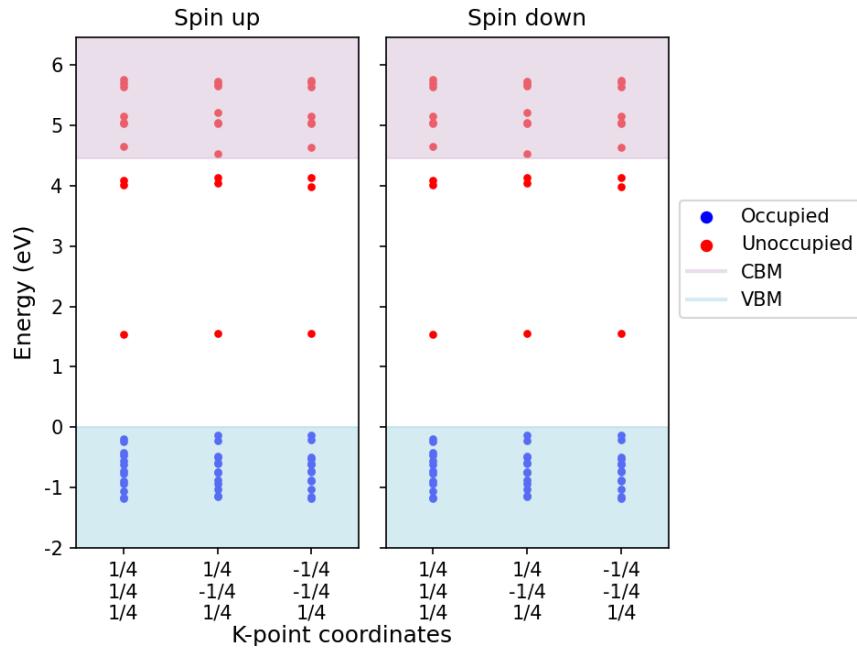


Figure 79: Kohn-Sham states.

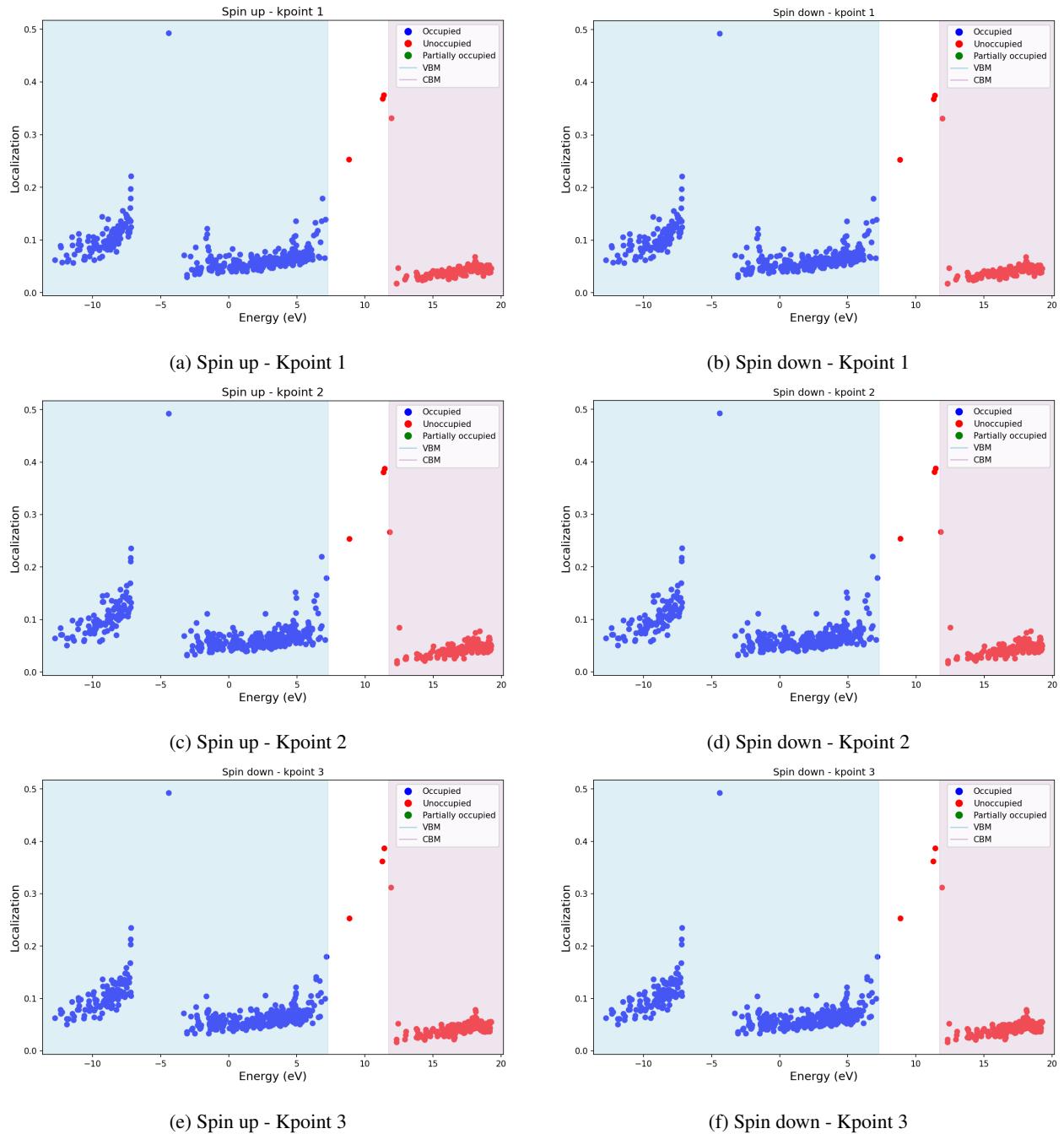


Figure 80: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

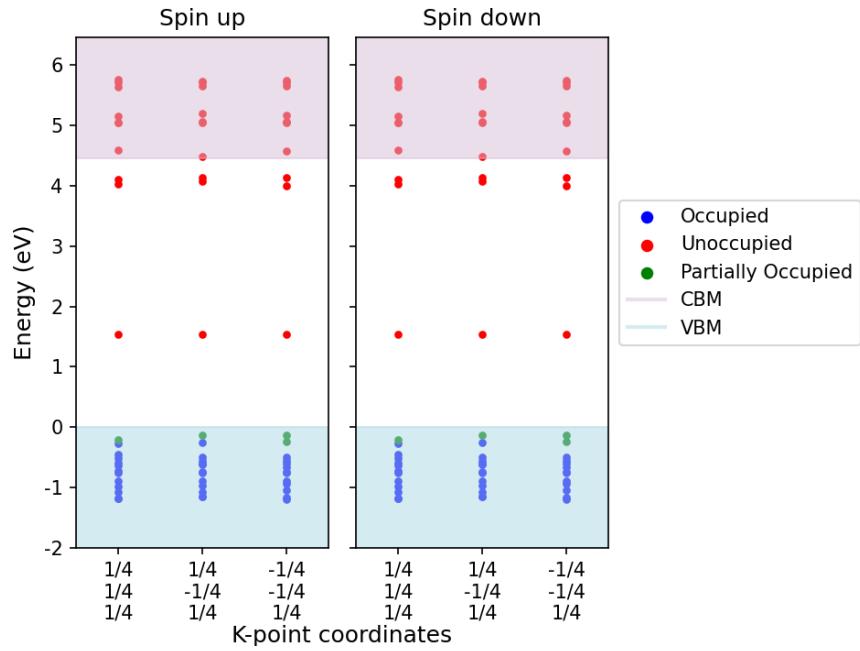


Figure 81: Kohn-Sham states.

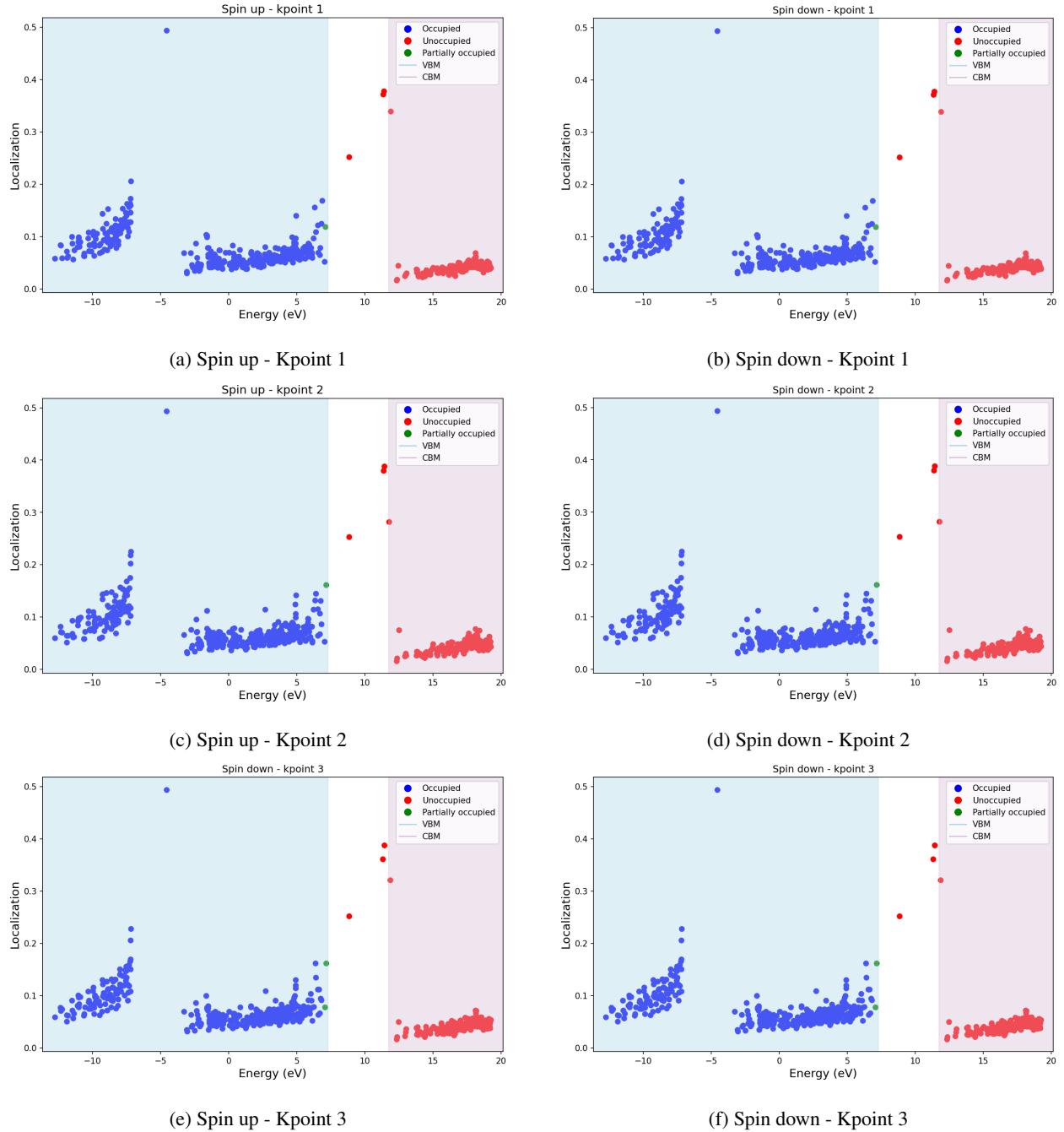


Figure 82: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

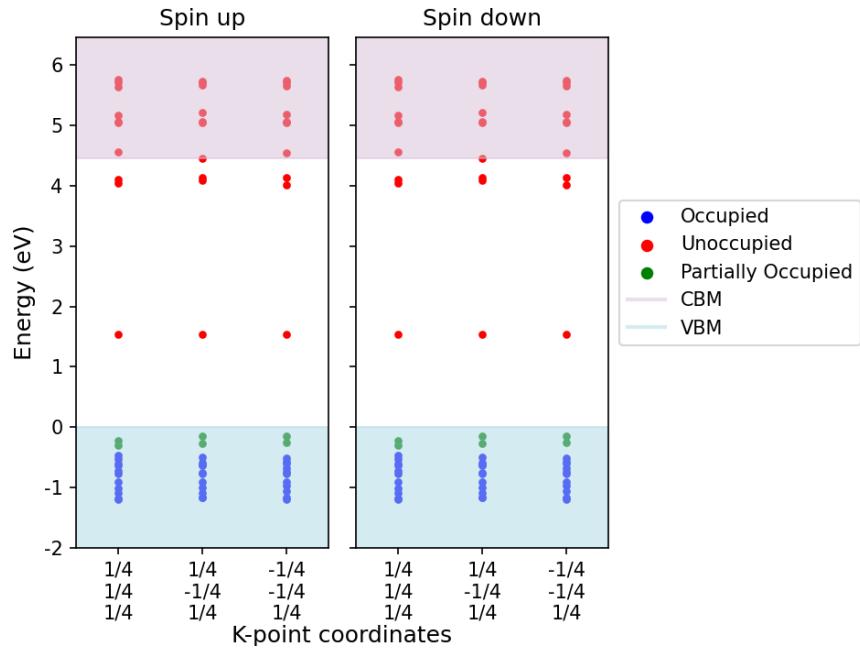


Figure 83: Kohn-Sham states.

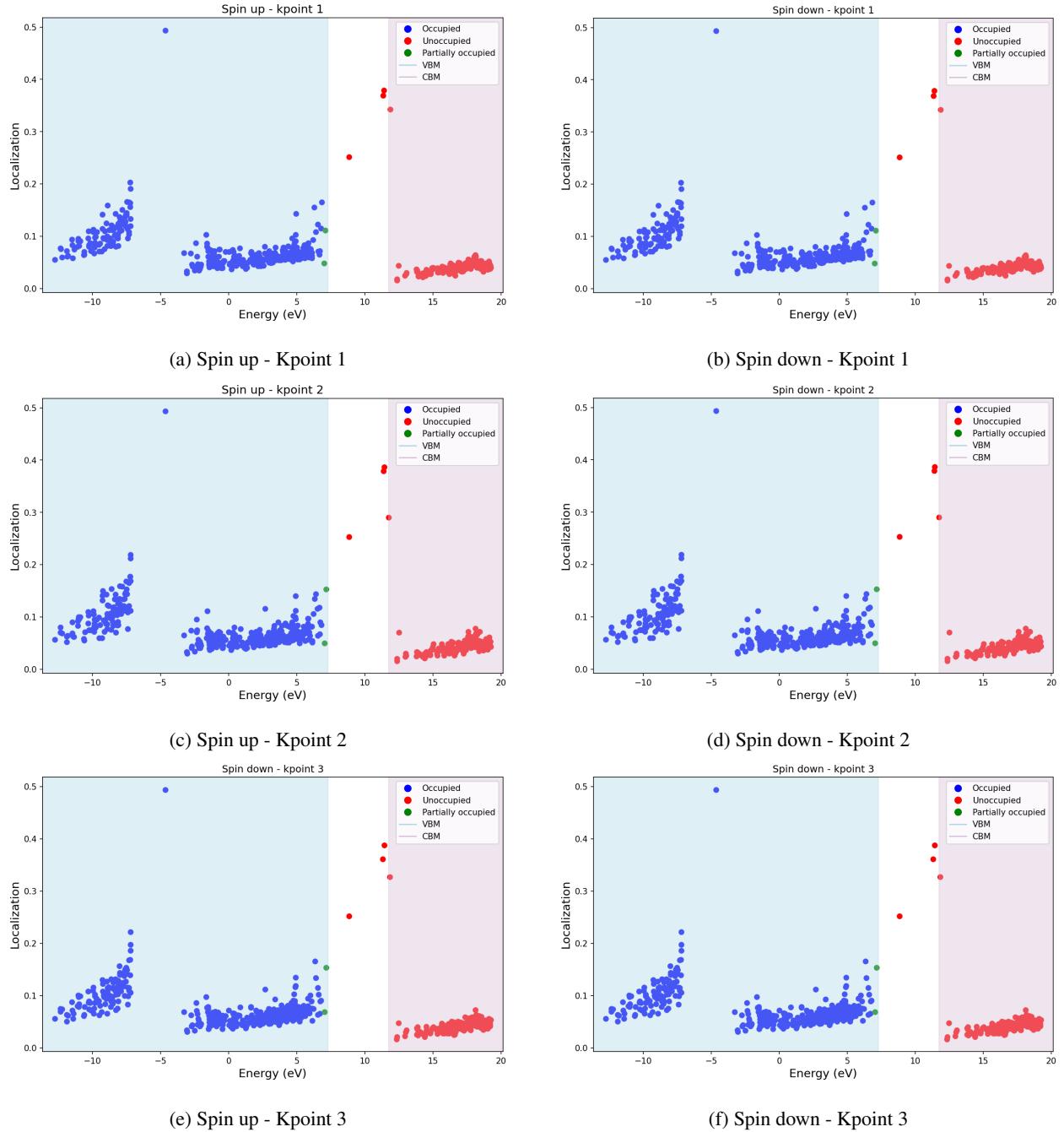


Figure 84: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

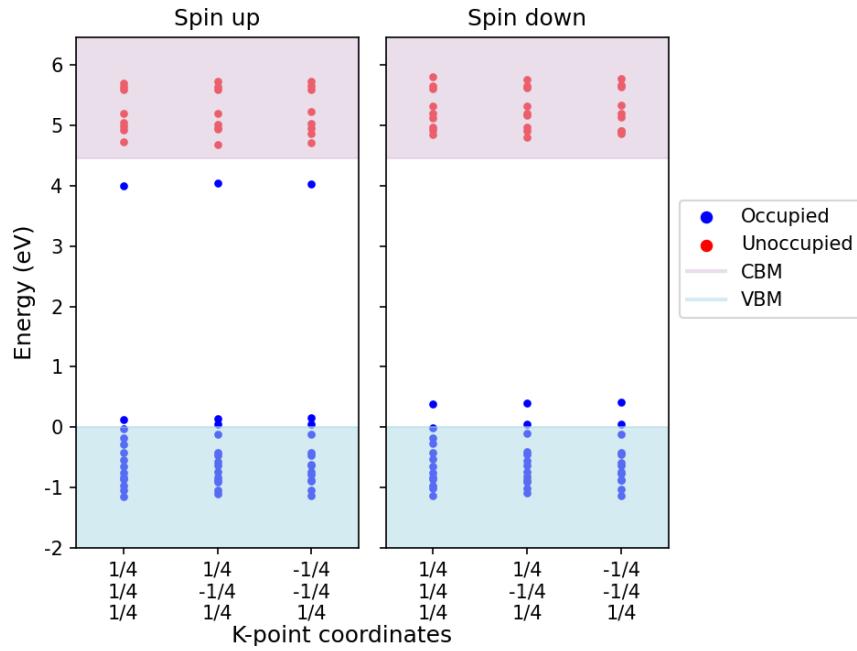


Figure 85: Kohn-Sham states.

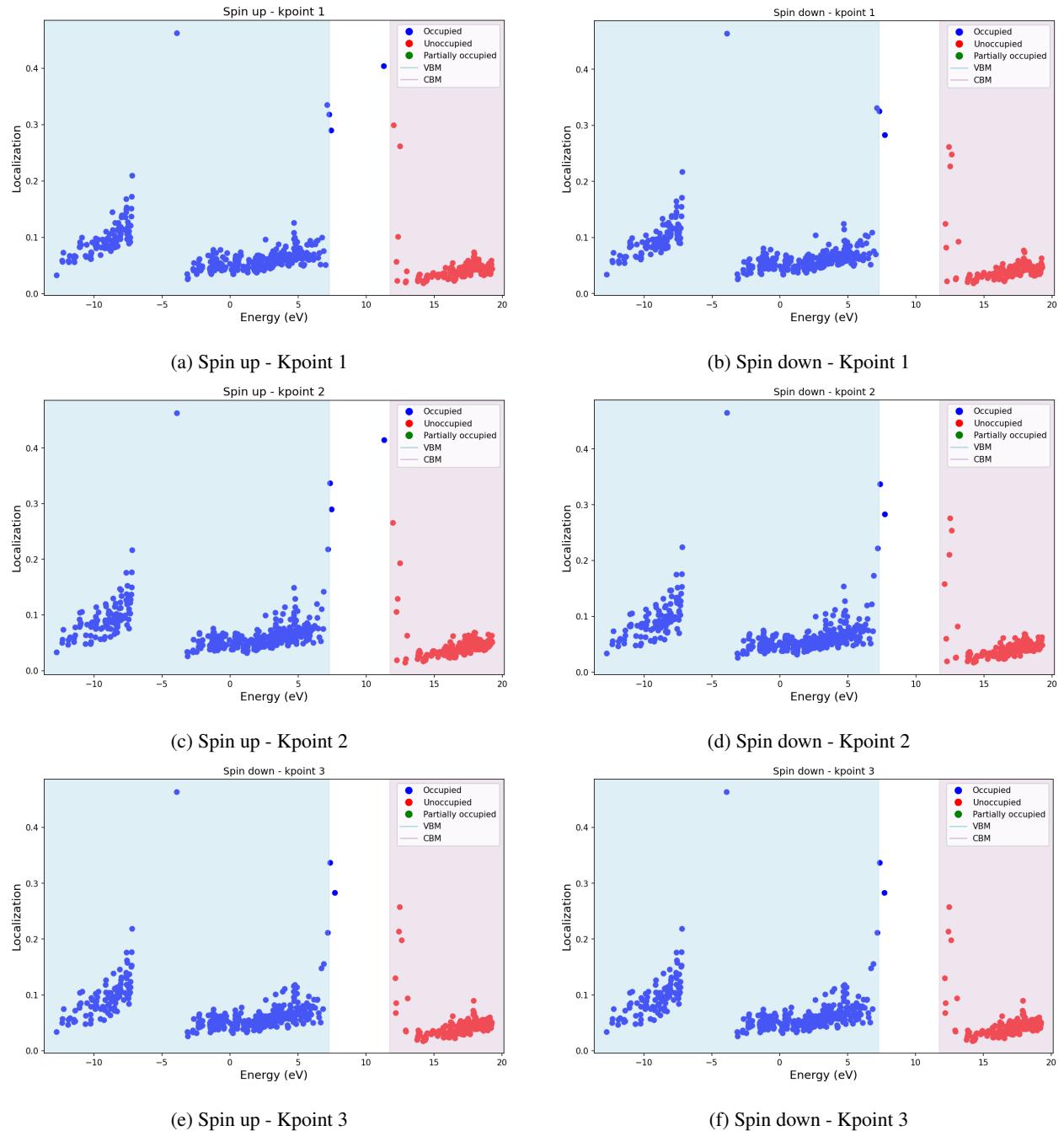


Figure 86: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

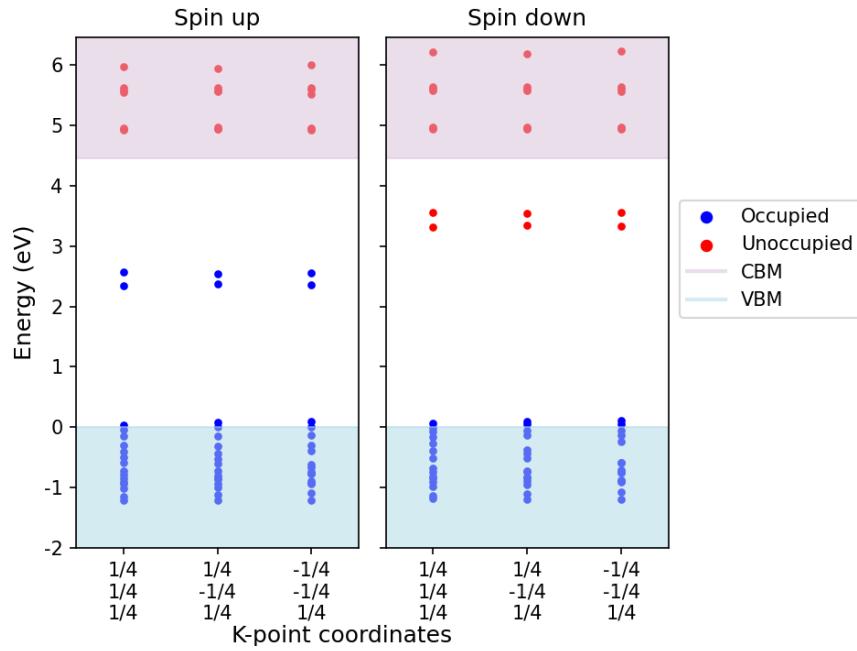


Figure 87: Kohn-Sham states.

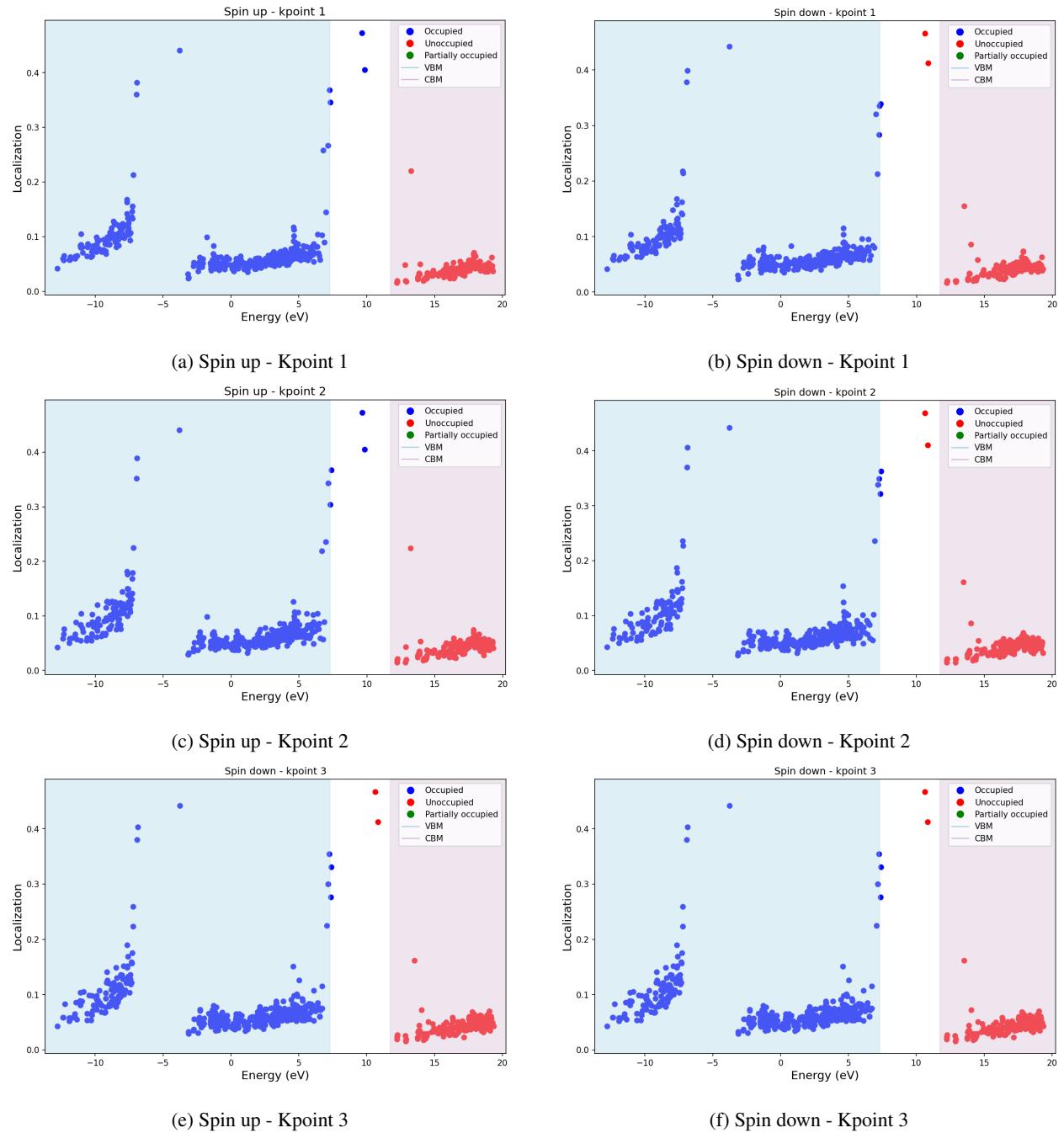


Figure 88: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

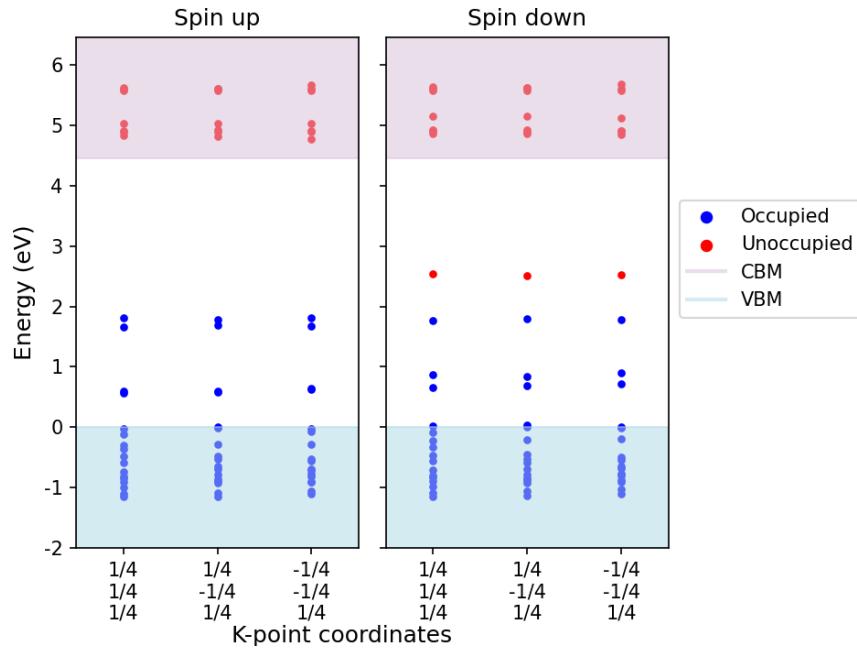


Figure 89: Kohn-Sham states.

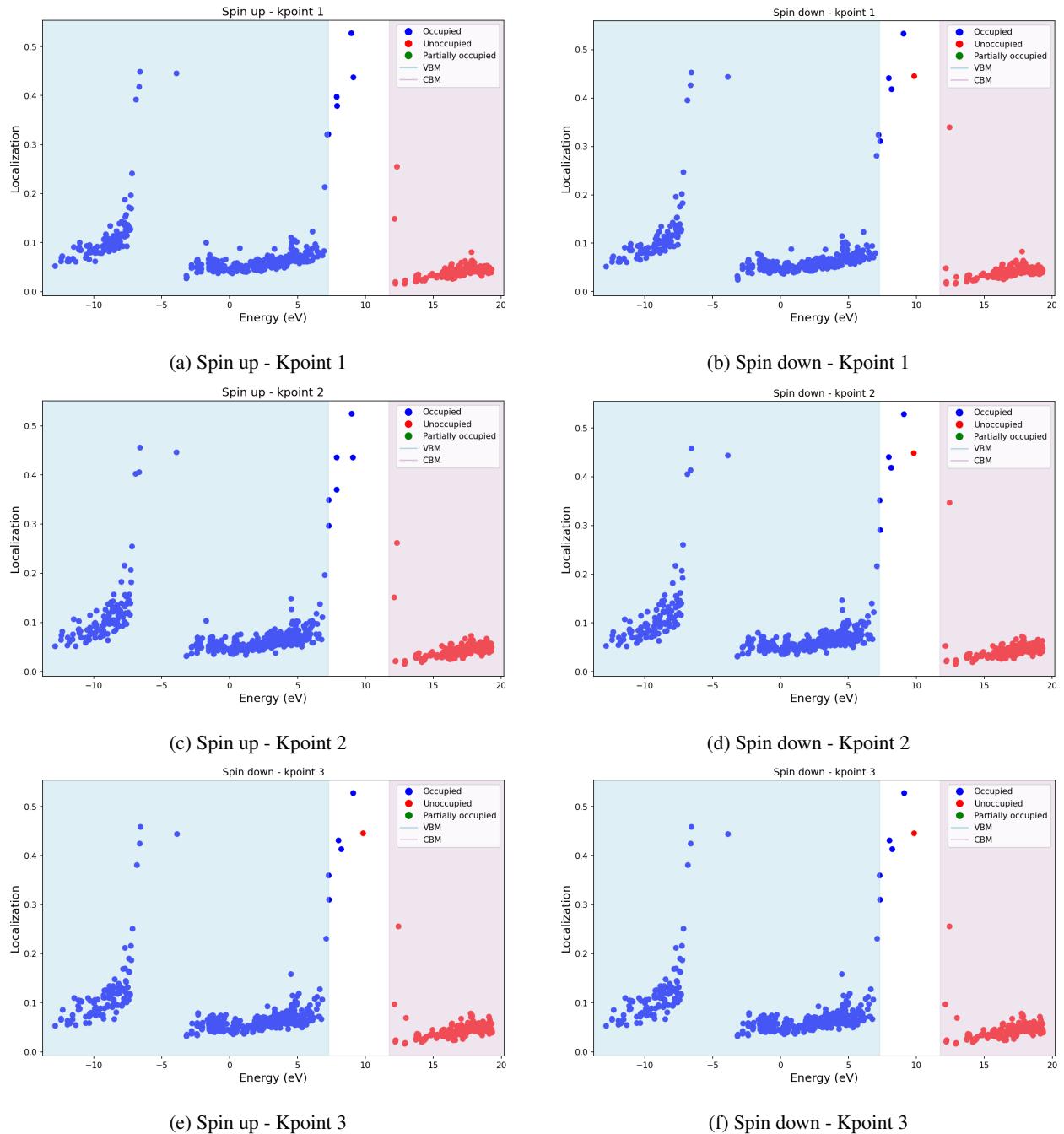


Figure 90: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

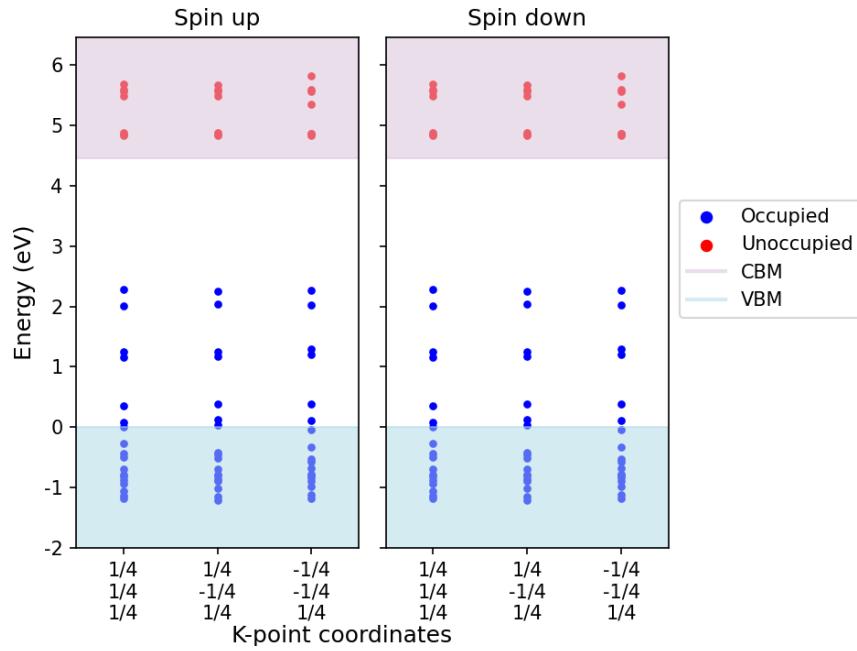


Figure 91: Kohn-Sham states.

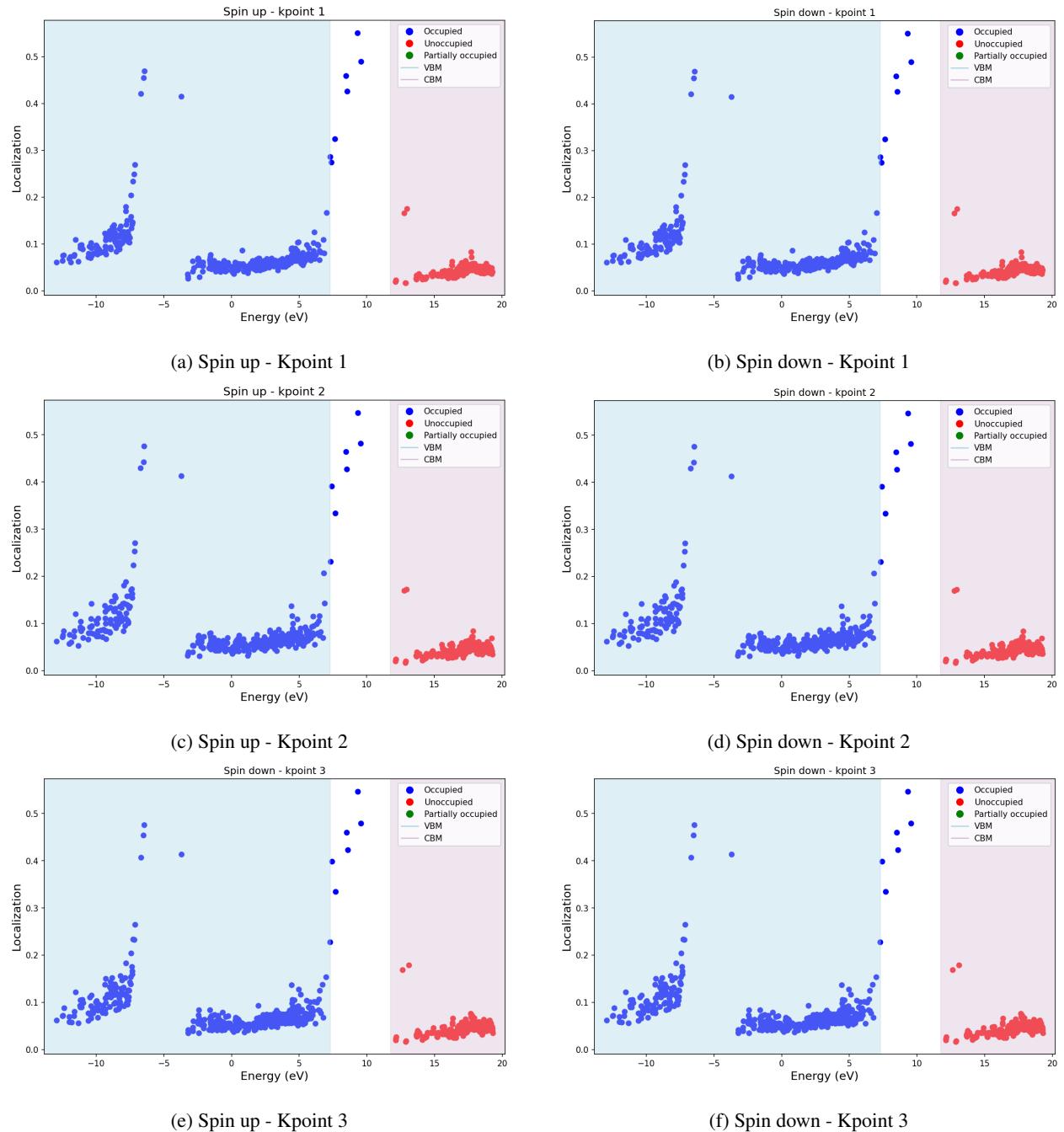


Figure 92: Localization factor using projected orbitals (s, p, and d).

### 1.47 Complex: $(B_N - V_B)^0$

[Go back to the Table 9](#)

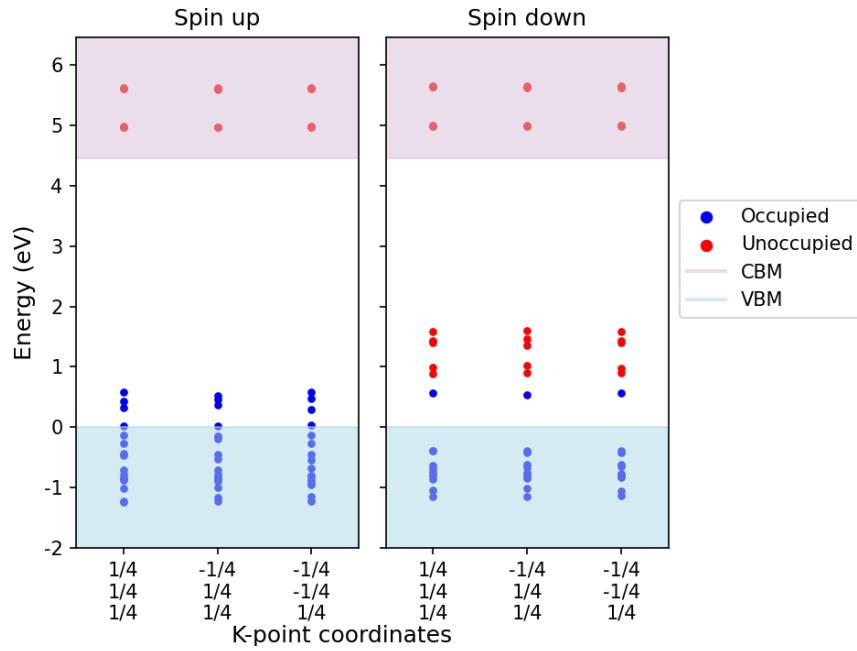


Figure 93: Kohn-Sham states.

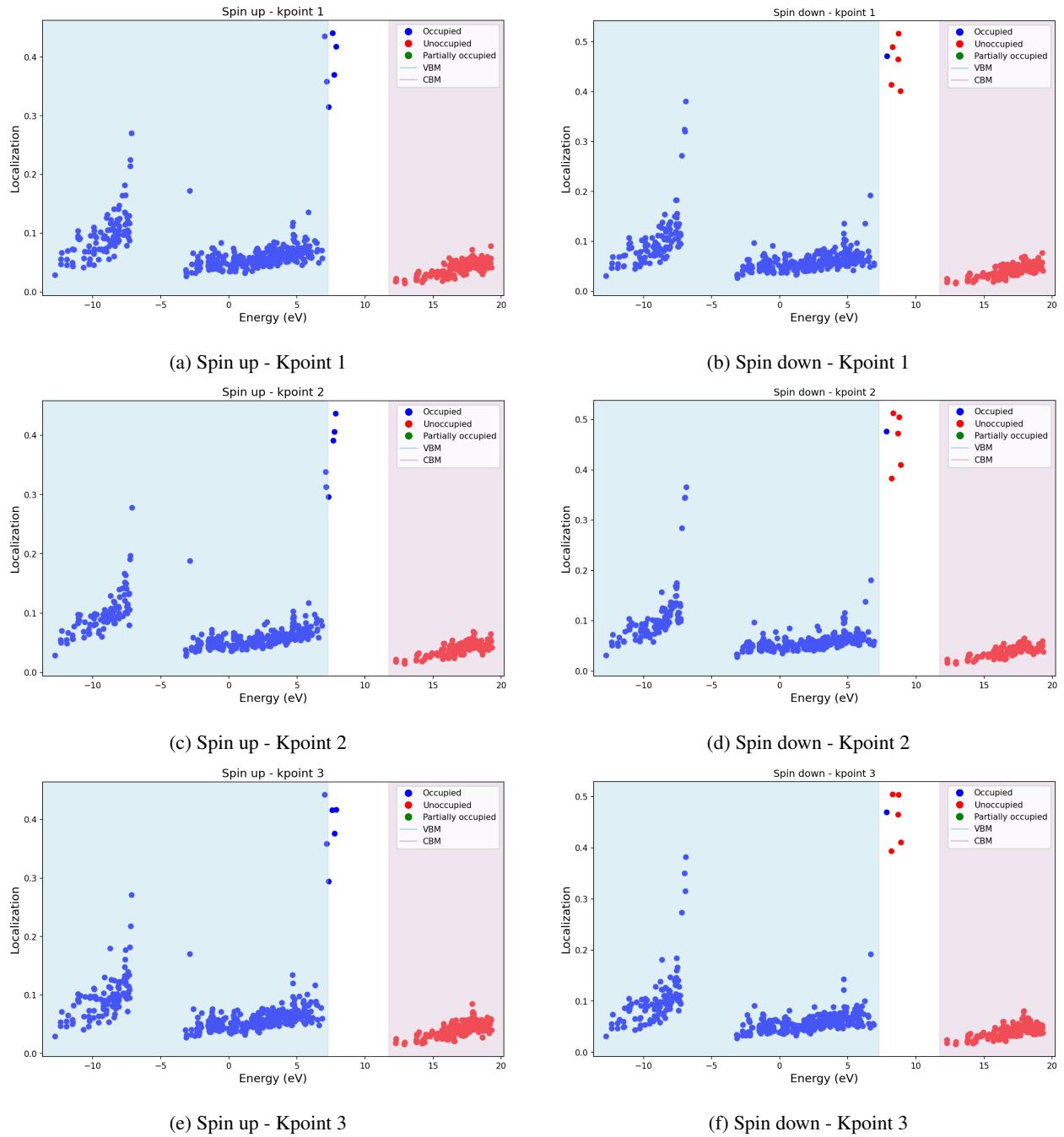


Figure 94: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

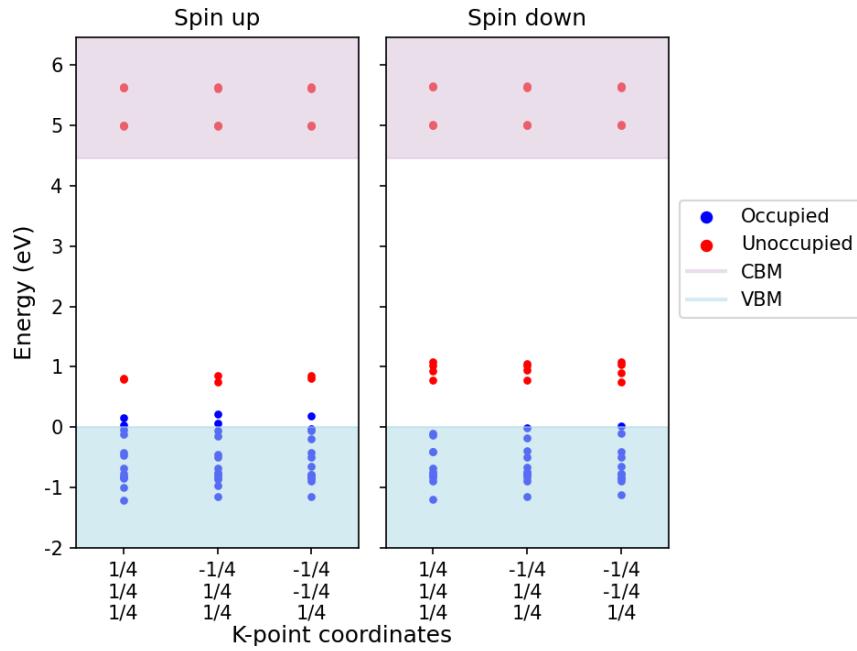


Figure 95: Kohn-Sham states.

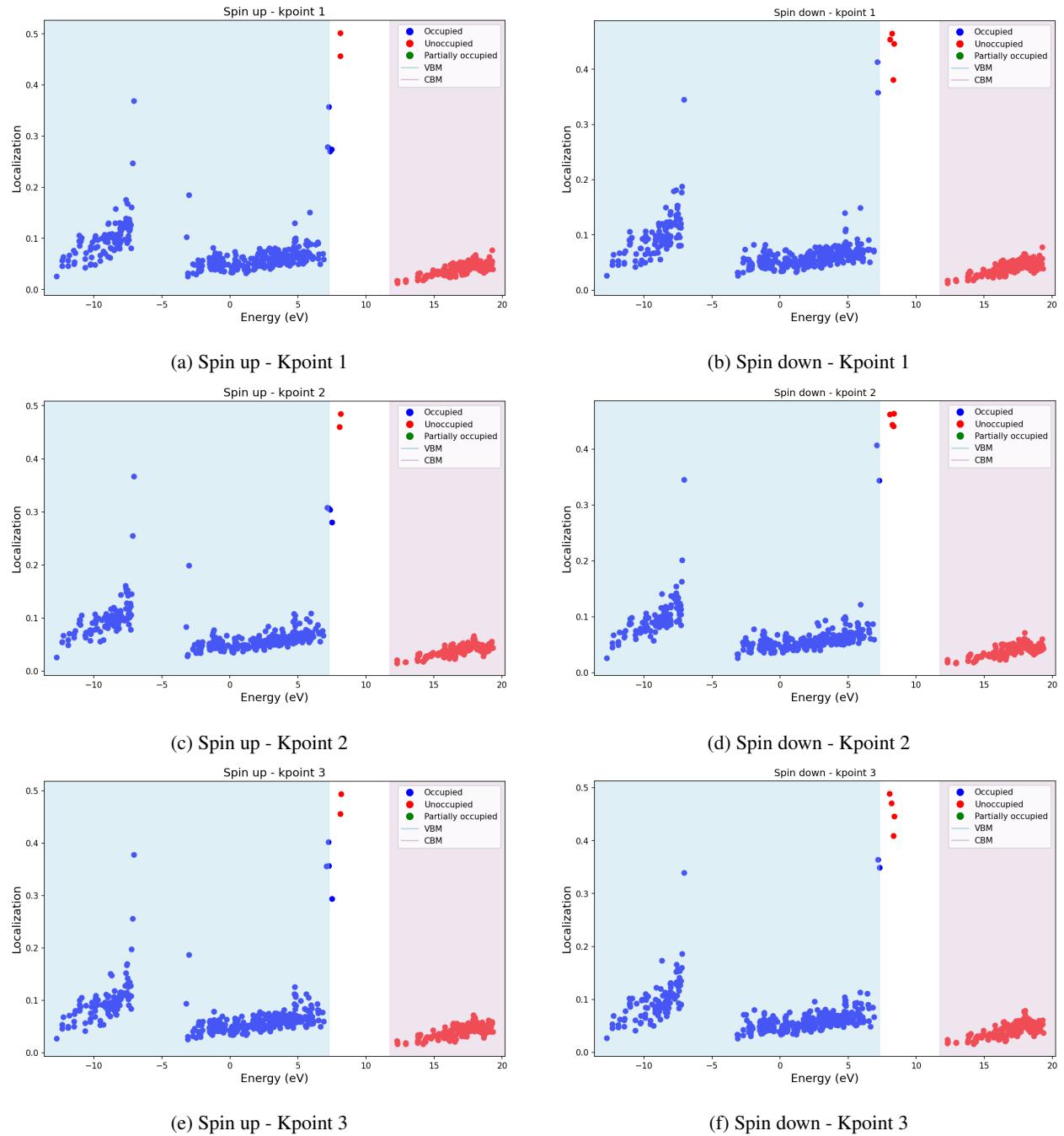


Figure 96: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

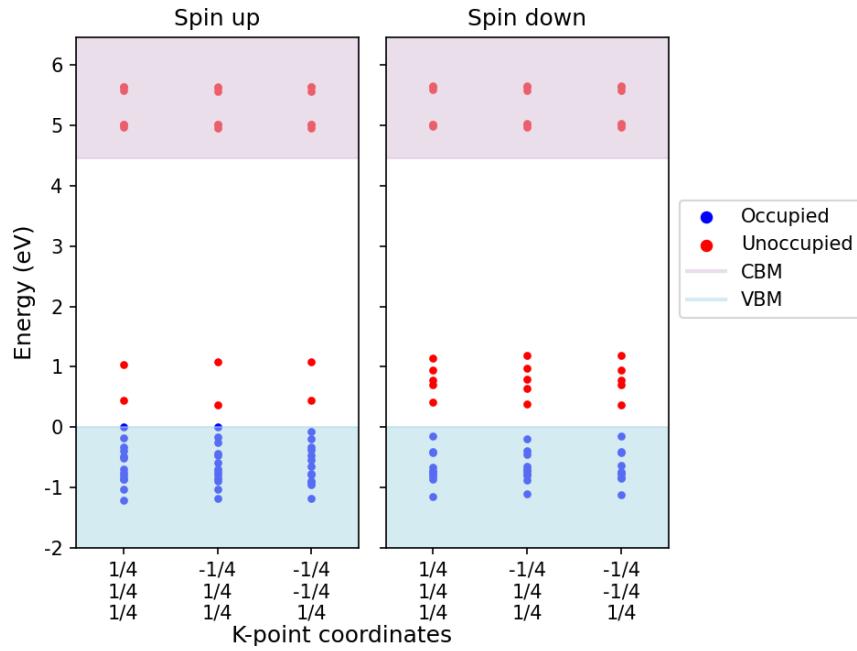


Figure 97: Kohn-Sham states.

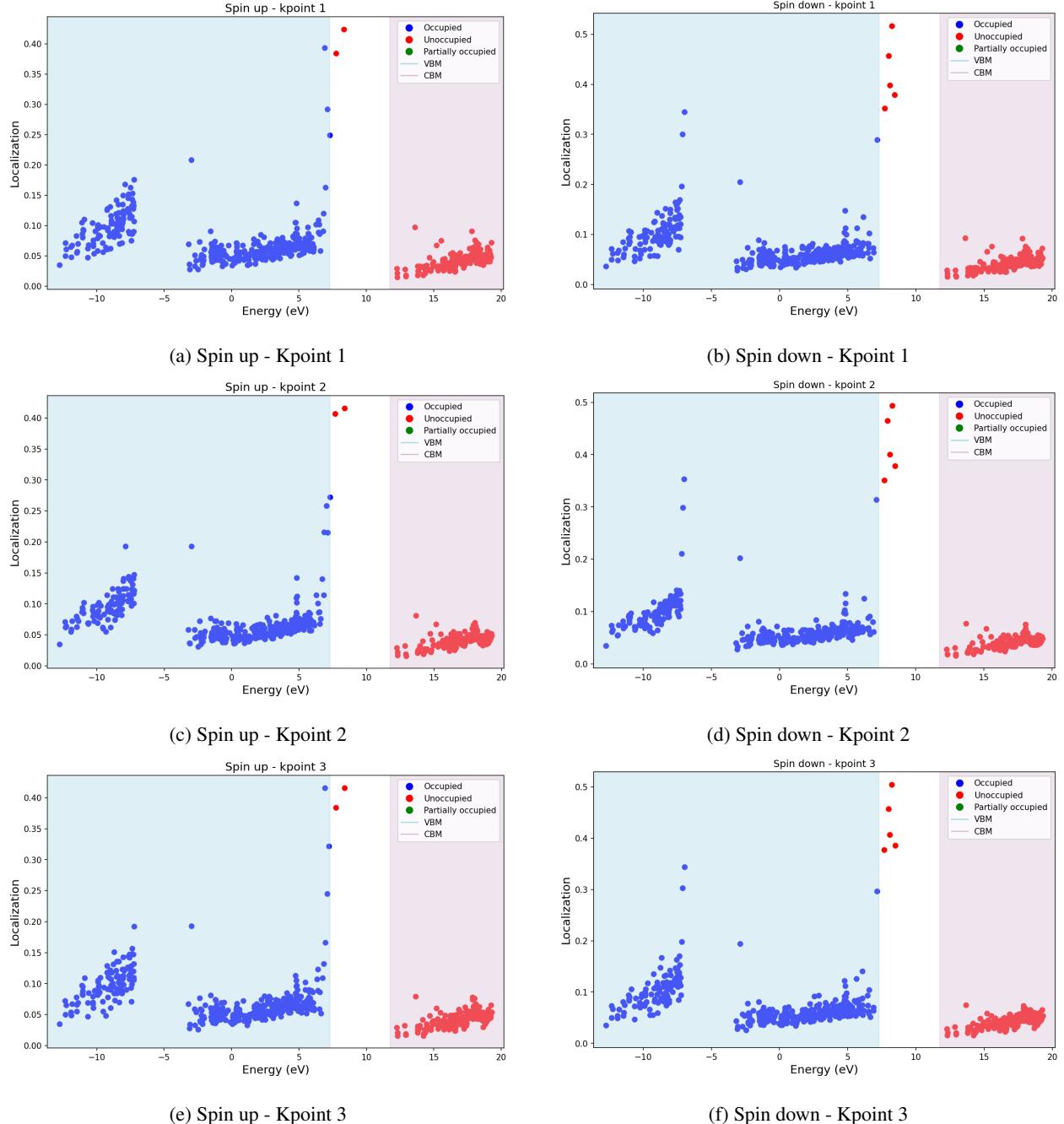


Figure 98: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

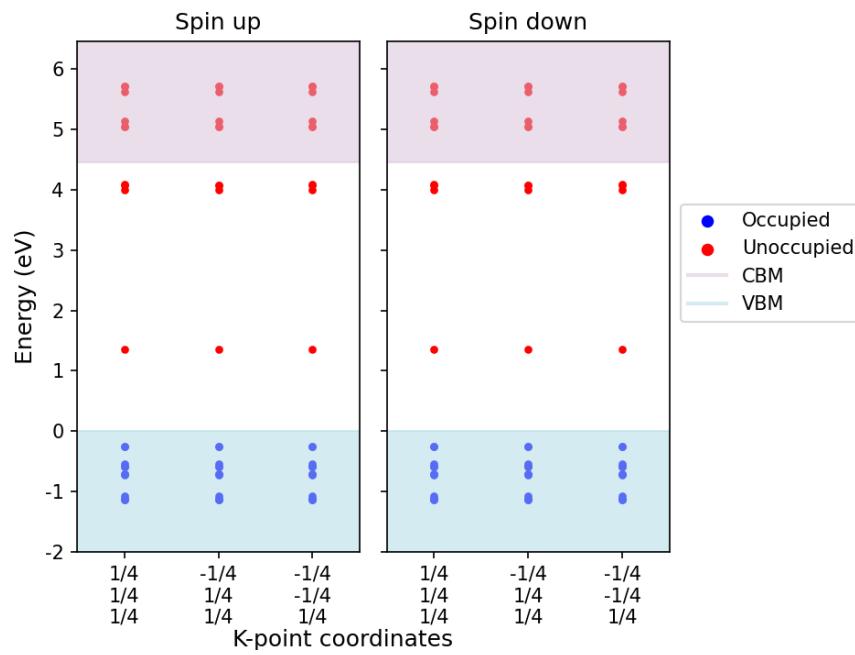


Figure 99: Kohn-Sham states.

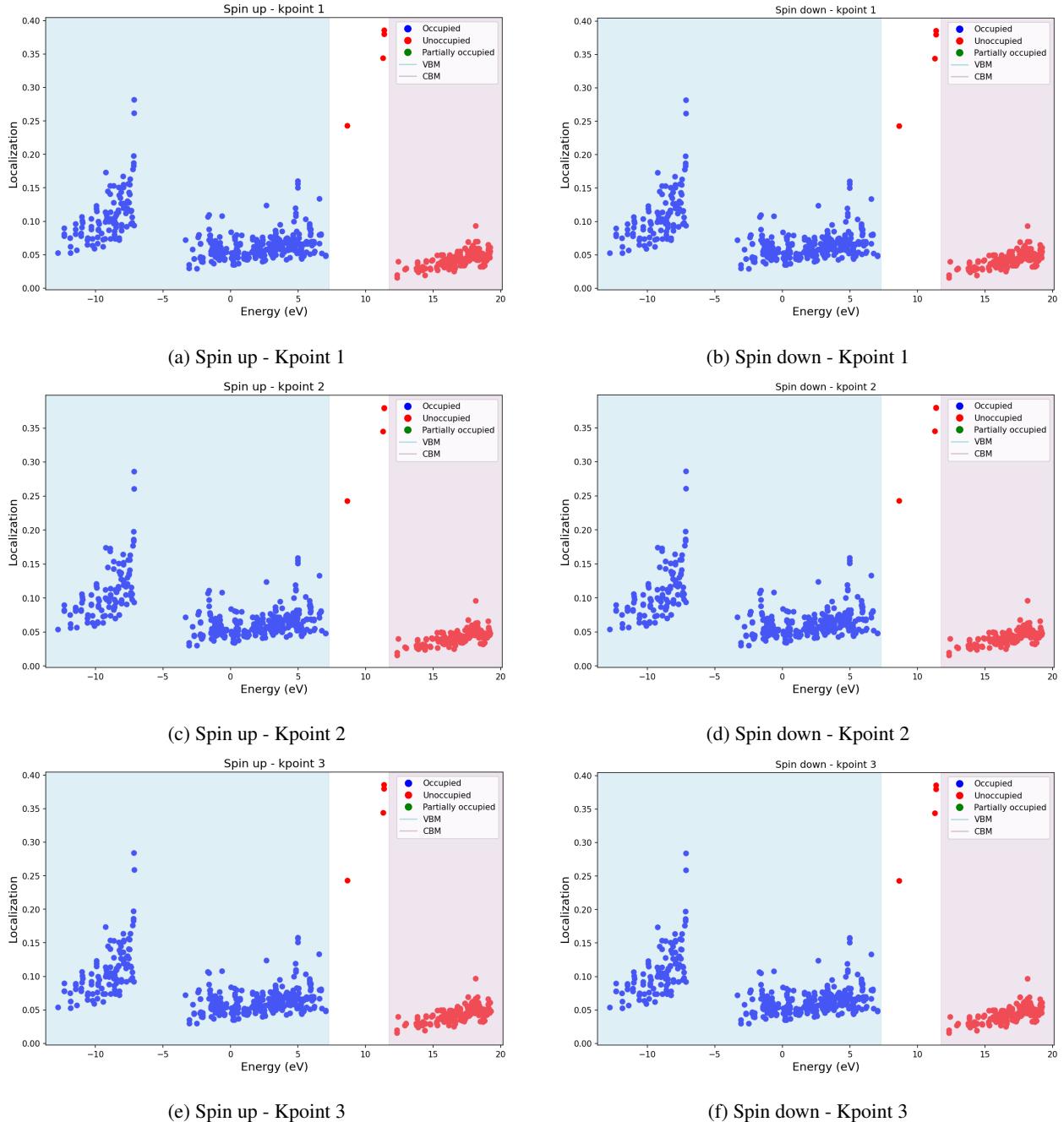


Figure 100: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

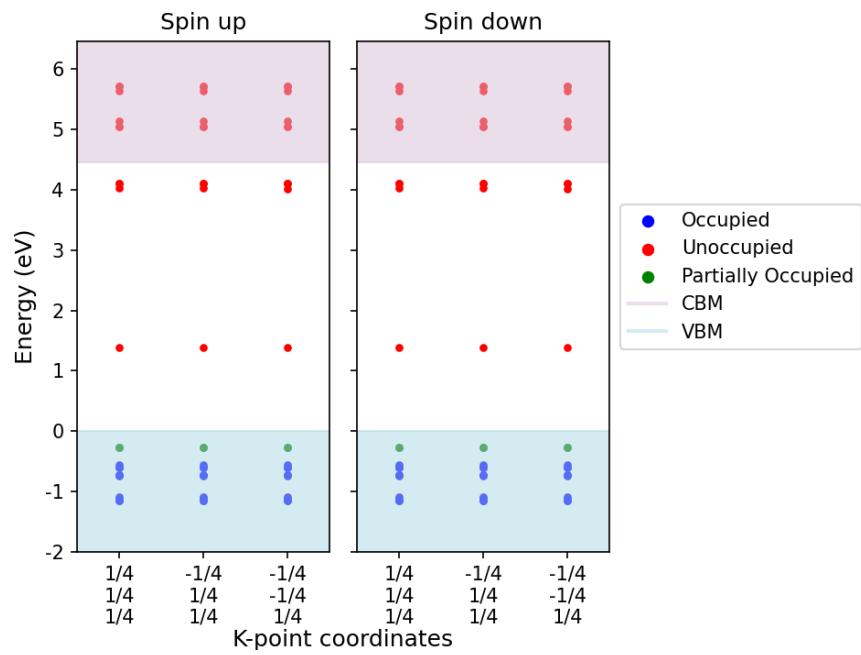


Figure 101: Kohn-Sham states.

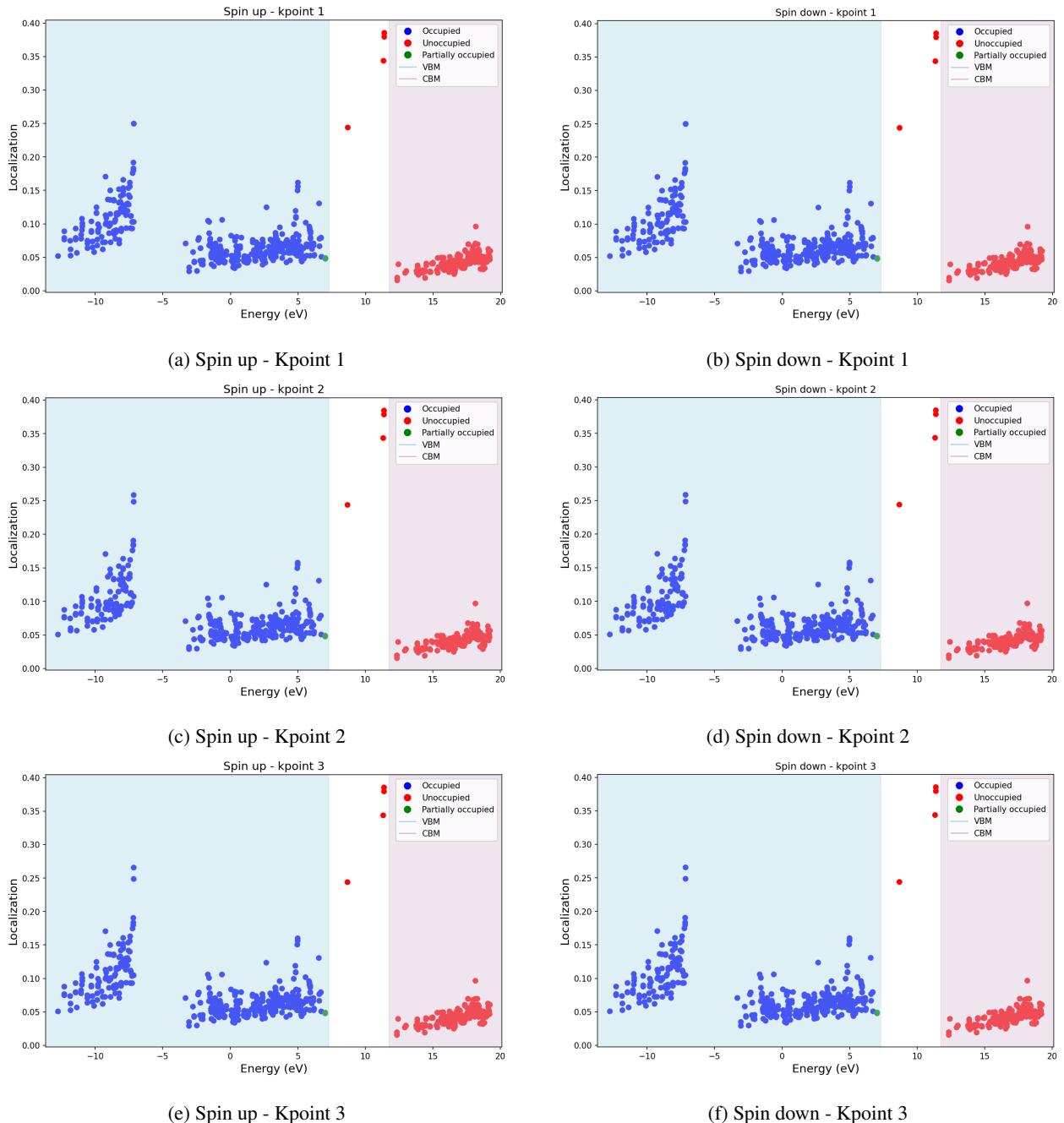


Figure 102: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

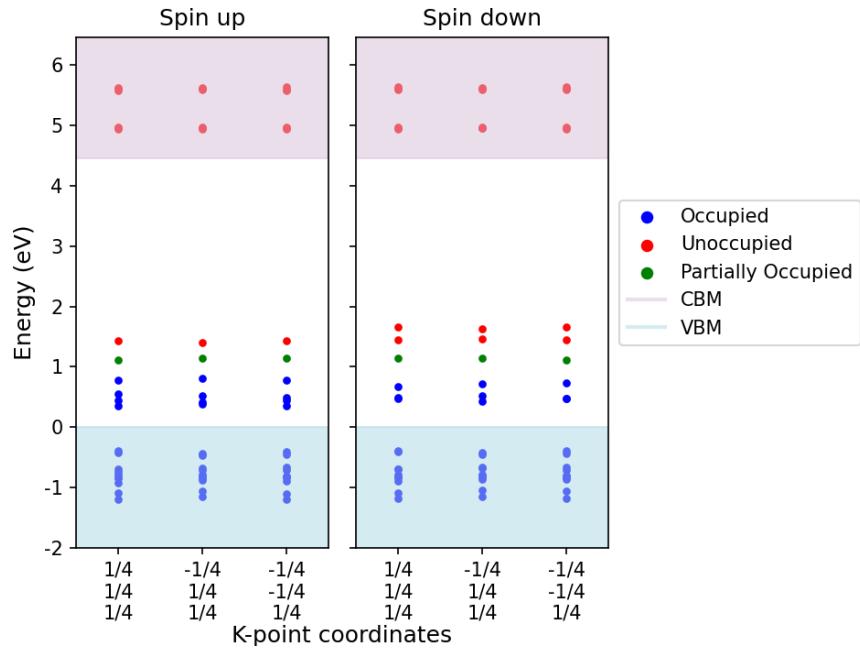


Figure 103: Kohn-Sham states.

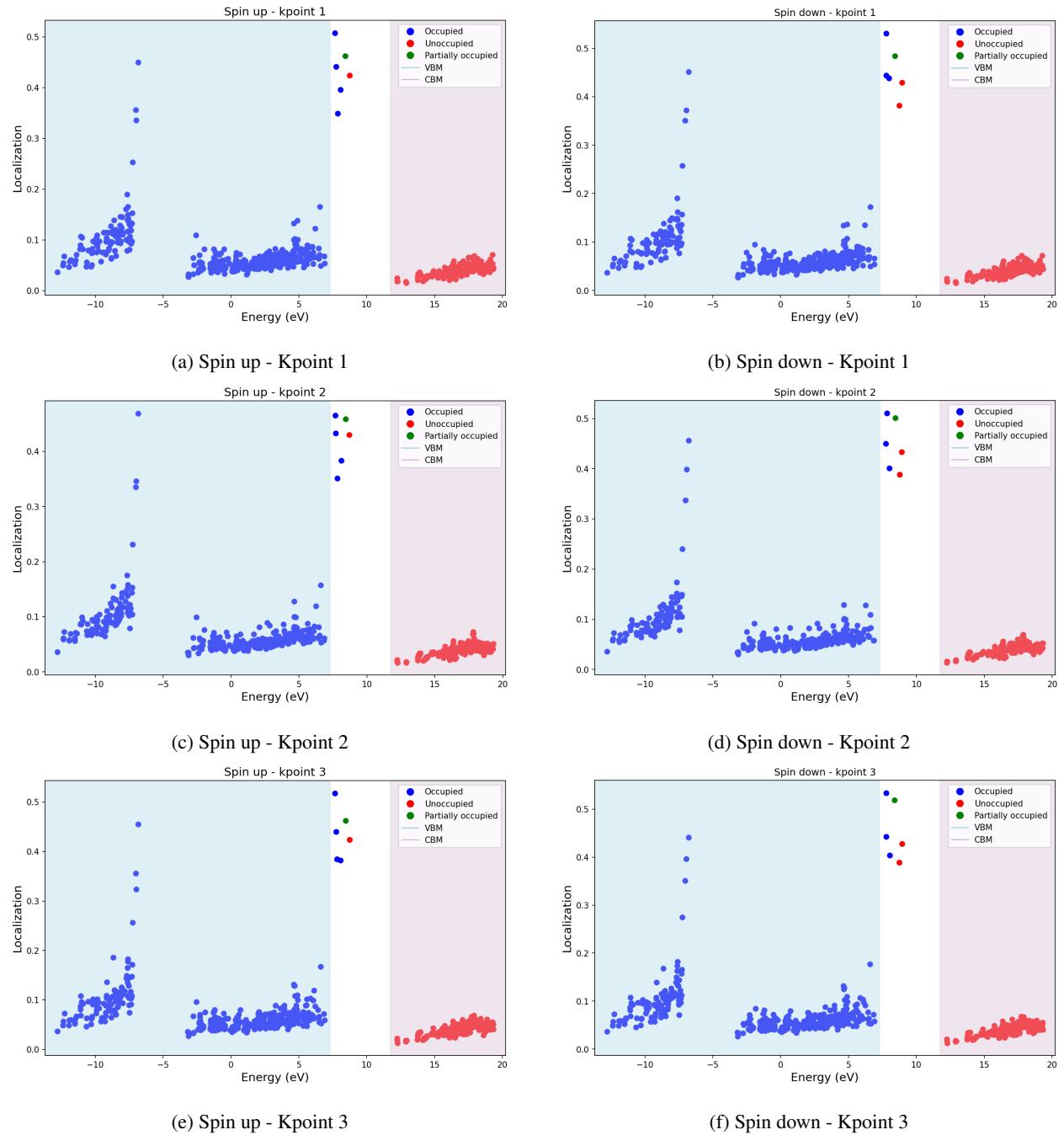


Figure 104: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

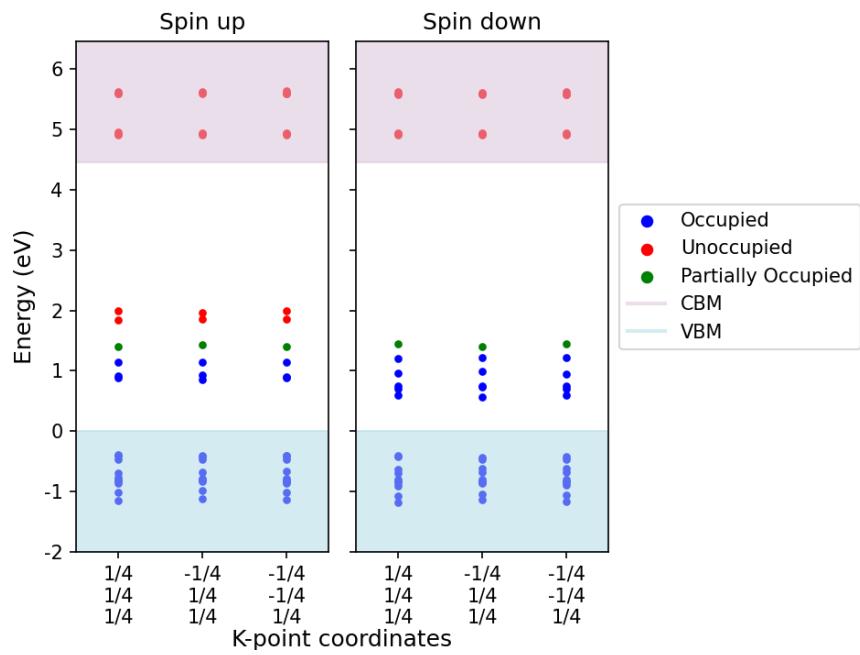


Figure 105: Kohn-Sham states.

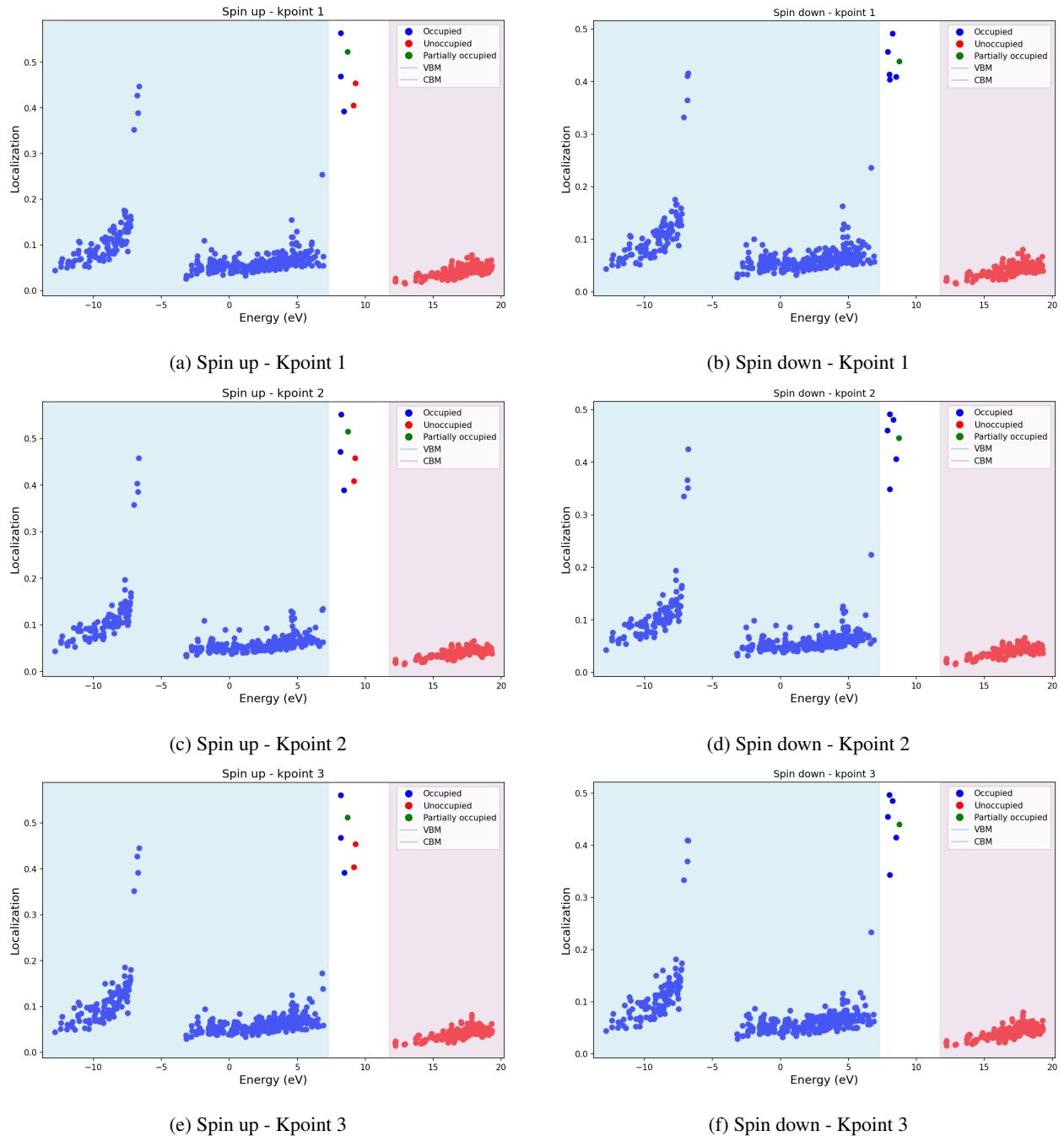


Figure 106: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

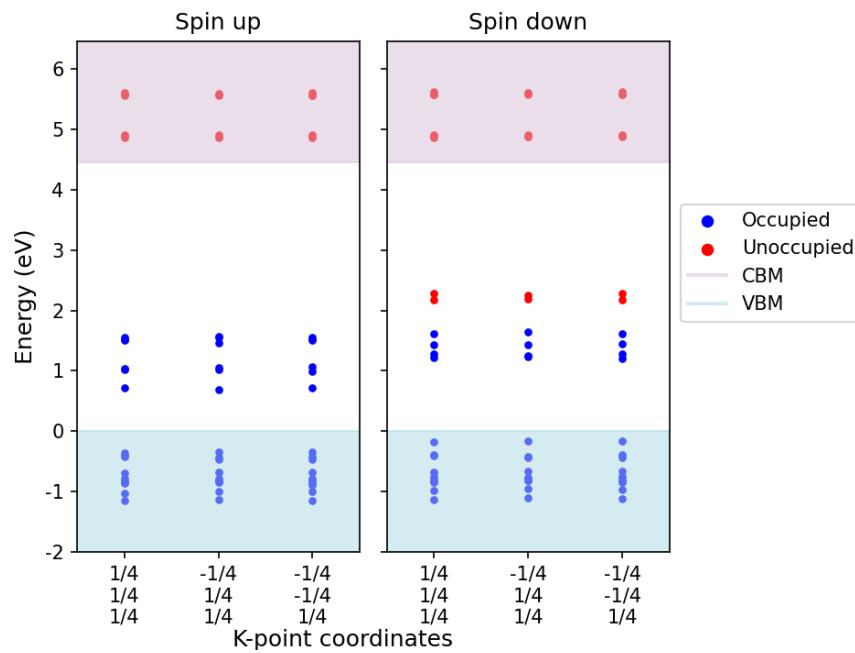


Figure 107: Kohn-Sham states.

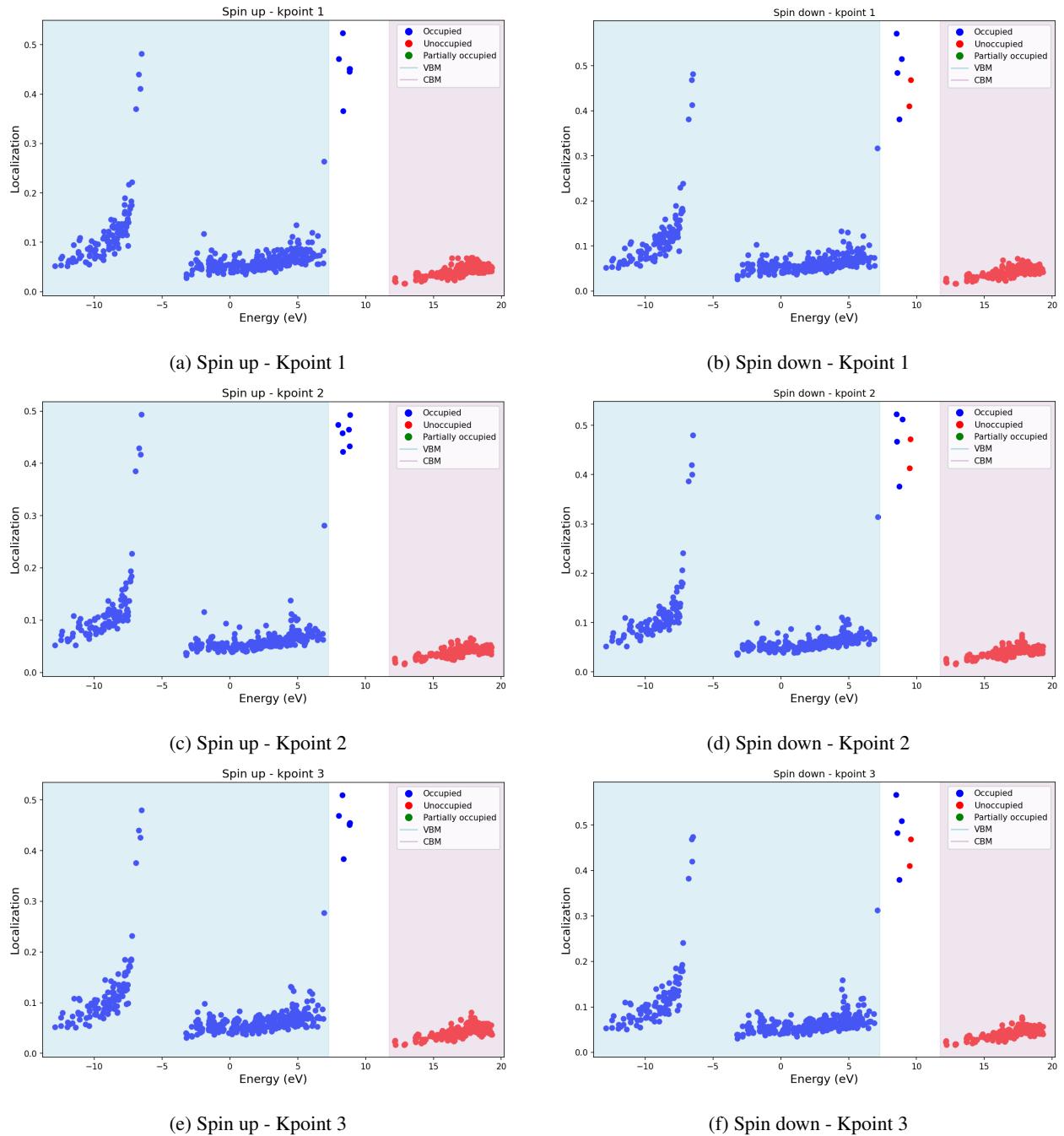


Figure 108: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

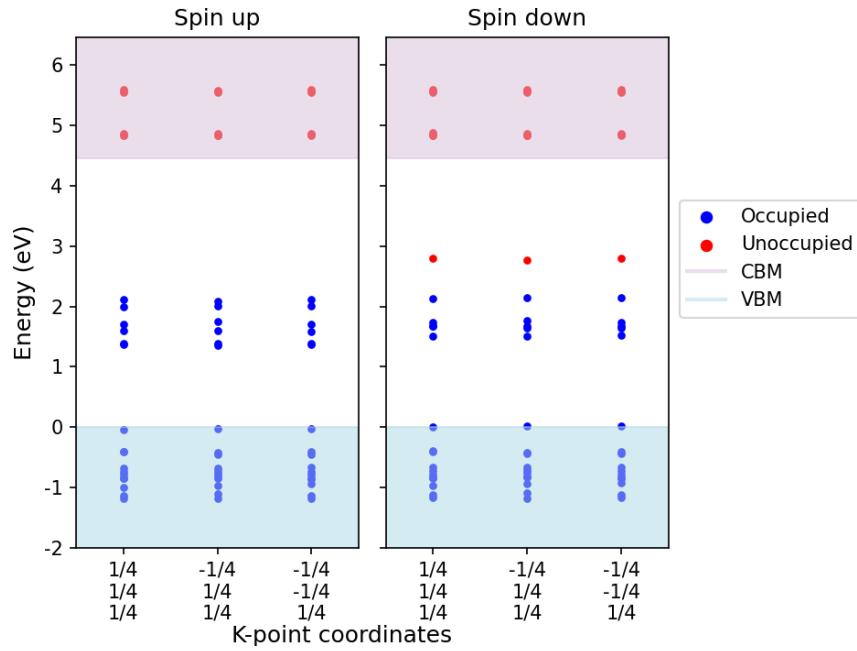


Figure 109: Kohn-Sham states.

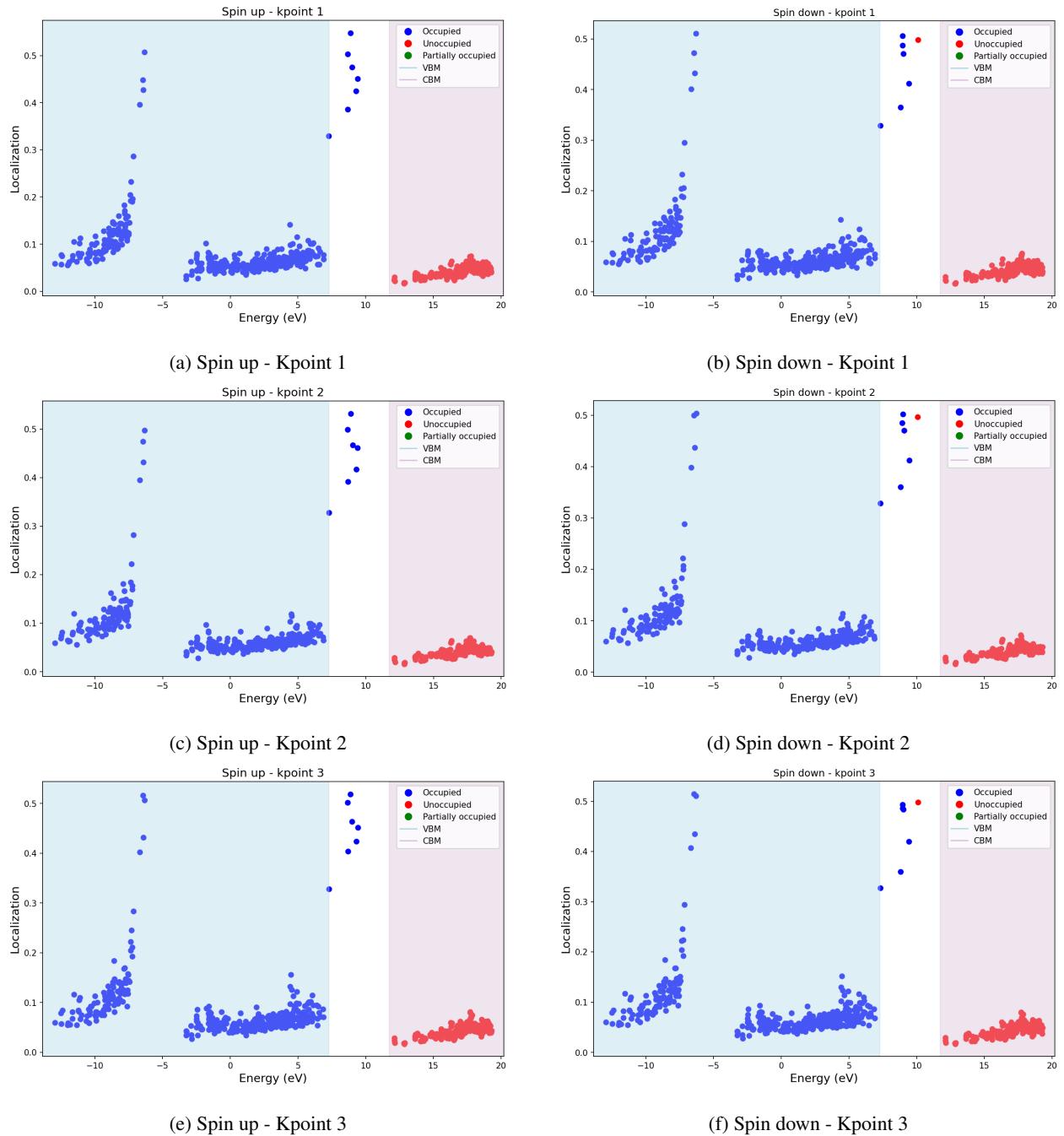


Figure 110: Localization factor using projected orbitals (s, p, and d).

## 1.56 Complex: $(N_B - V_N)^0$

[Go back to the Table 9](#)

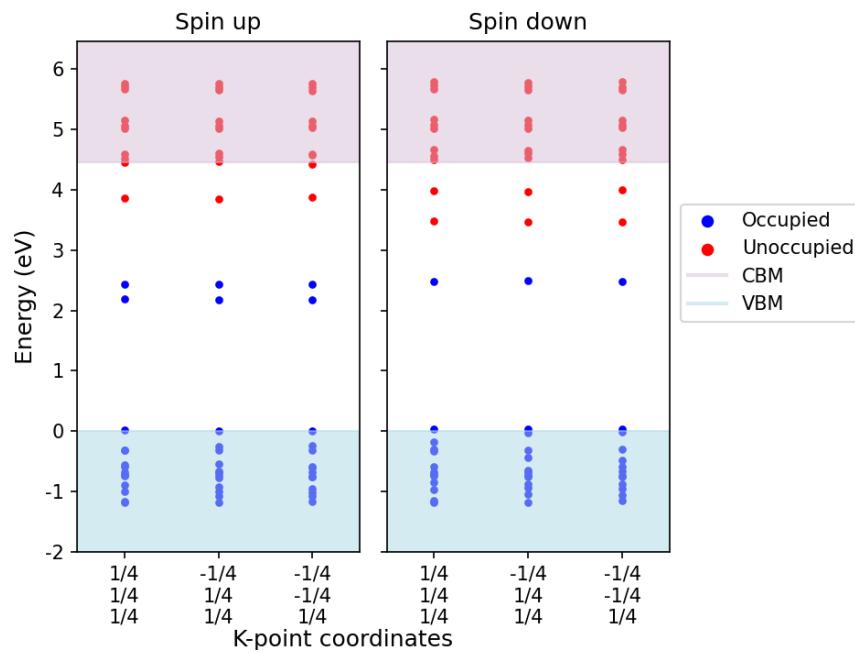


Figure 111: Kohn-Sham states.

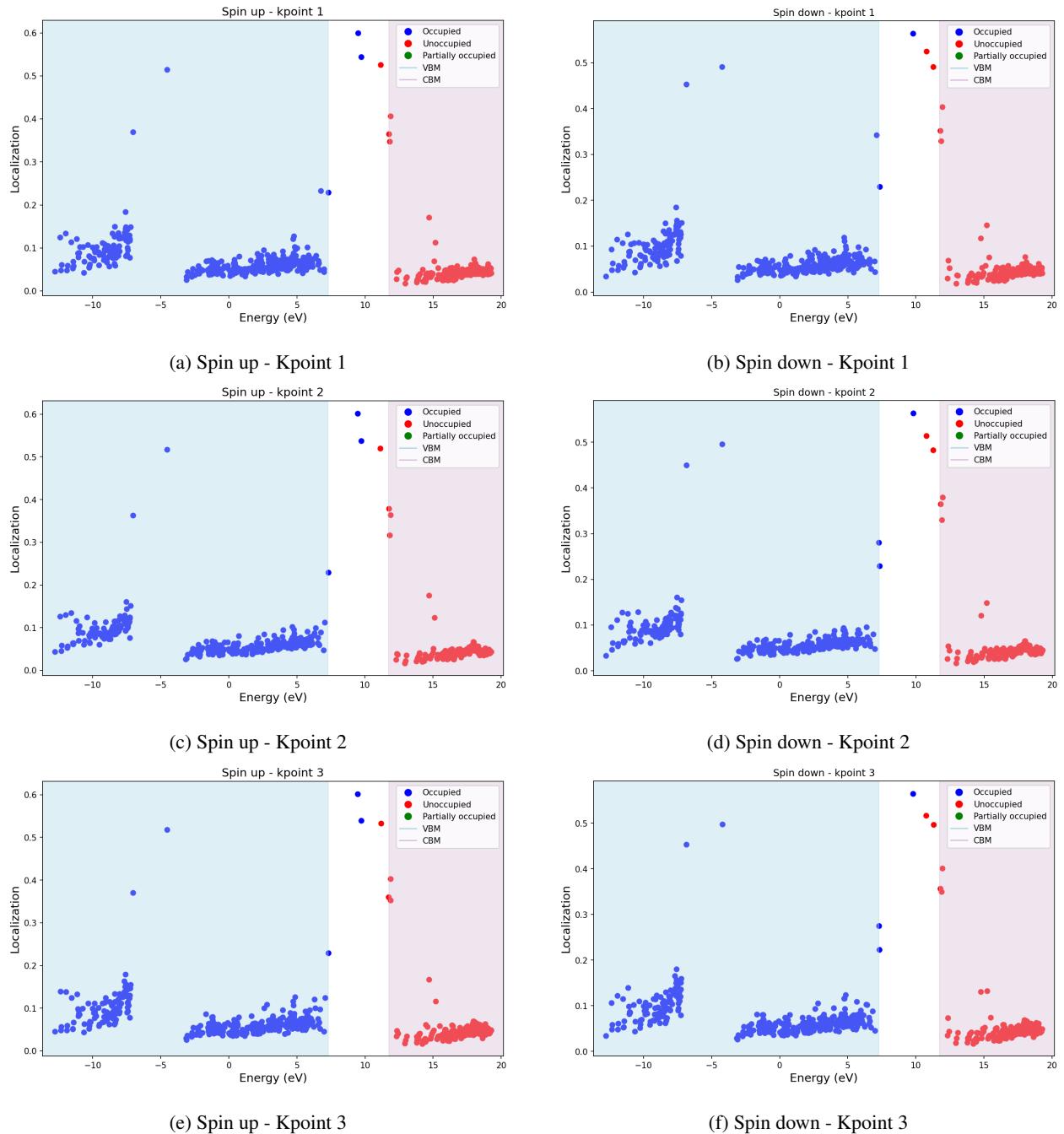


Figure 112: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

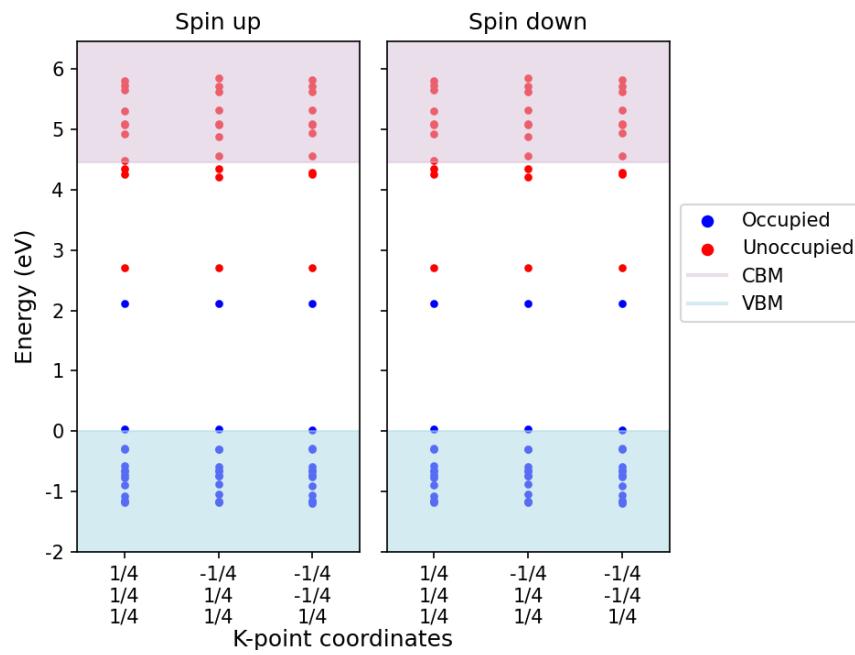


Figure 113: Kohn-Sham states.

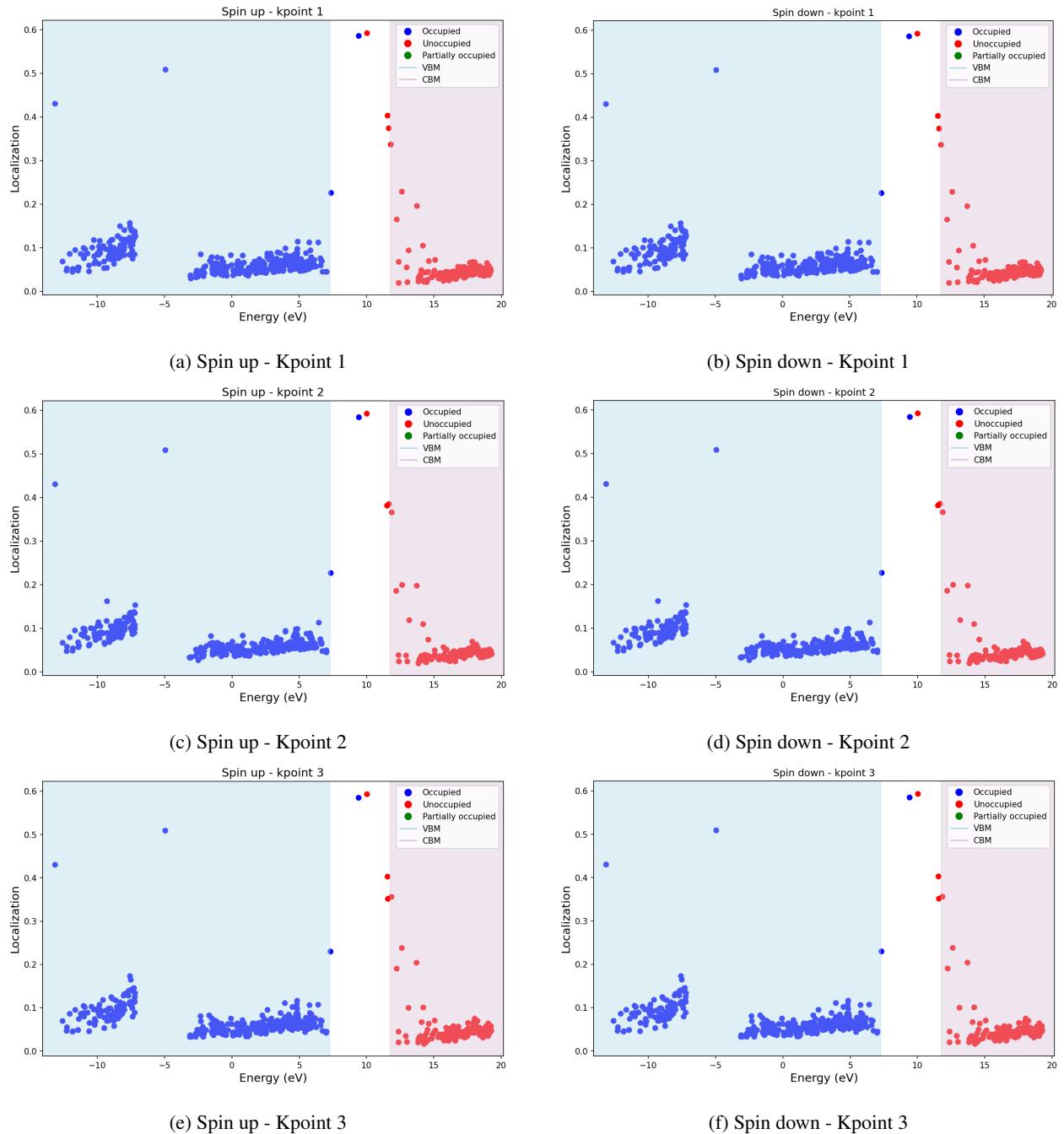


Figure 114: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

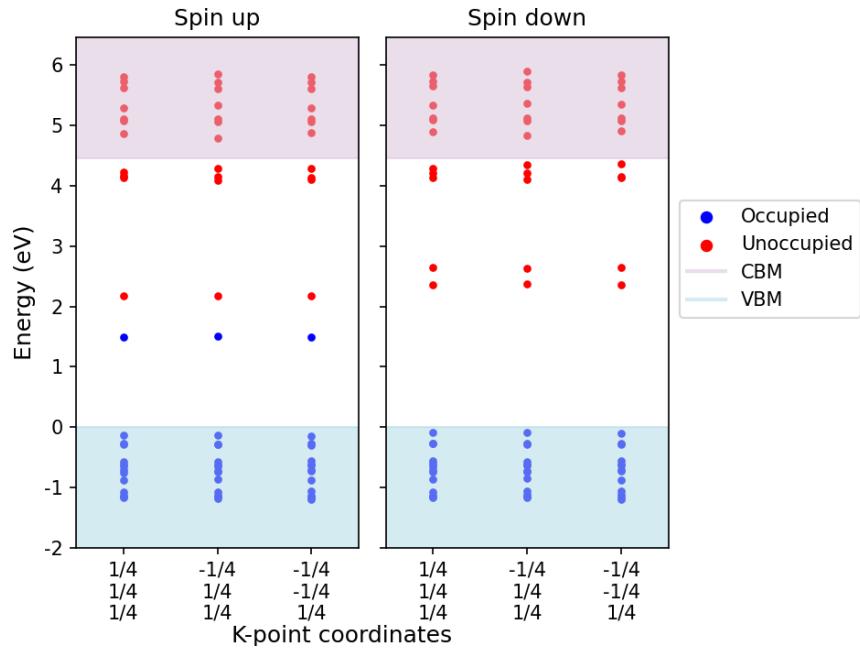


Figure 115: Kohn-Sham states.

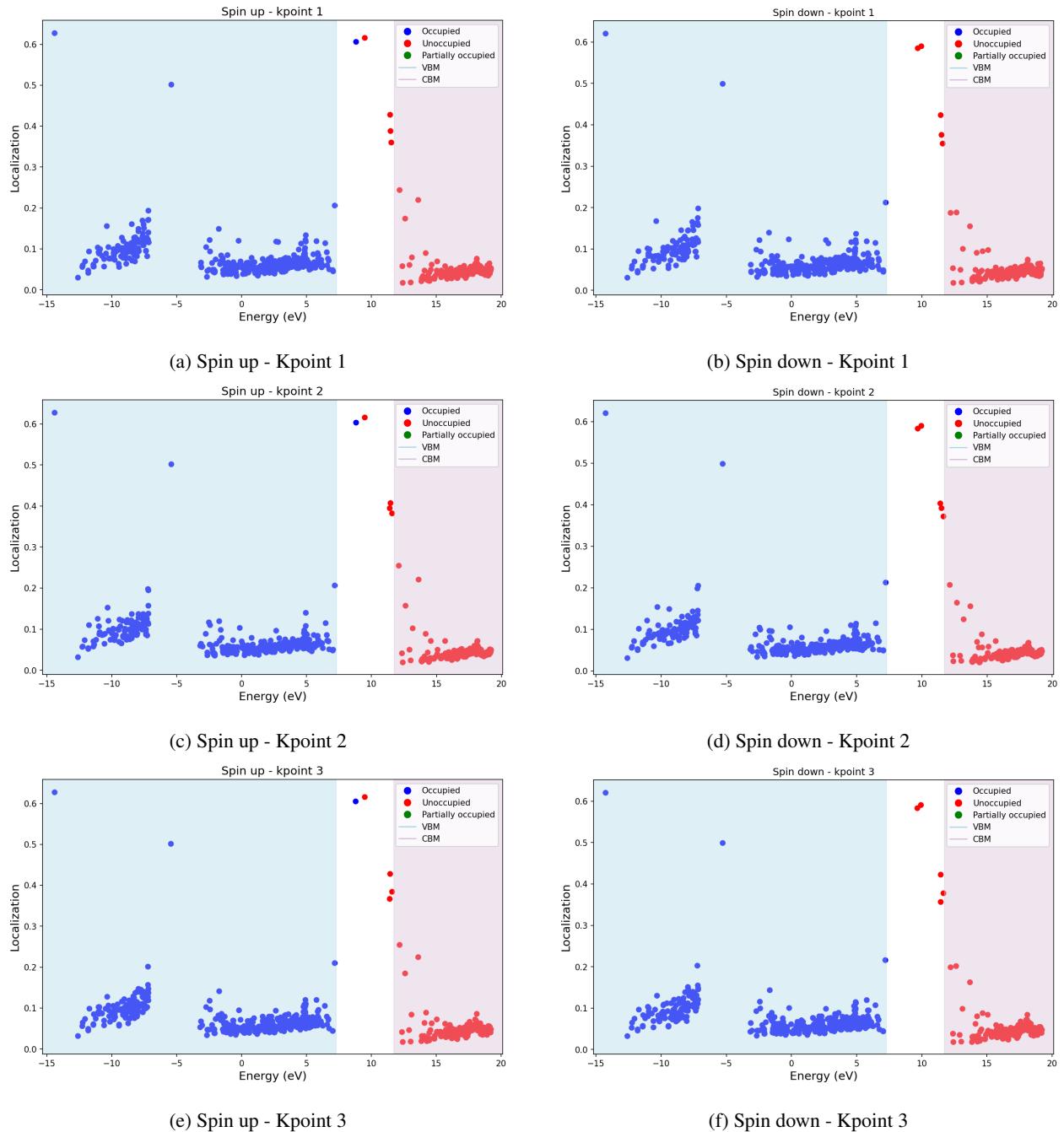


Figure 116: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

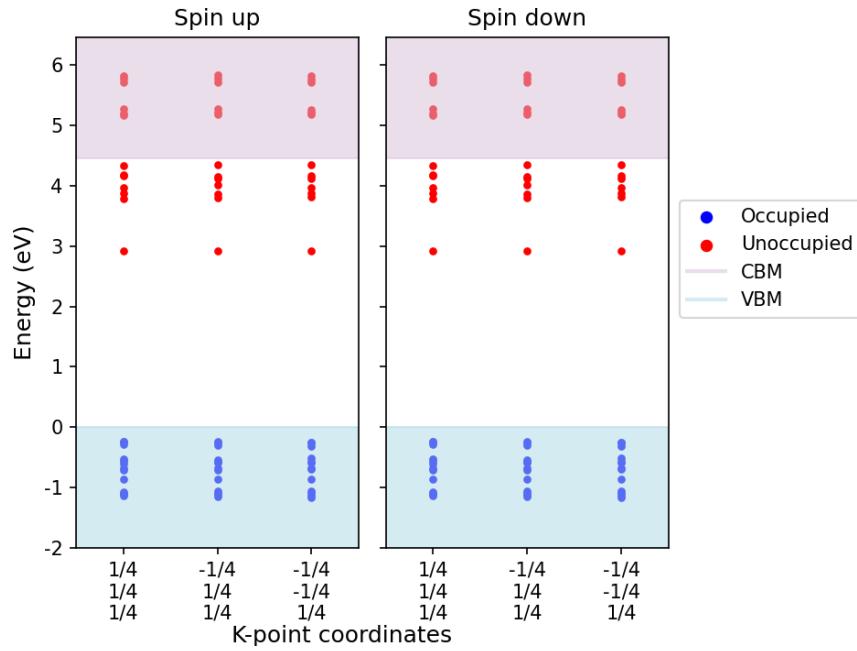


Figure 117: Kohn-Sham states.

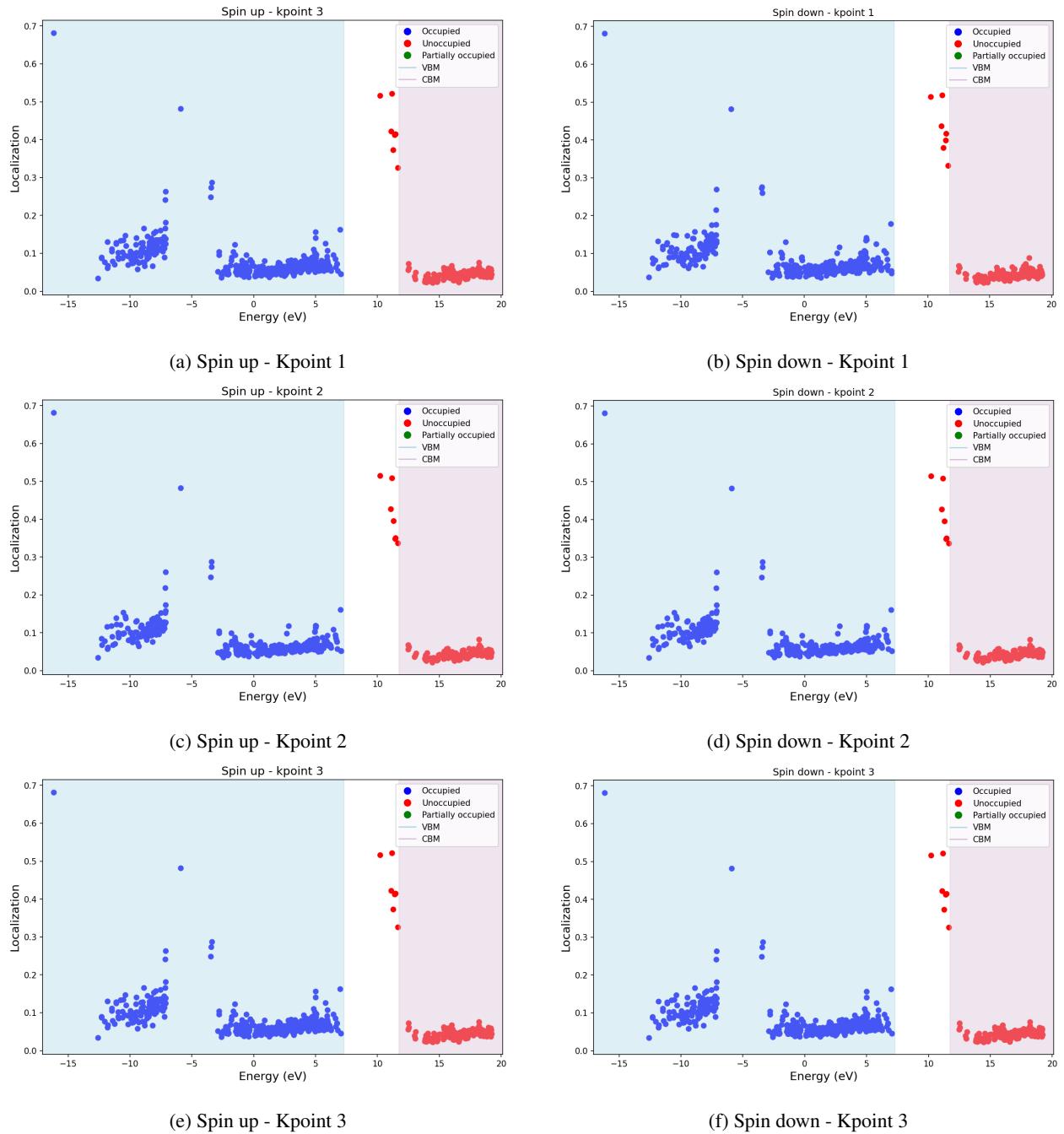


Figure 118: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

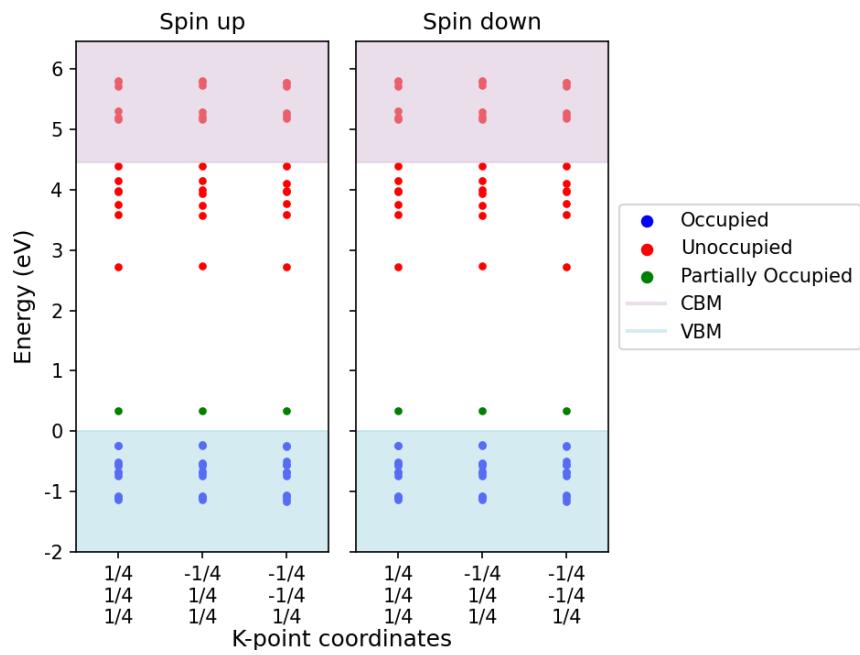


Figure 119: Kohn-Sham states.

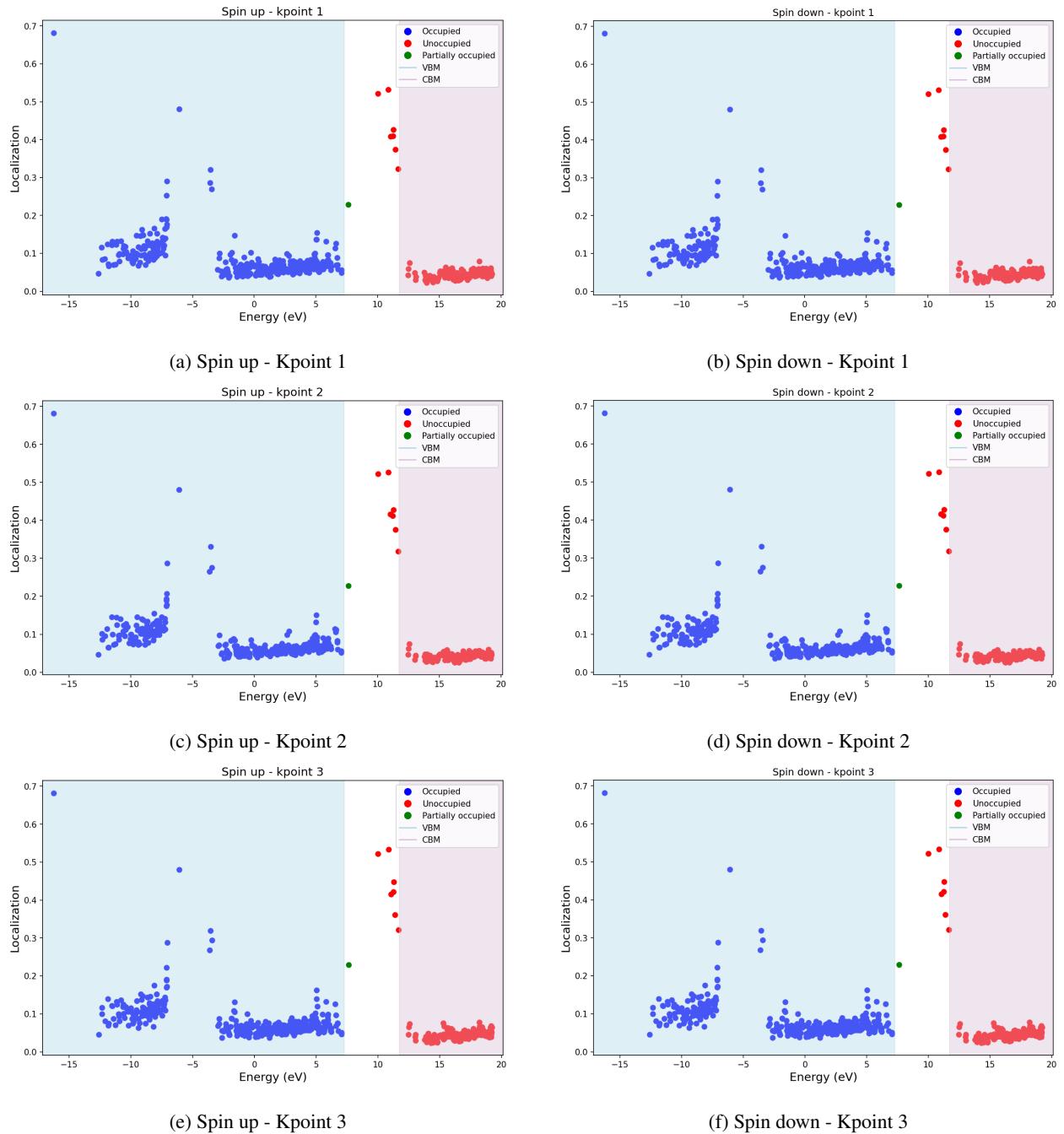


Figure 120: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

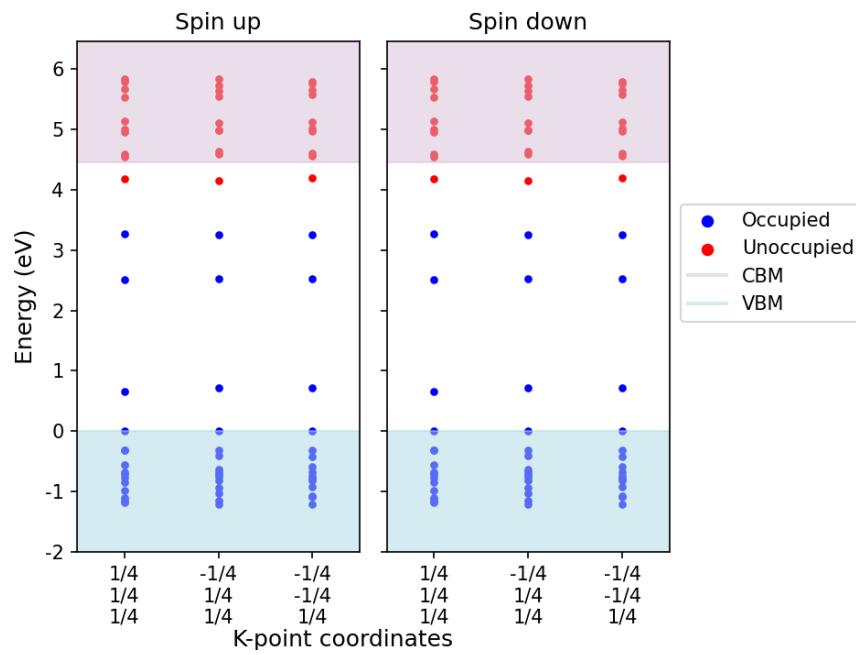


Figure 121: Kohn-Sham states.

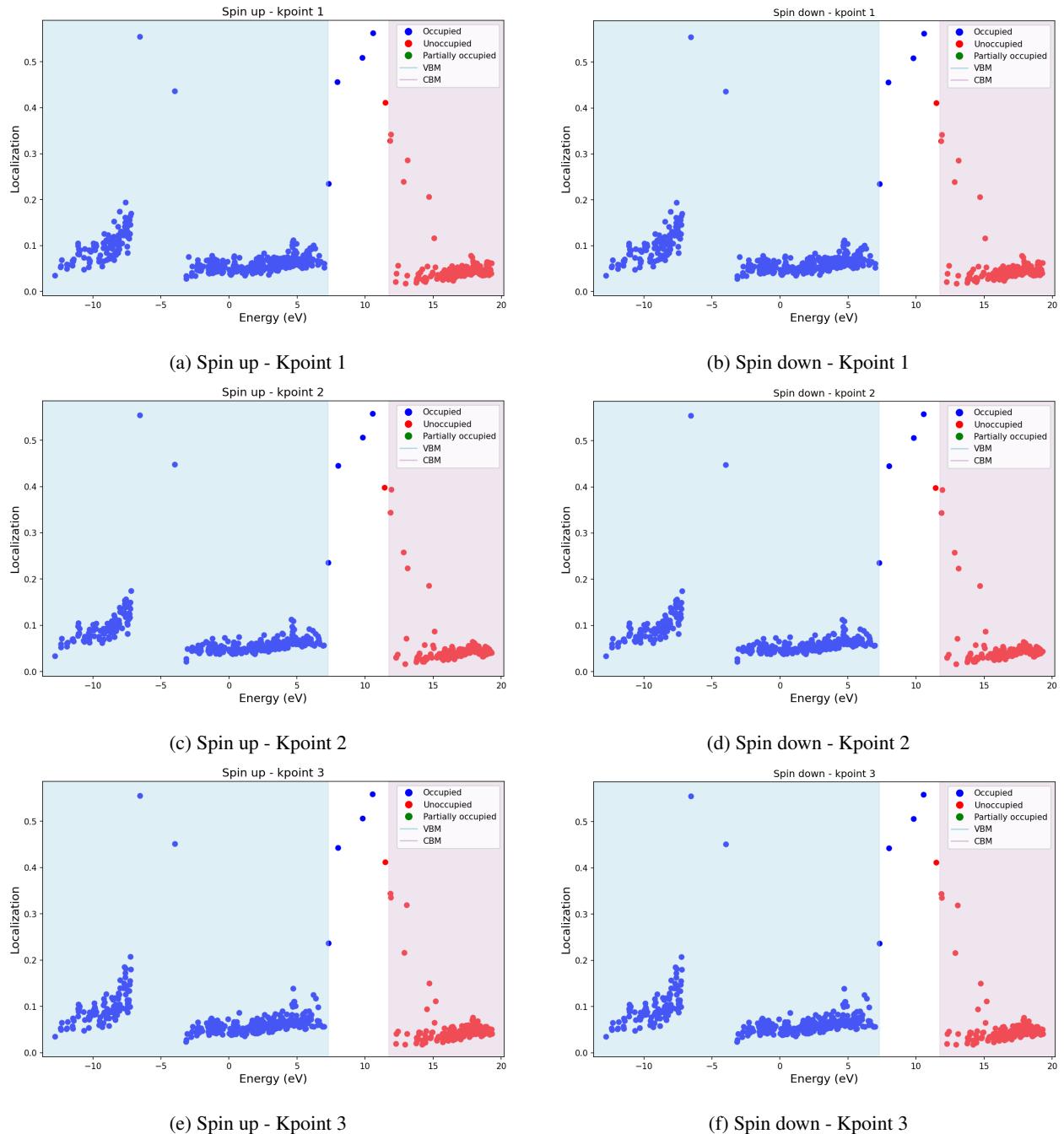


Figure 122: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

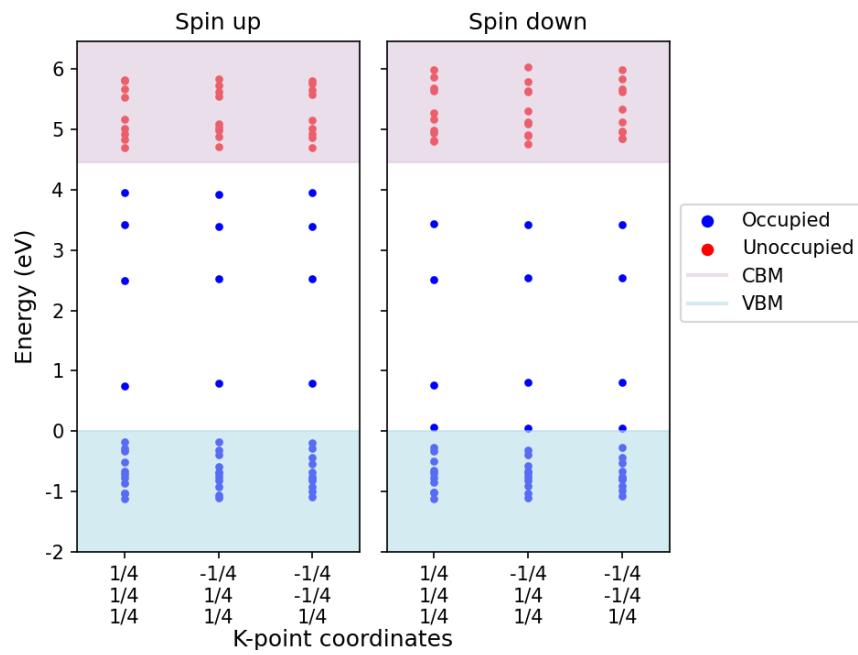


Figure 123: Kohn-Sham states.

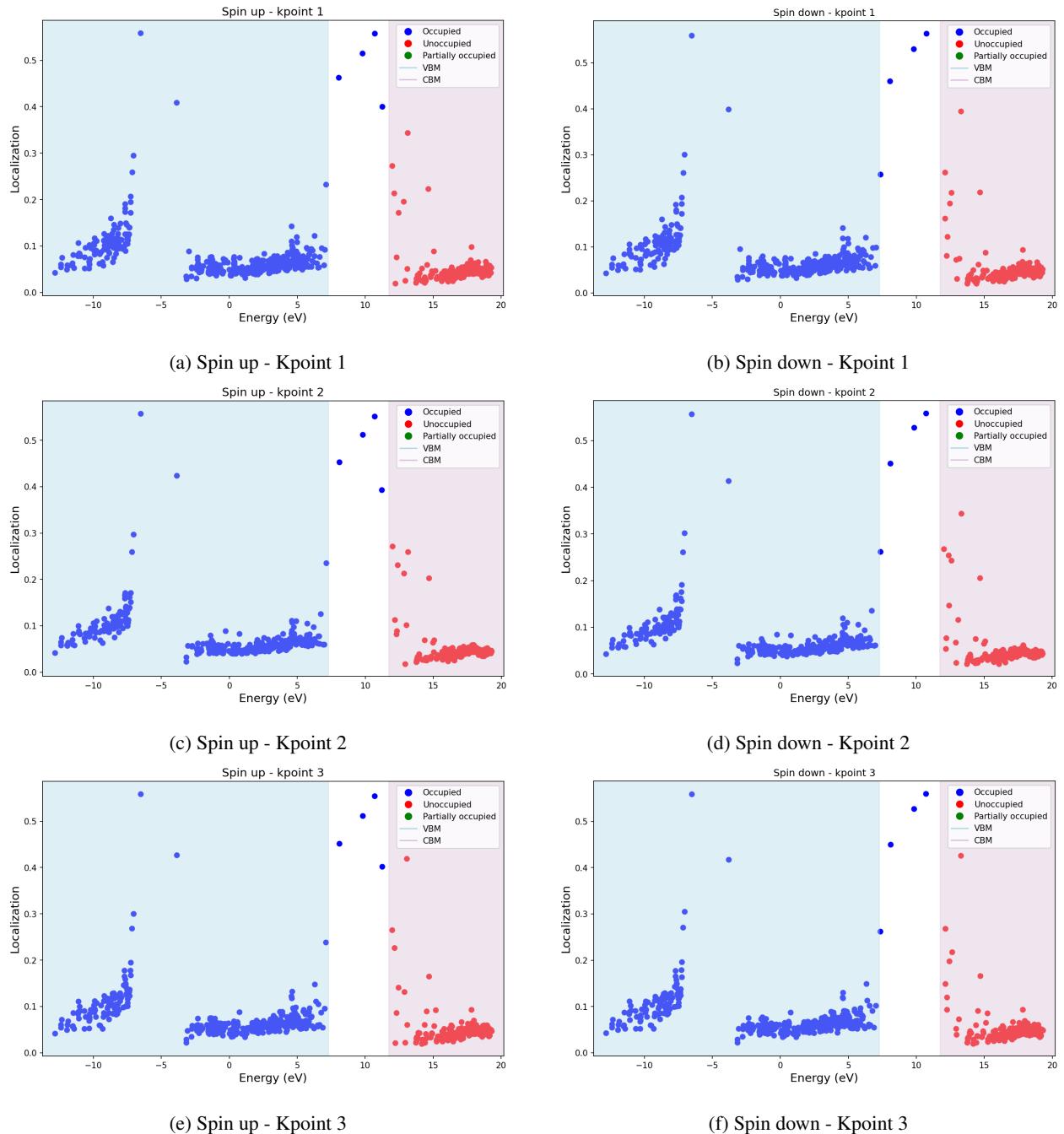


Figure 124: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

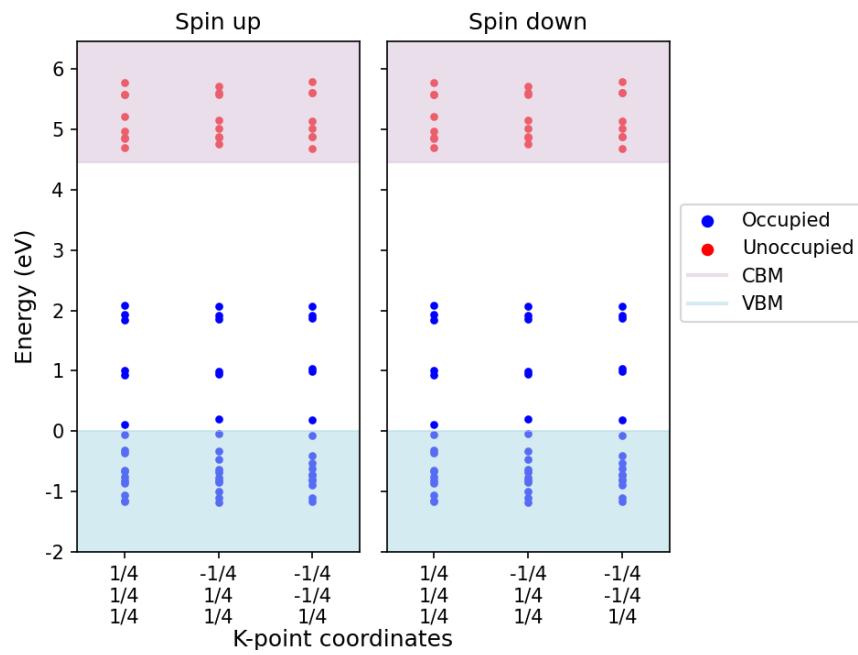


Figure 125: Kohn-Sham states.

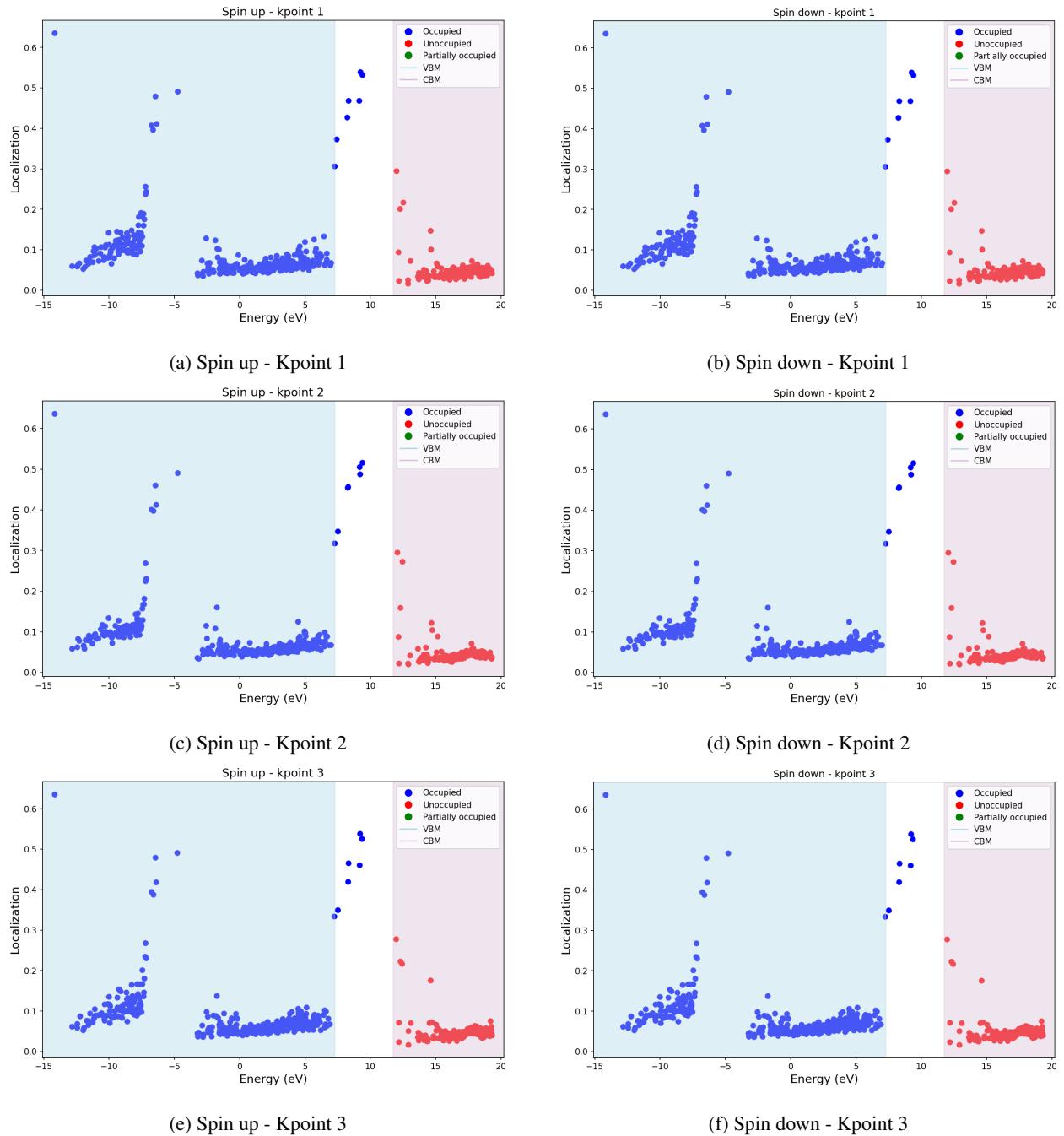


Figure 126: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

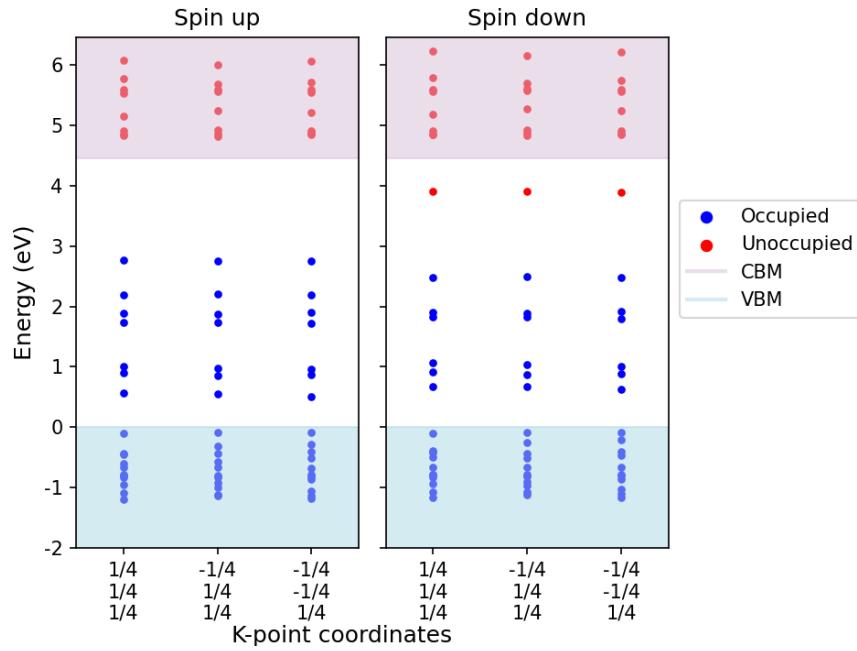


Figure 127: Kohn-Sham states.

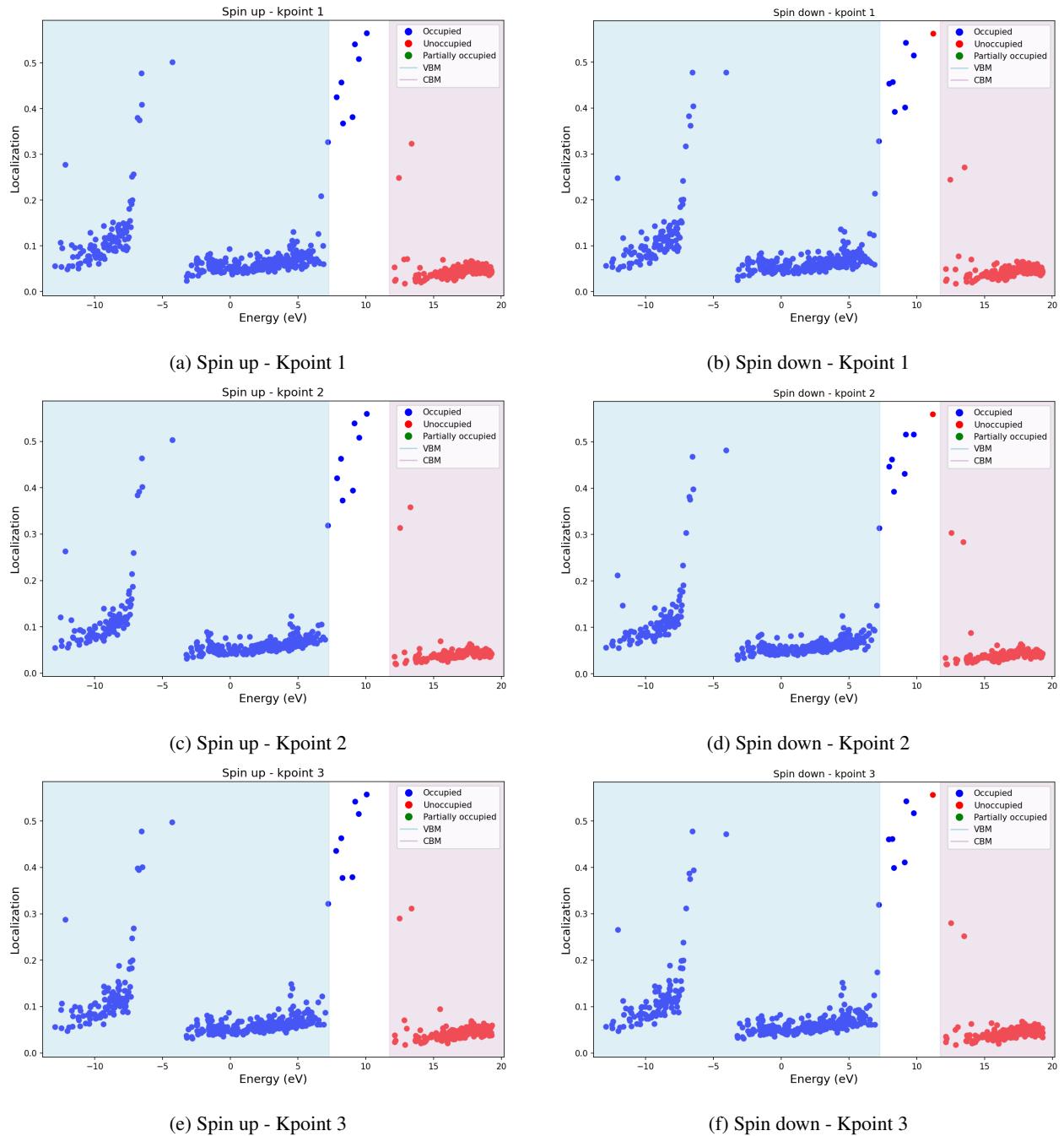


Figure 128: Localization factor using projected orbitals (s, p, and d).

## 1.65 Complex: $(V_B - V_N)^0$

[Go back to the Table 9](#)

Table 47:  $(V_B - V_N)^0$ 

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

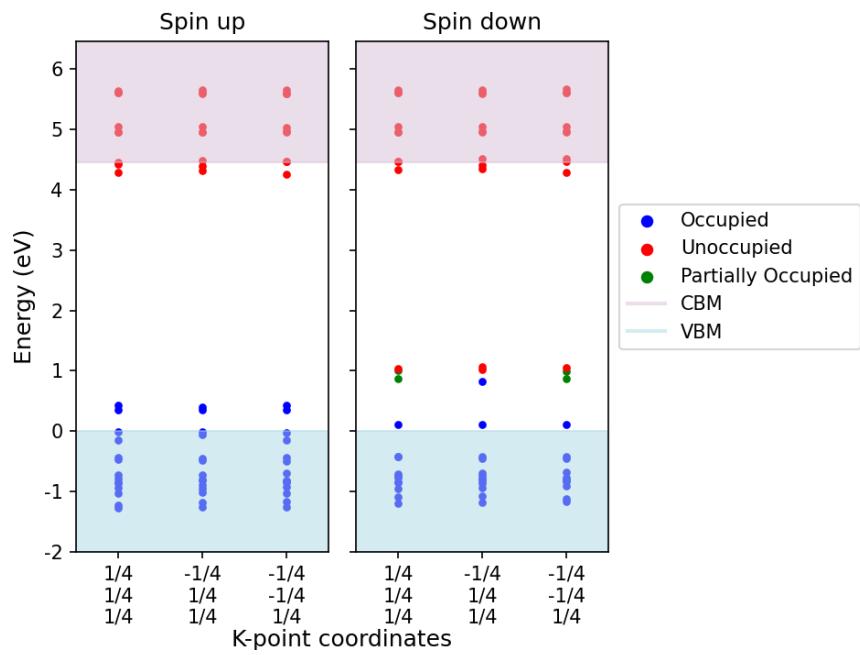


Figure 129: Kohn-Sham states.

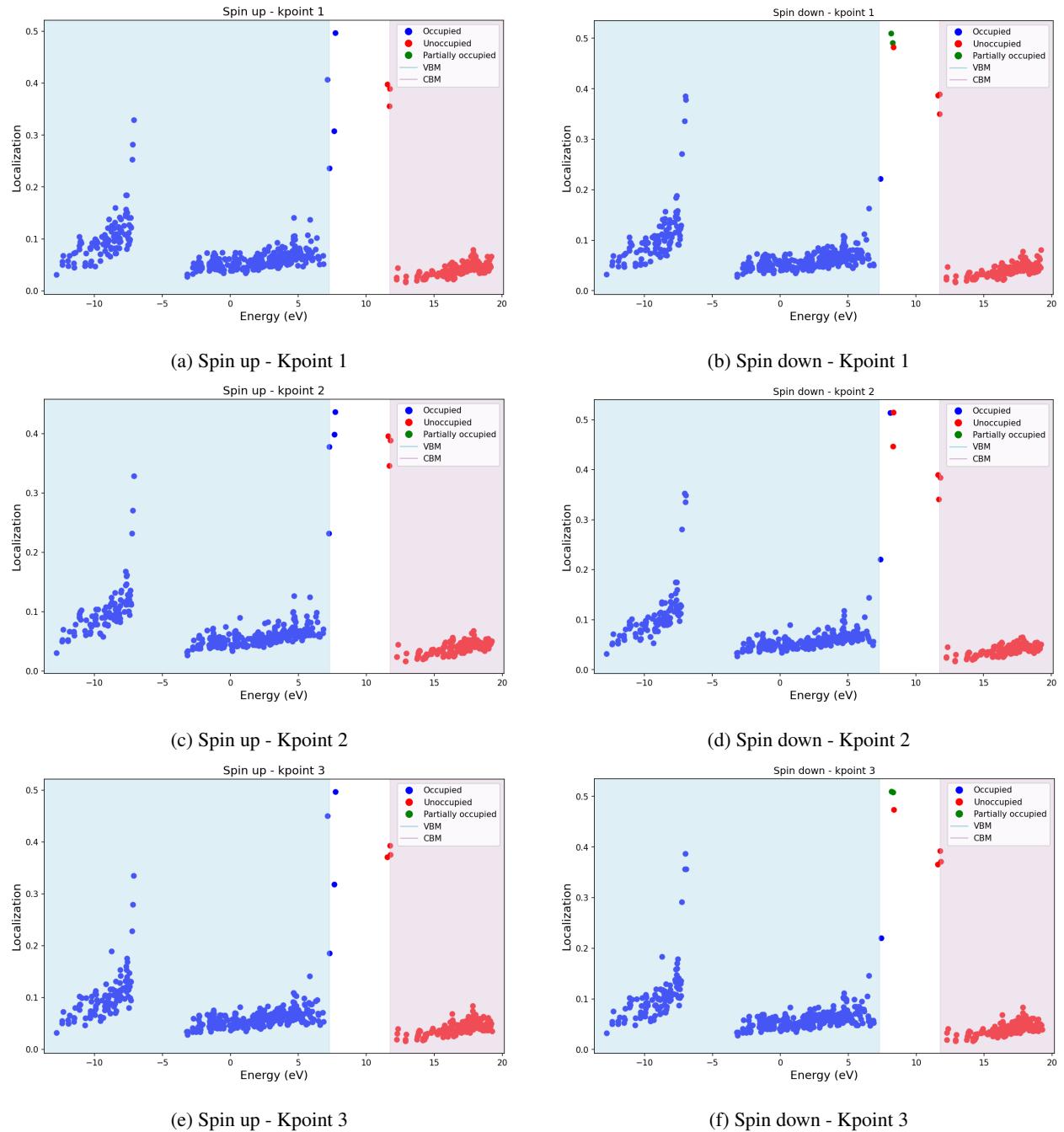


Figure 130: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

Table 48:  $(V_B - V_N)^{+1}$ 

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

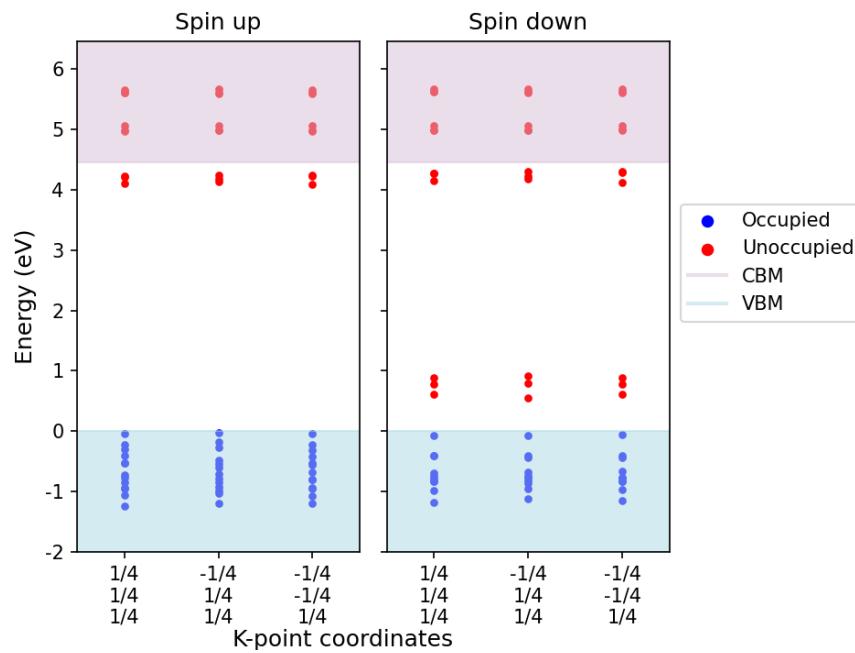


Figure 131: Kohn-Sham states.

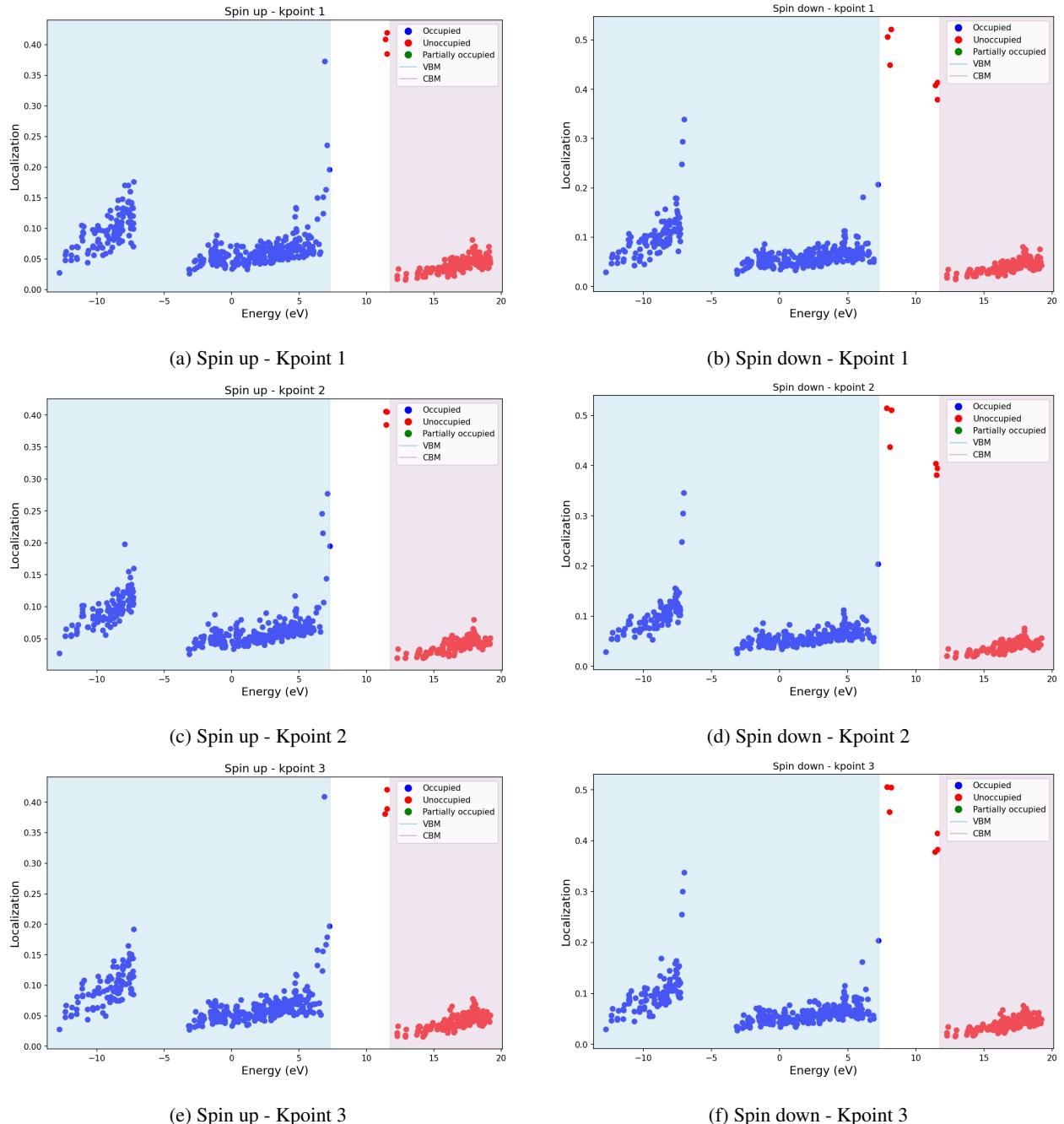


Figure 132: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

Table 49:  $(V_B - V_N)^{+2}$ 

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	$\bar{1}30$	< 0.1	–
	3	430	26, 41	0.212, 0.108	Y, Y
	3	431	41	0.137	Y

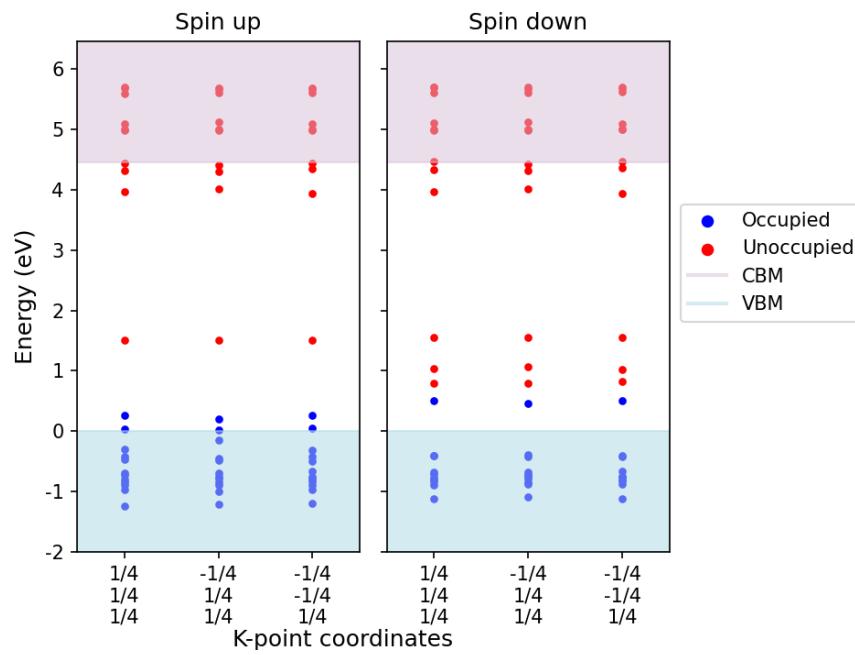


Figure 133: Kohn-Sham states.

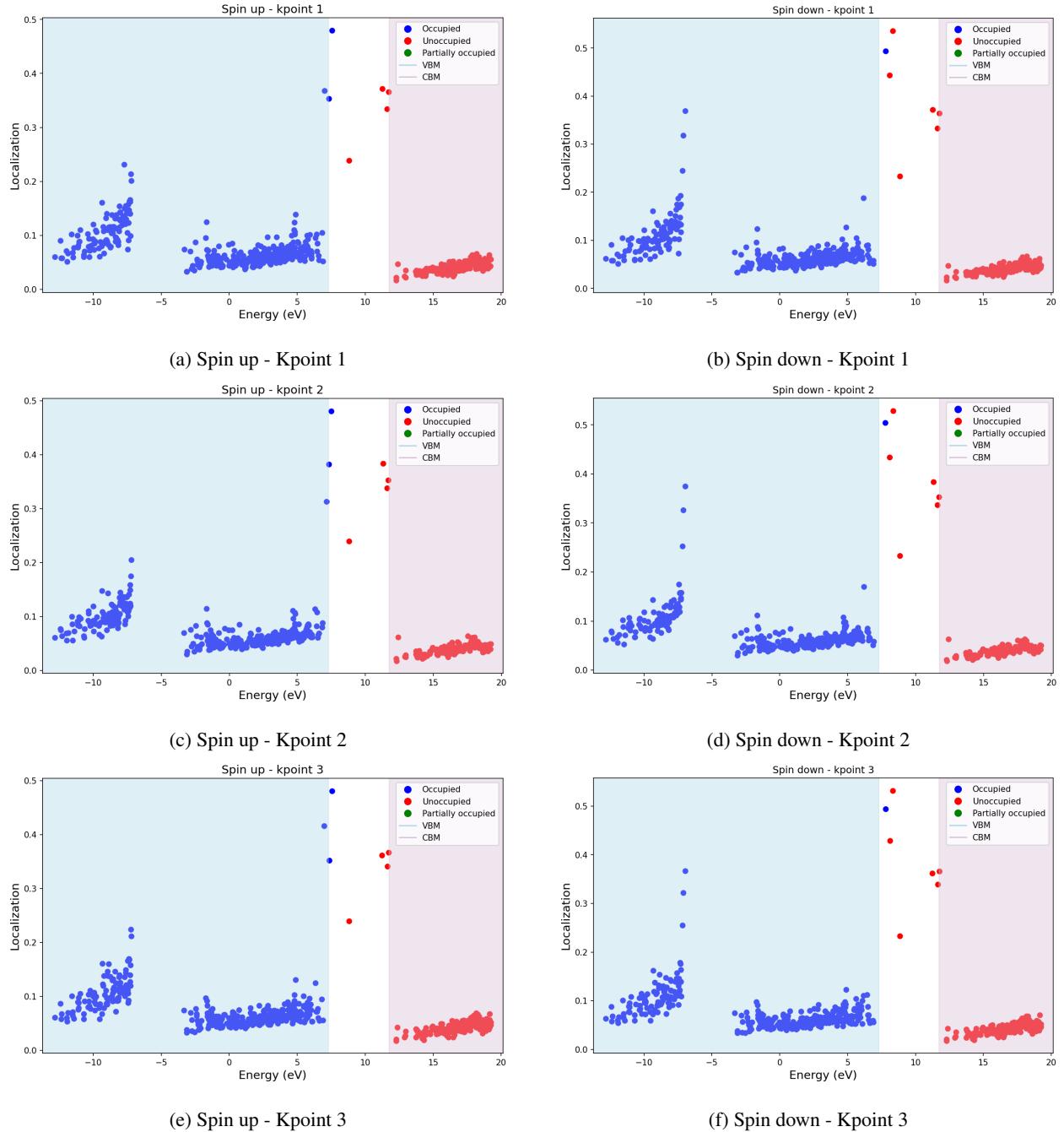


Figure 134: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

Table 50:  $(V_B - V_N)^{+3}$ 

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

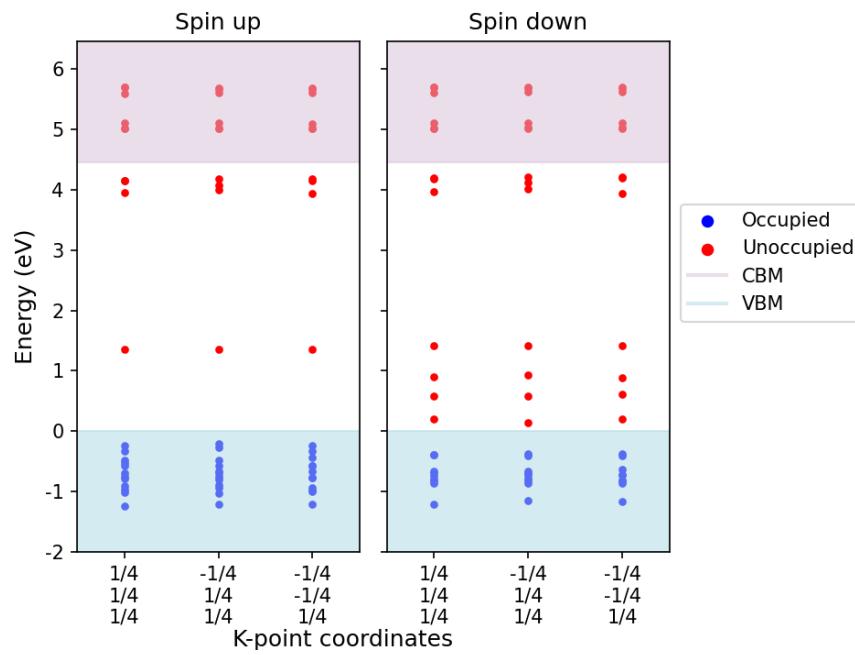


Figure 135: Kohn-Sham states.

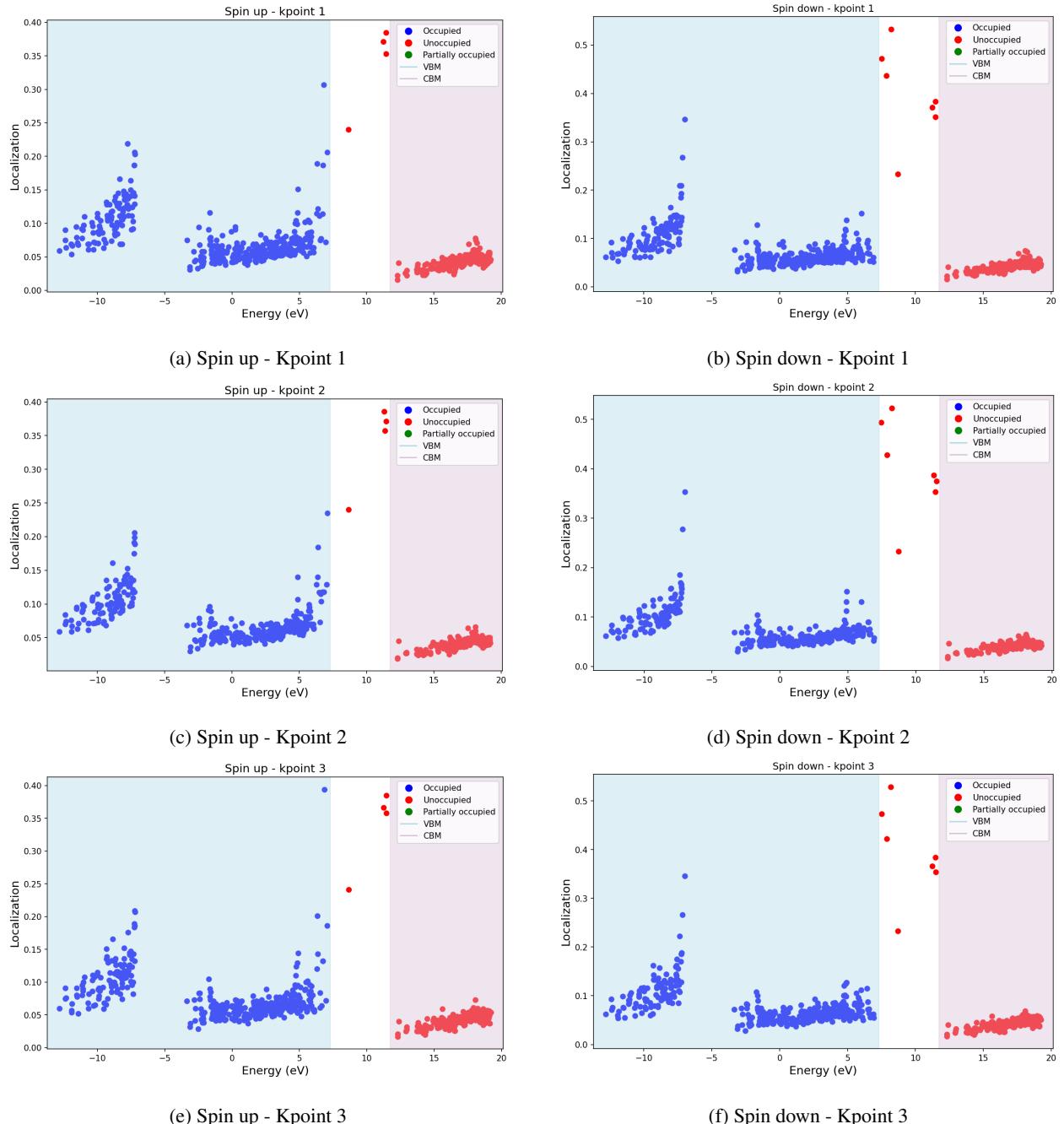


Figure 136: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

Table 51:  $(V_B - V_N)^{+4}$ 

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

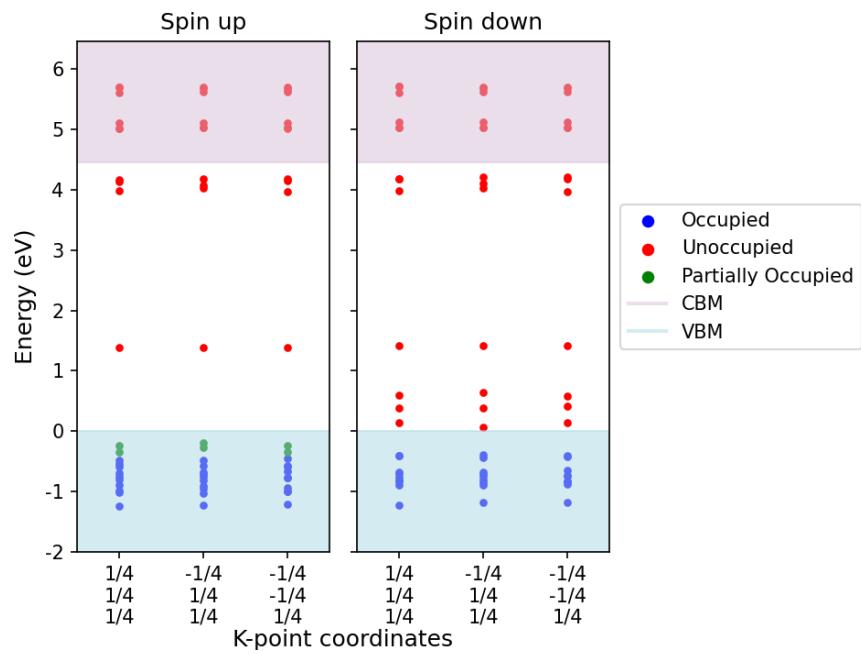


Figure 137: Kohn-Sham states.

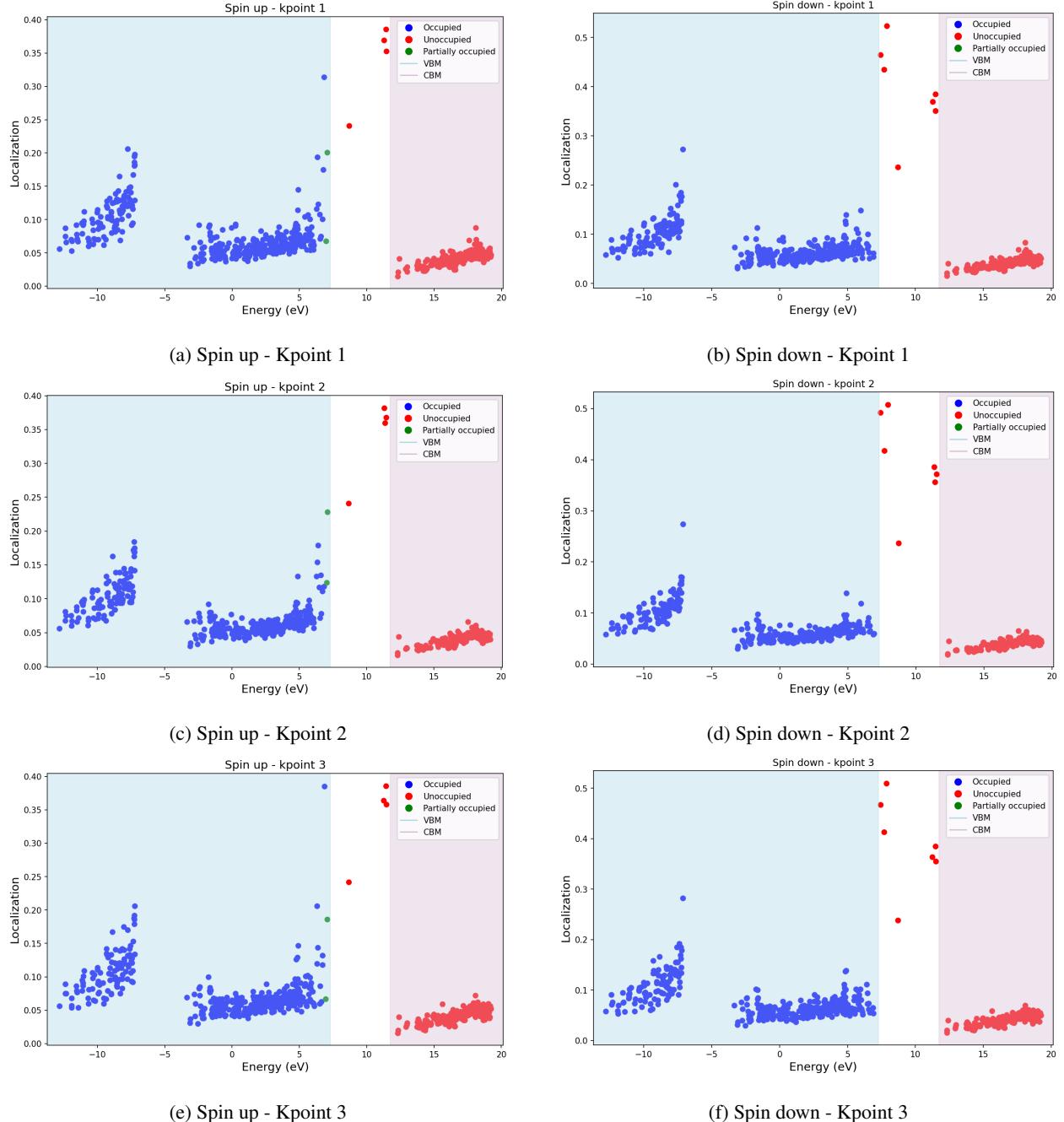


Figure 138: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

Table 52:  $(V_B - V_N)^{-1}$ 

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	–

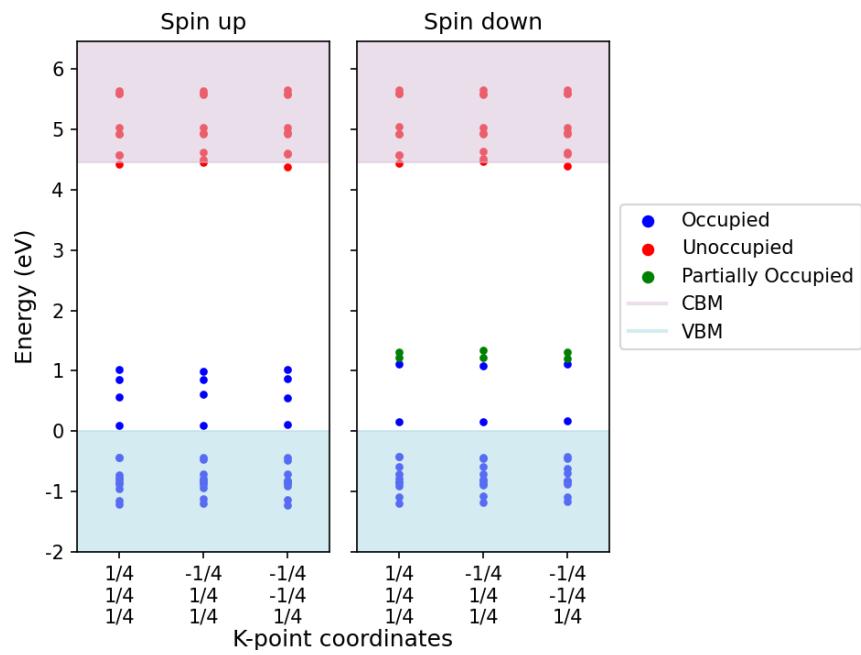


Figure 139: Kohn-Sham states.

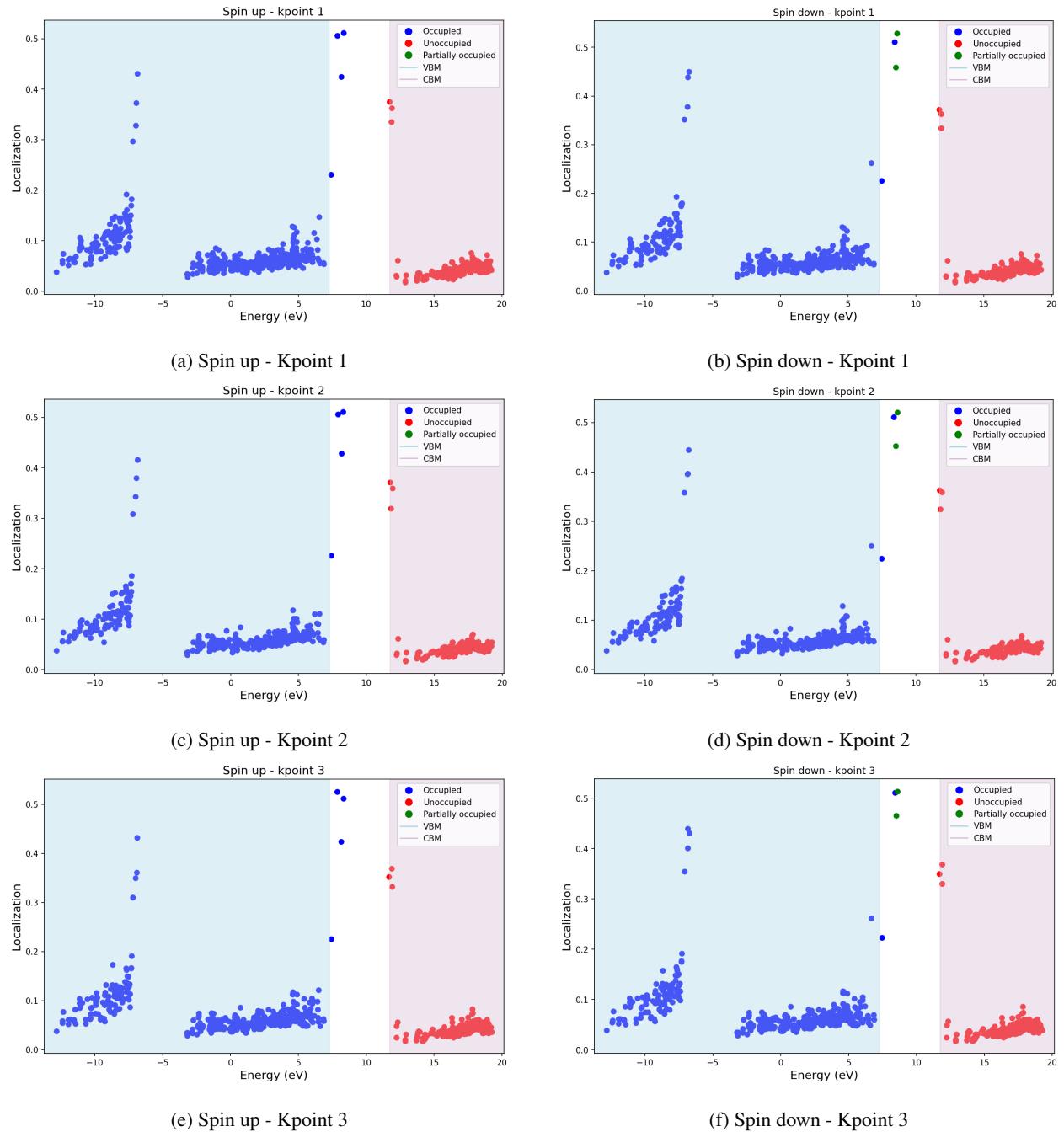


Figure 140: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

Table 53:  $(V_B - V_N)^{-2}$ 

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

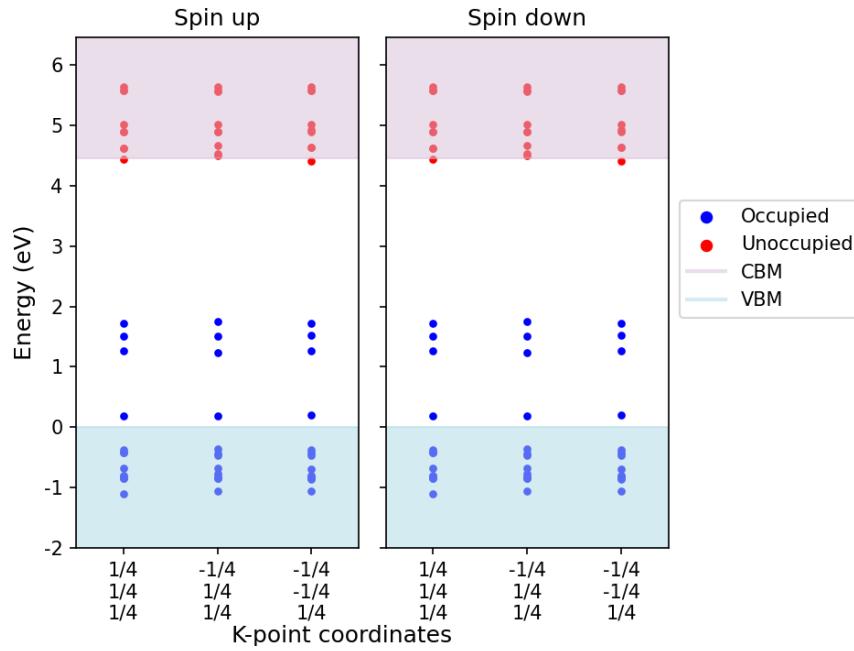


Figure 141: Kohn-Sham states.

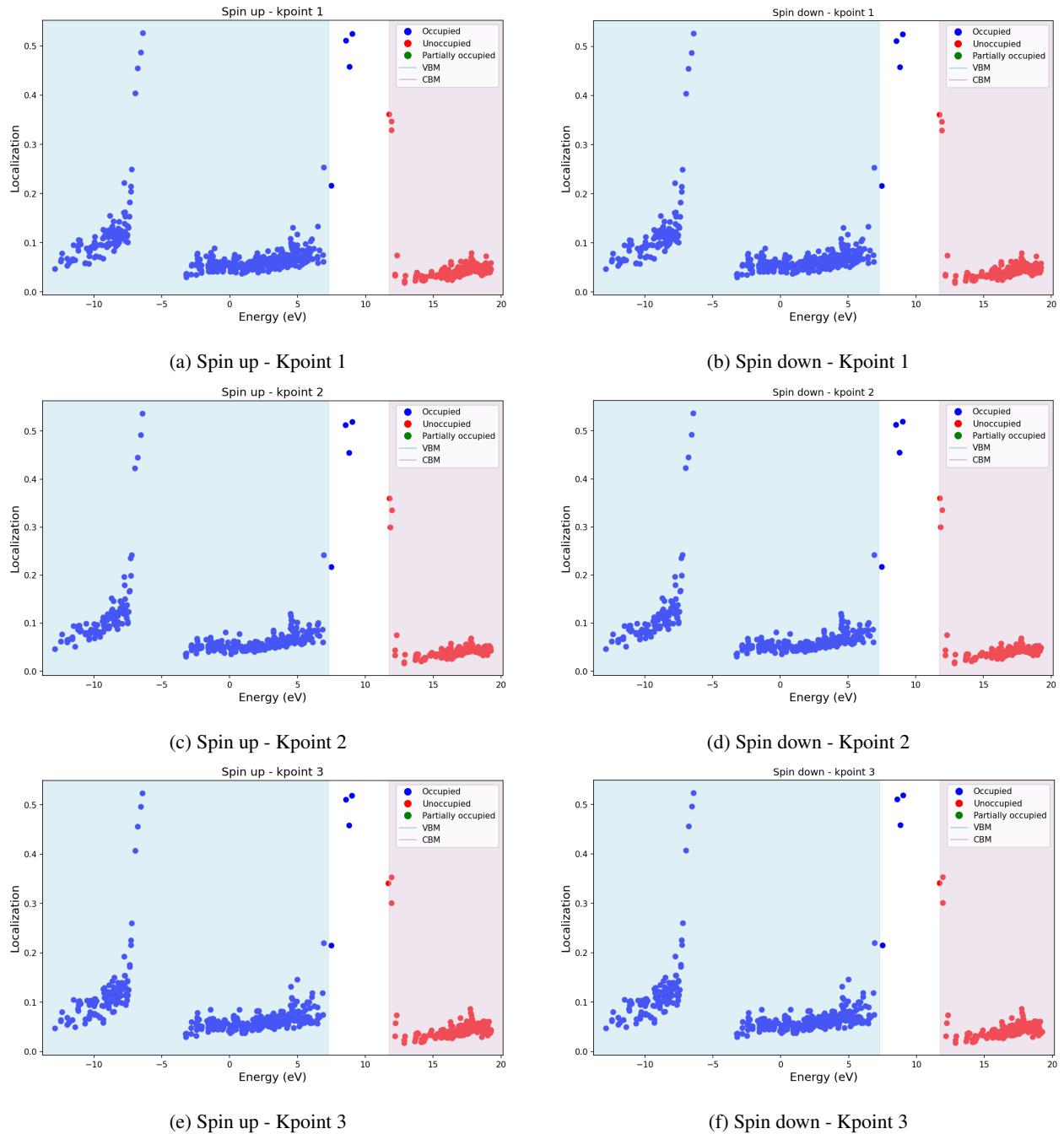


Figure 142: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

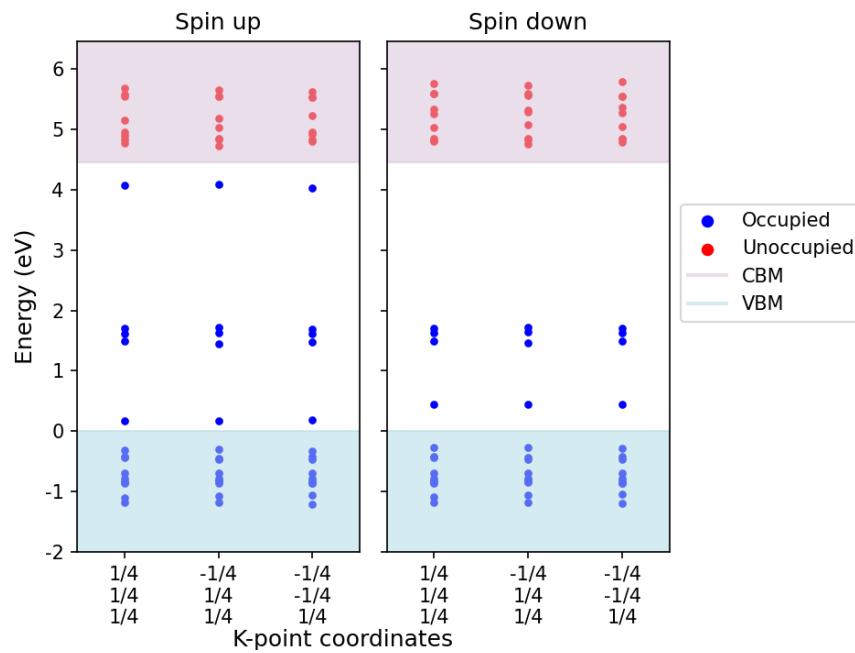


Figure 143: Kohn-Sham states.

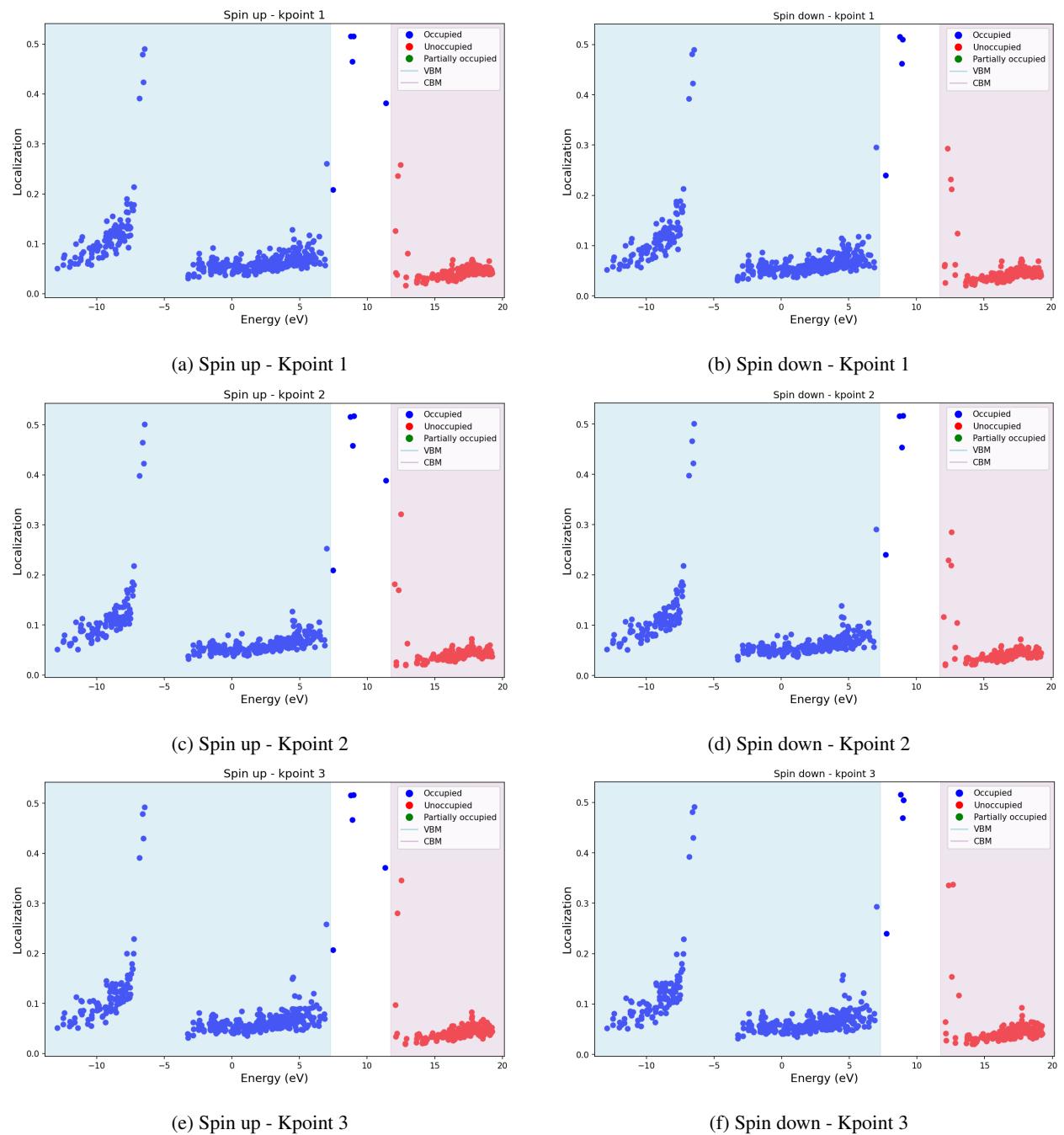


Figure 144: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

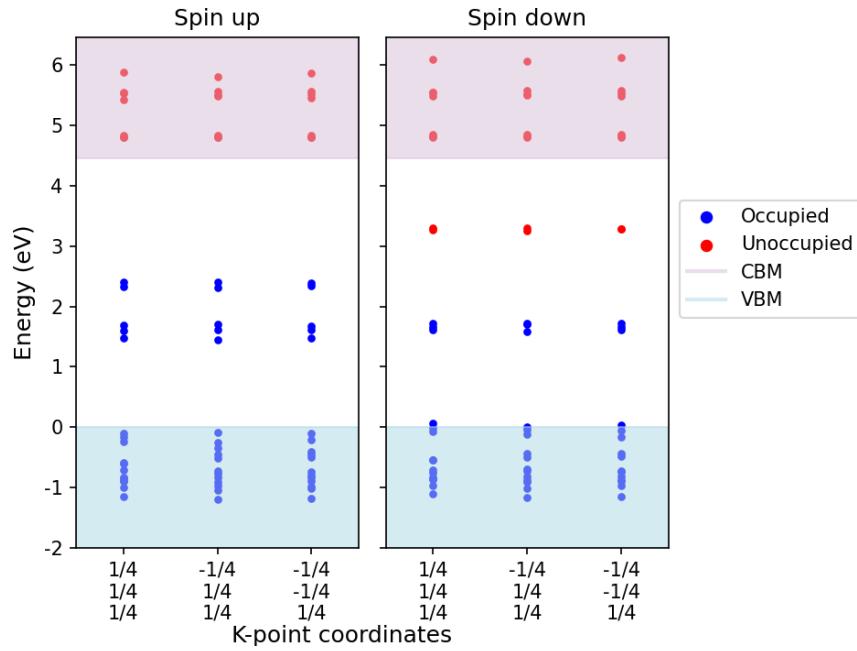


Figure 145: Kohn-Sham states.

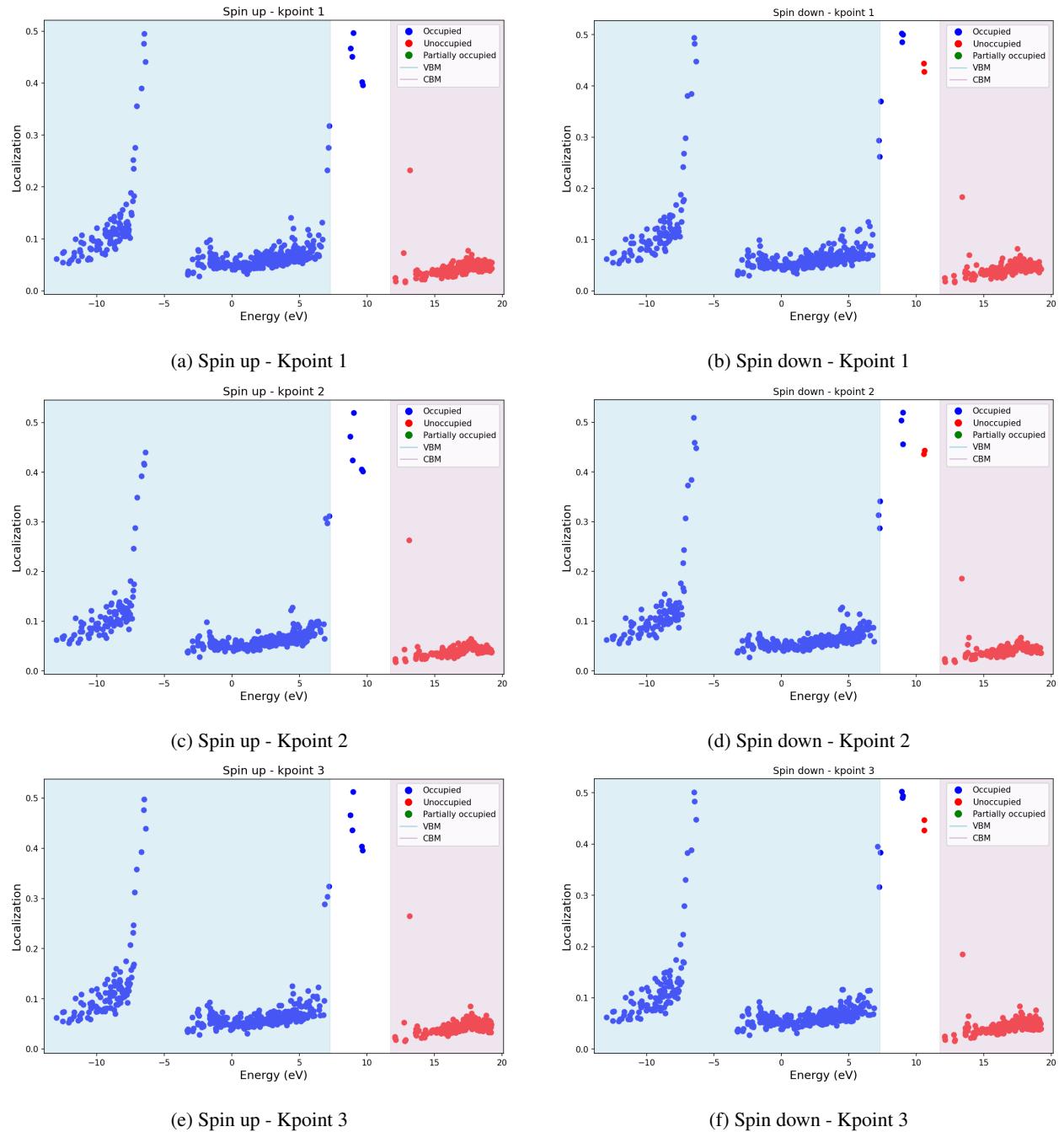


Figure 146: Localization factor using projected orbitals (s, p, and d).

## 1.74 Complex: $(C_B - V_N)^0$

[Go back to the Table 9](#)

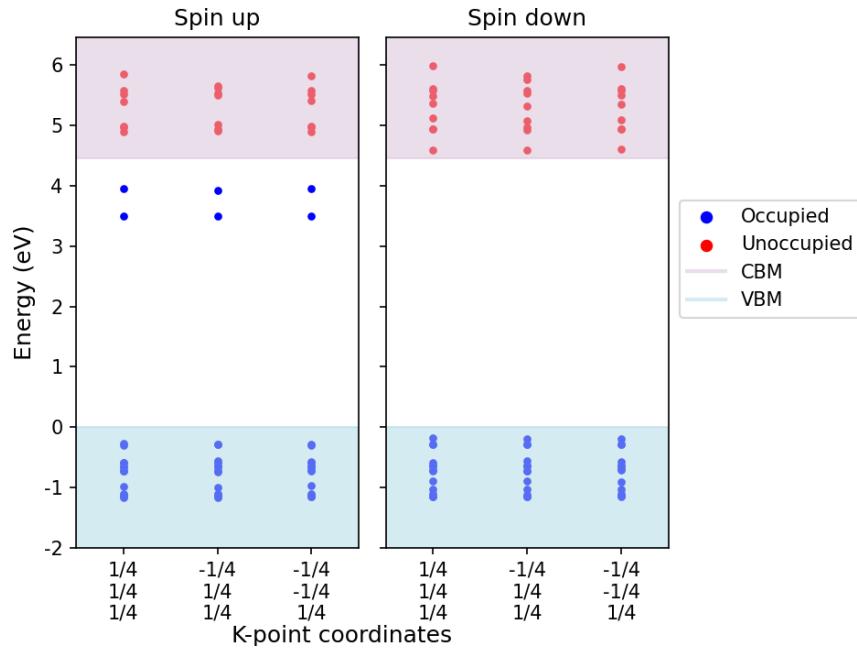


Figure 147: Kohn-Sham states.

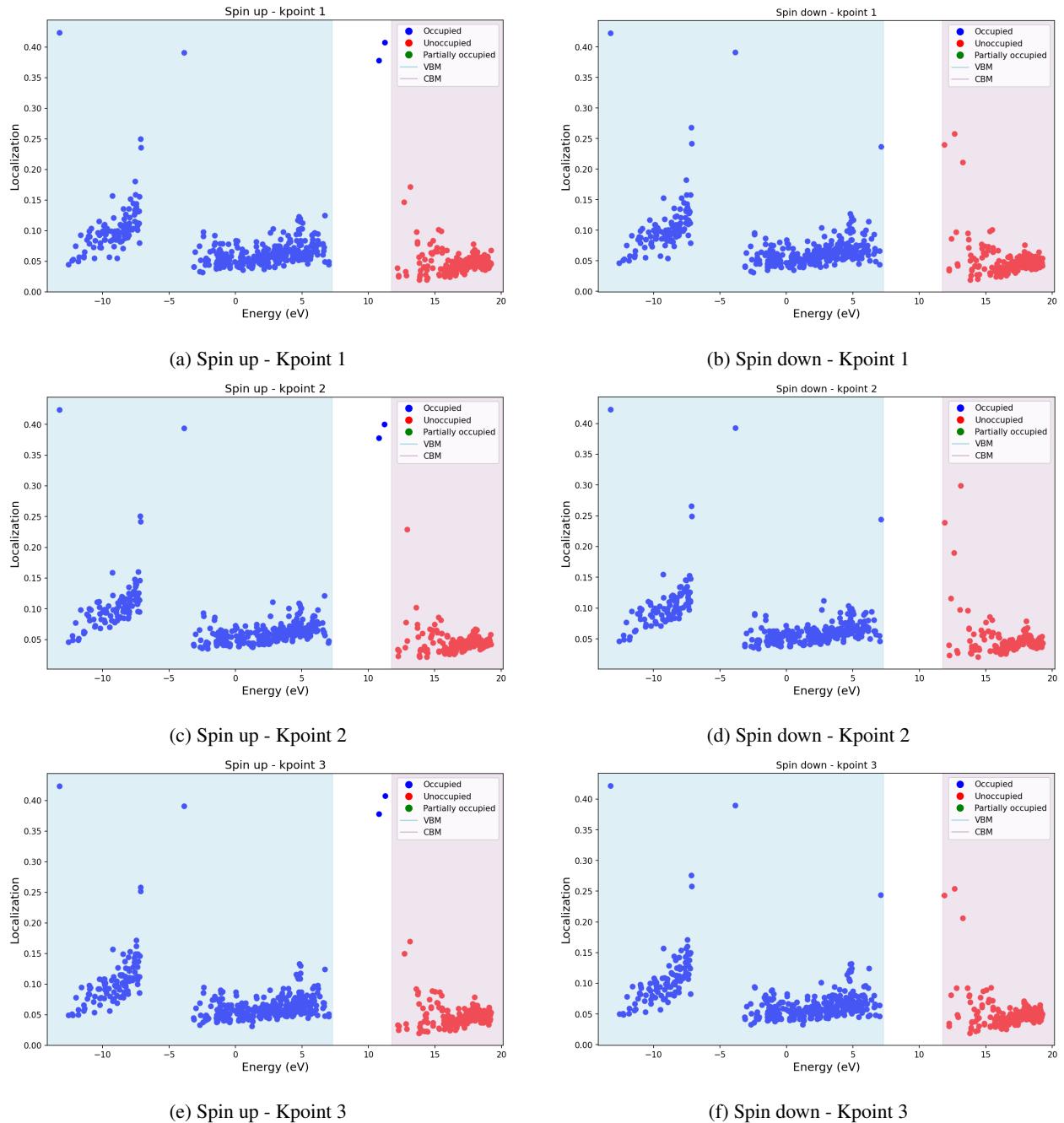


Figure 148: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

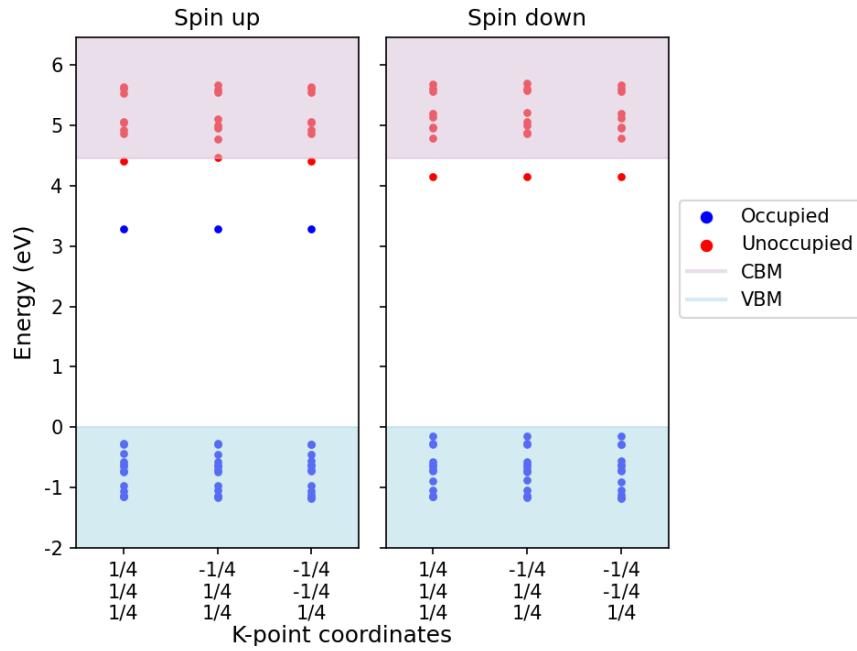


Figure 149: Kohn-Sham states.

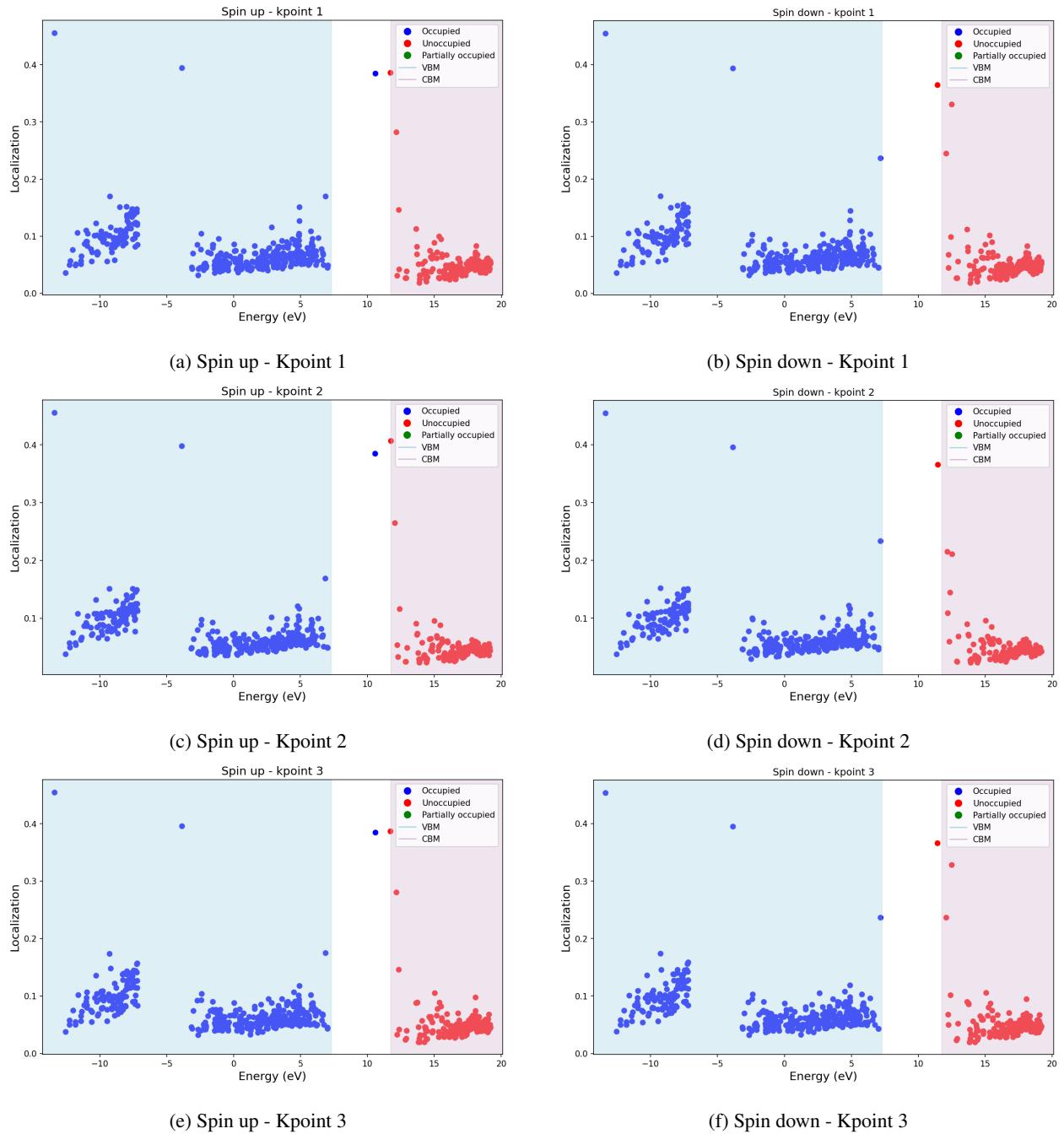


Figure 150: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

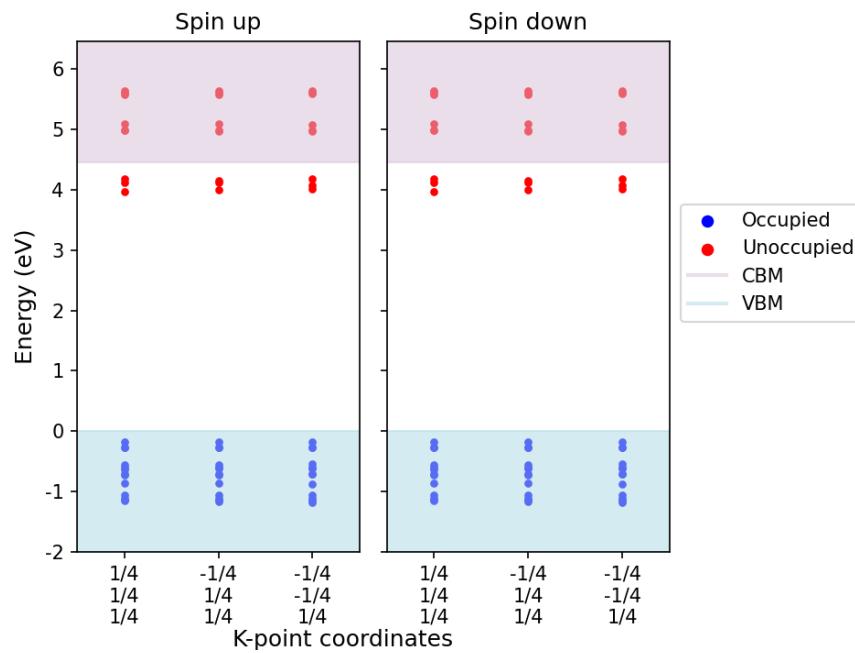


Figure 151: Kohn-Sham states.

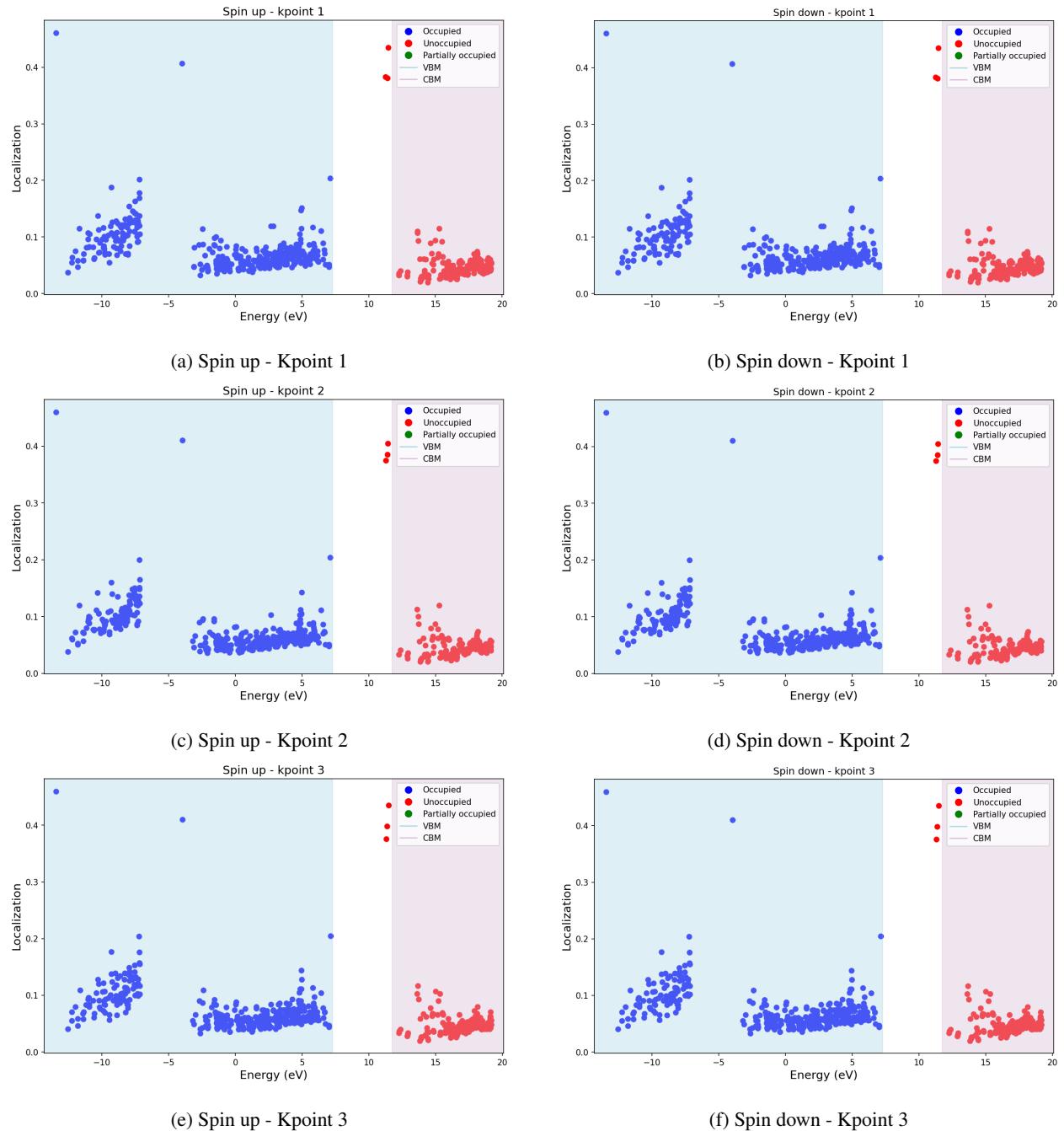


Figure 152: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

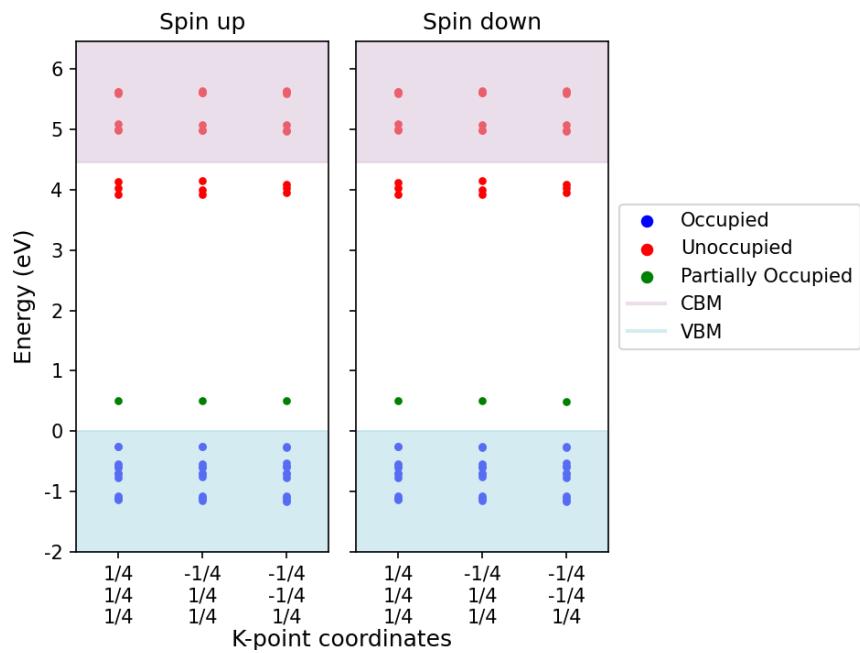


Figure 153: Kohn-Sham states.

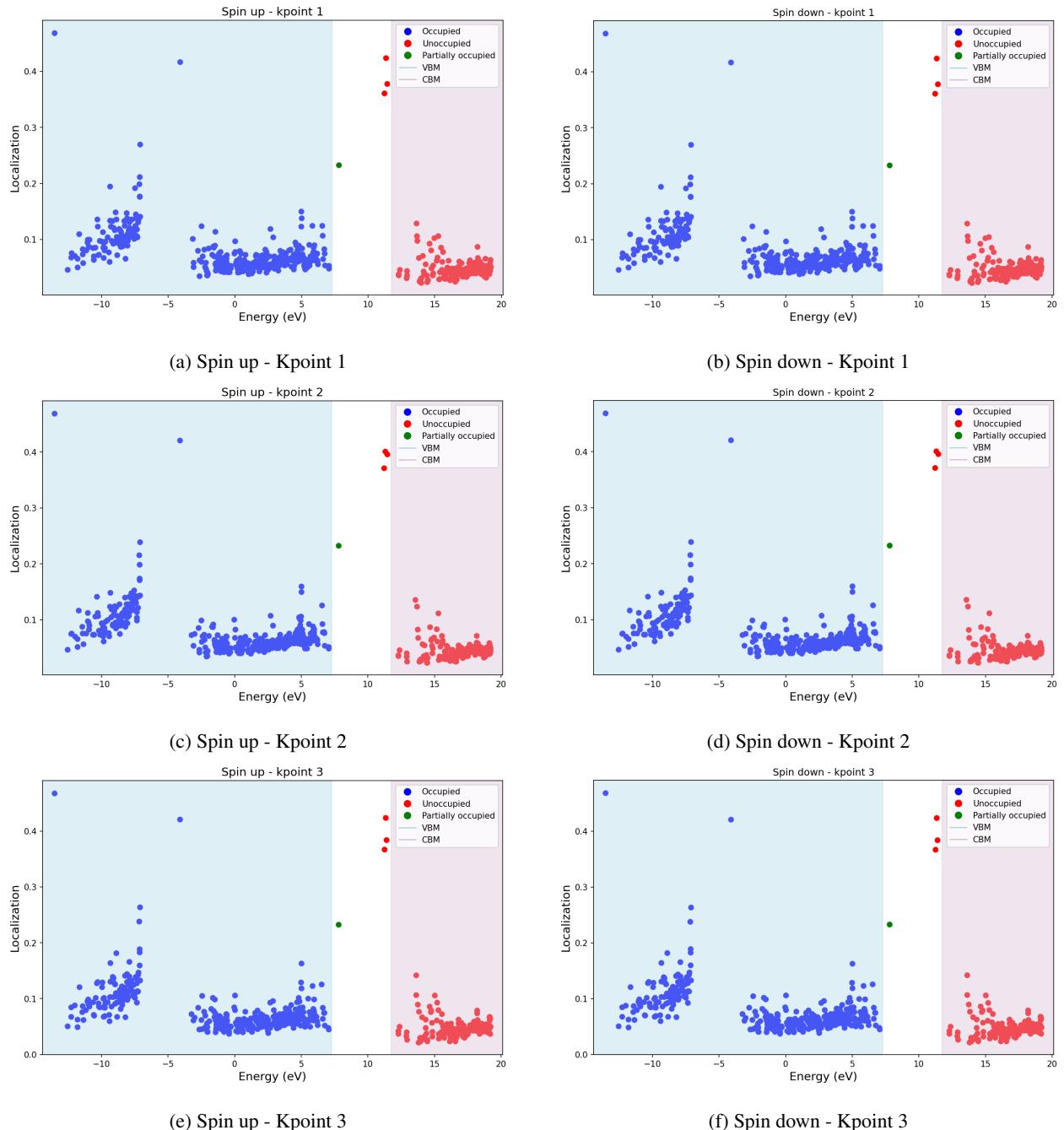


Figure 154: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

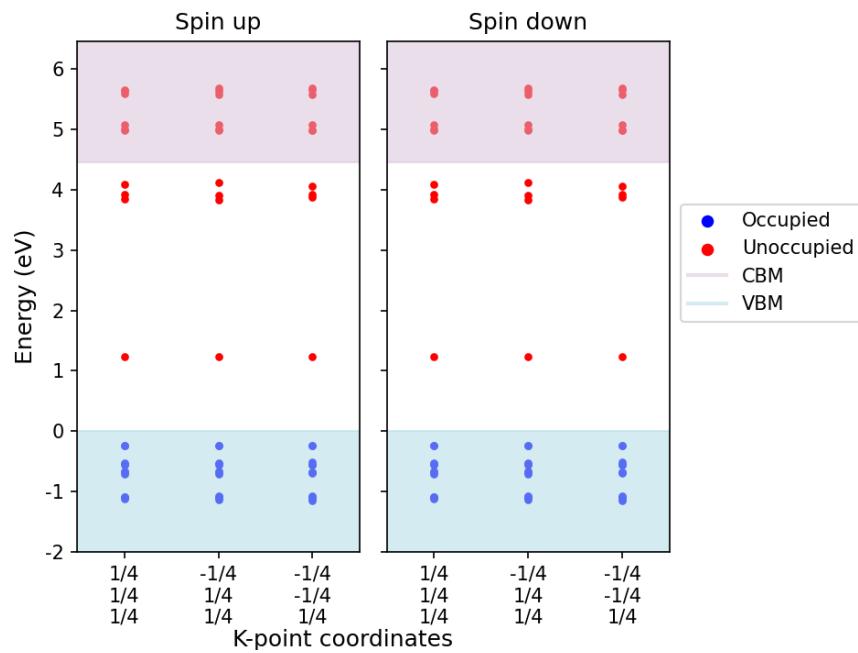


Figure 155: Kohn-Sham states.

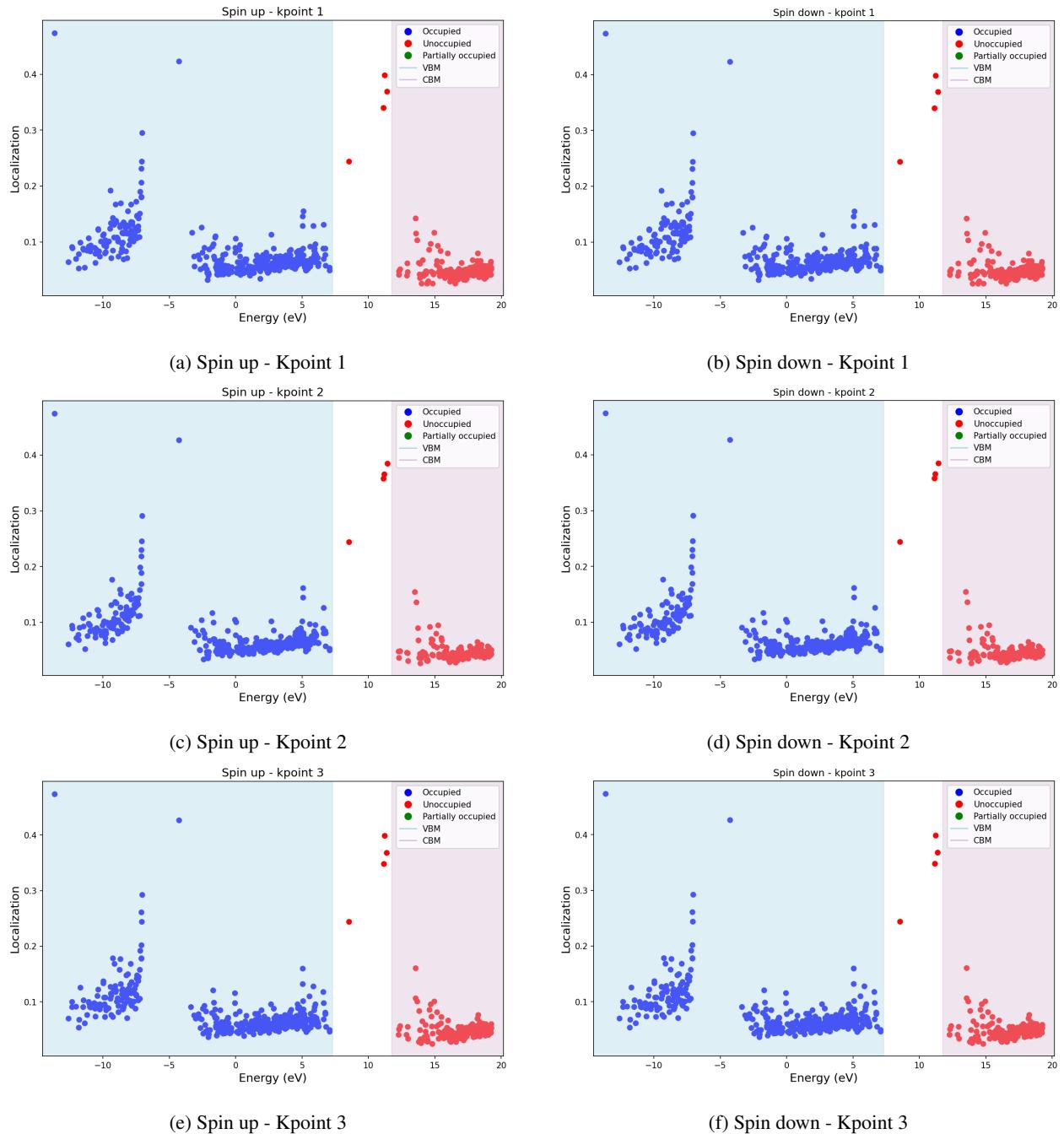


Figure 156: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

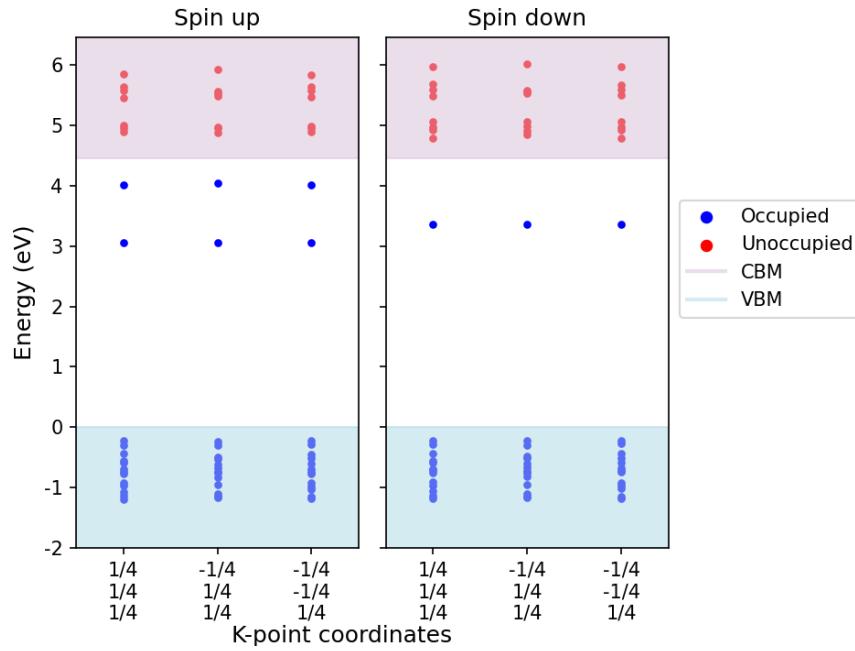


Figure 157: Kohn-Sham states.

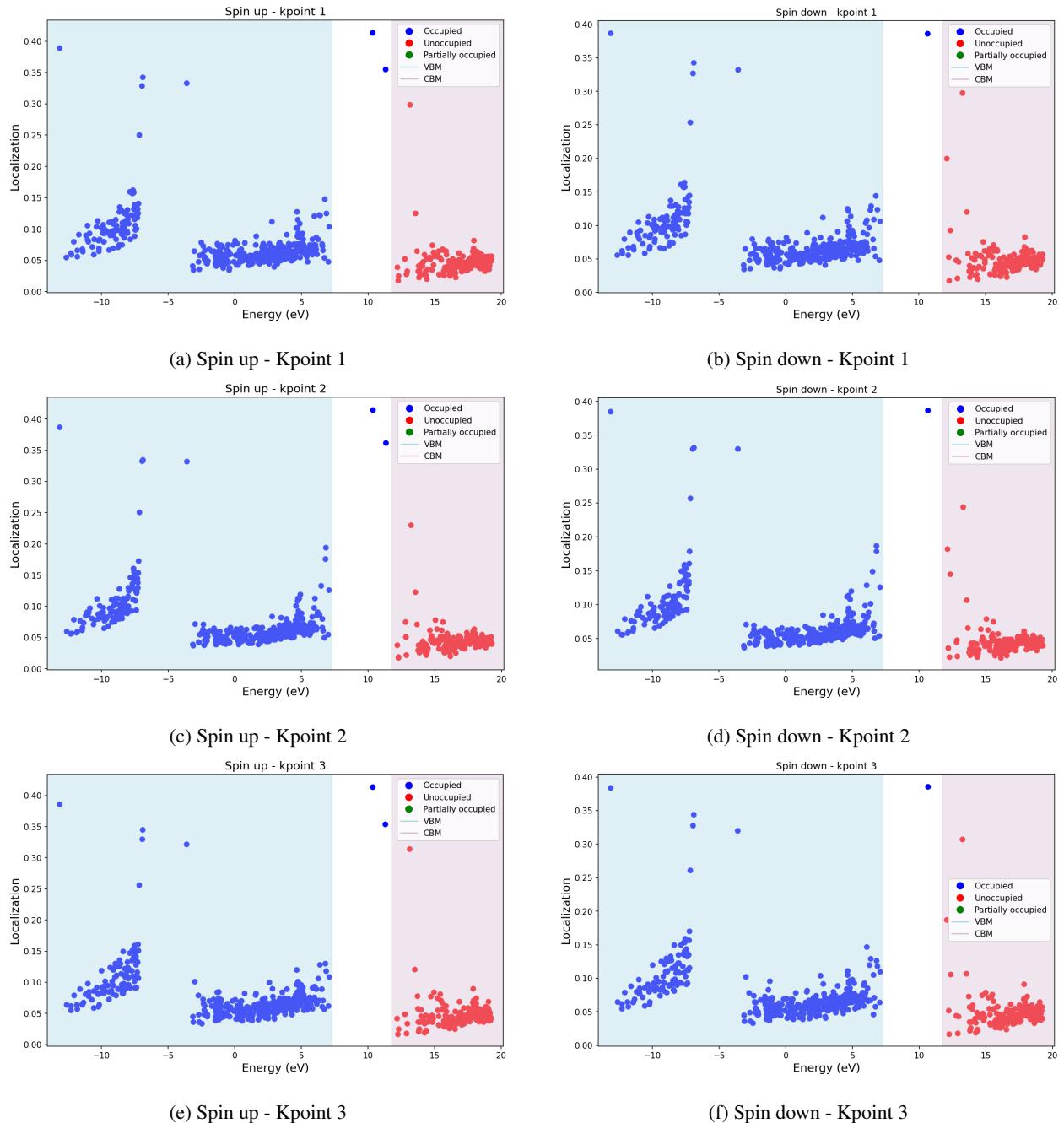


Figure 158: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

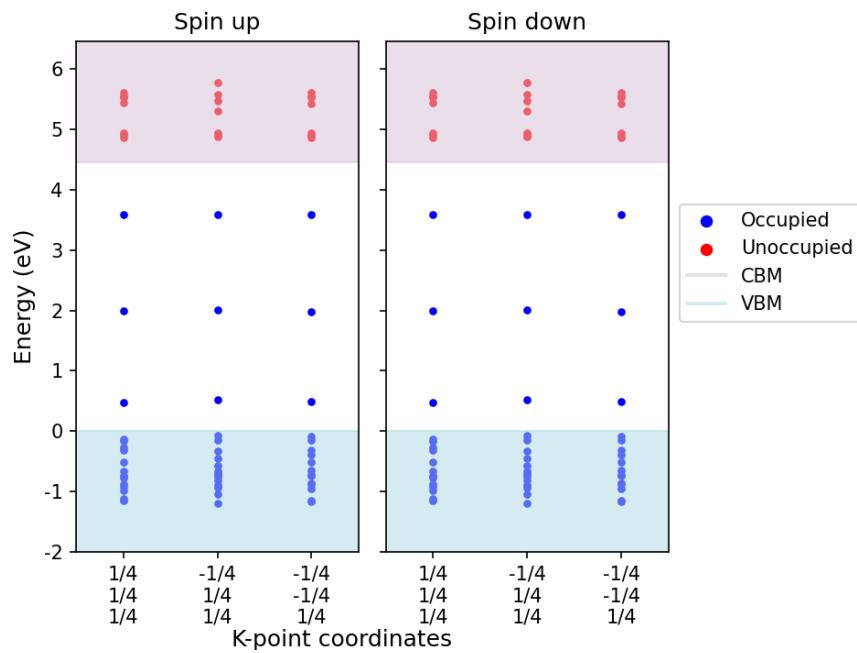


Figure 159: Kohn-Sham states.

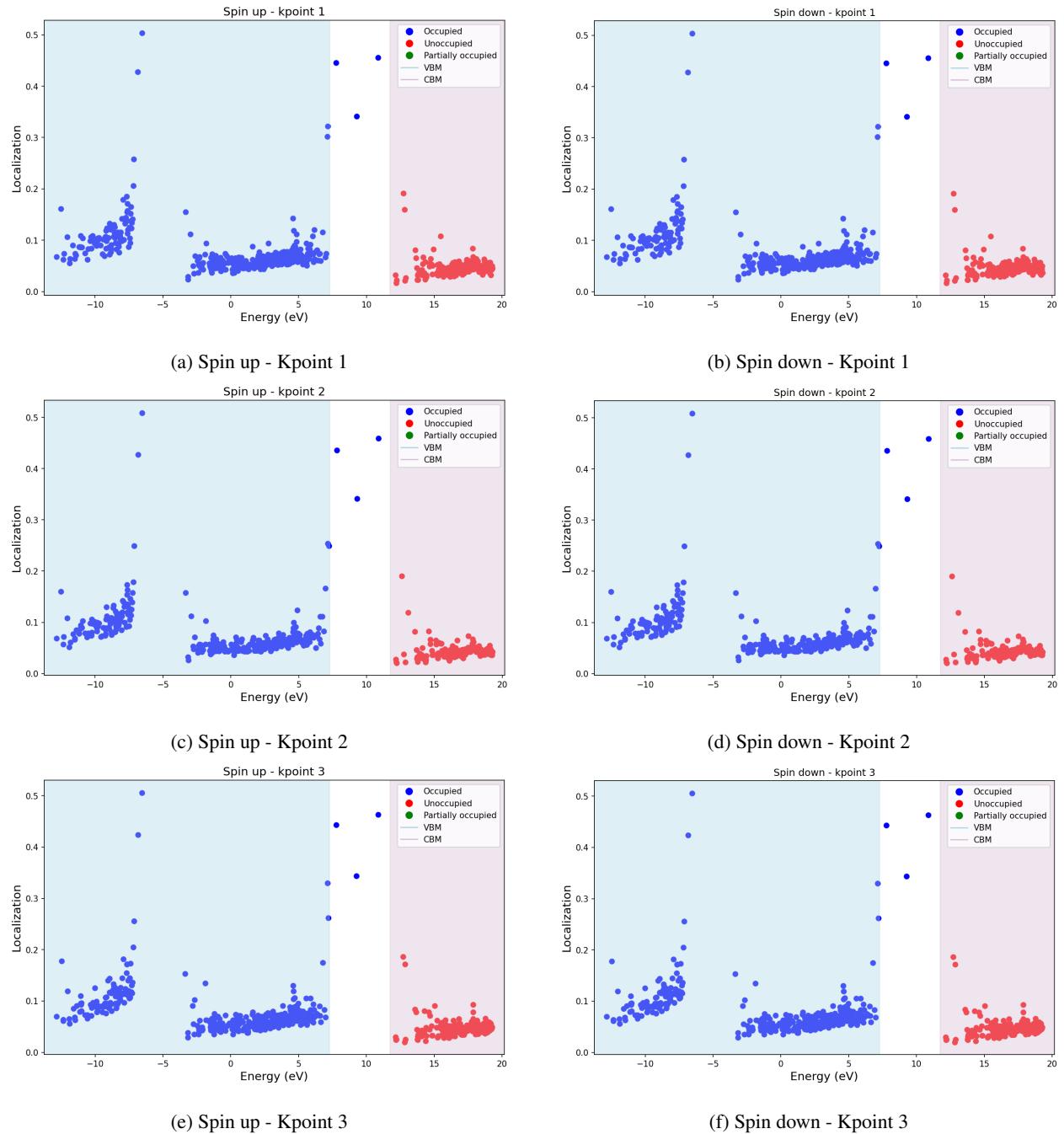


Figure 160: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

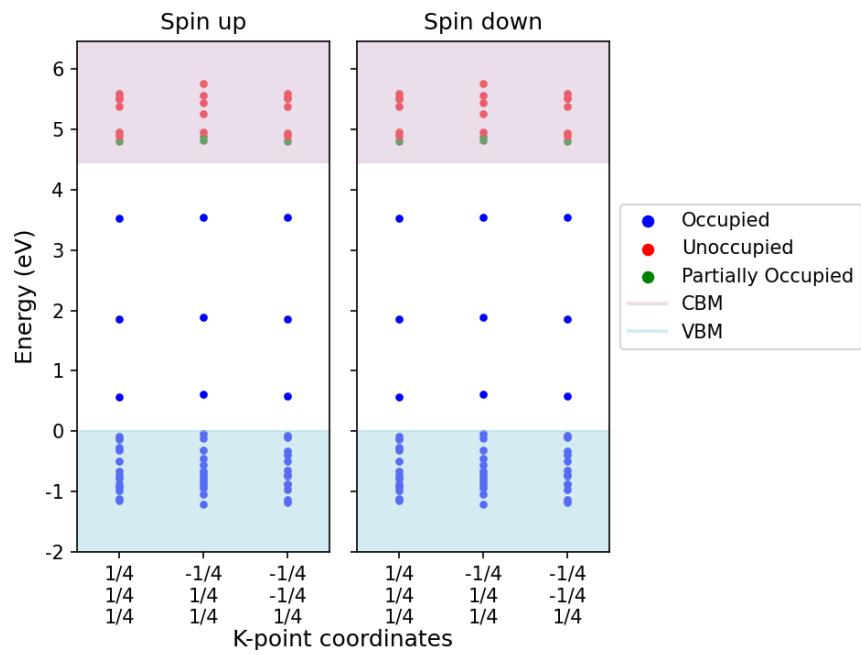


Figure 161: Kohn-Sham states.

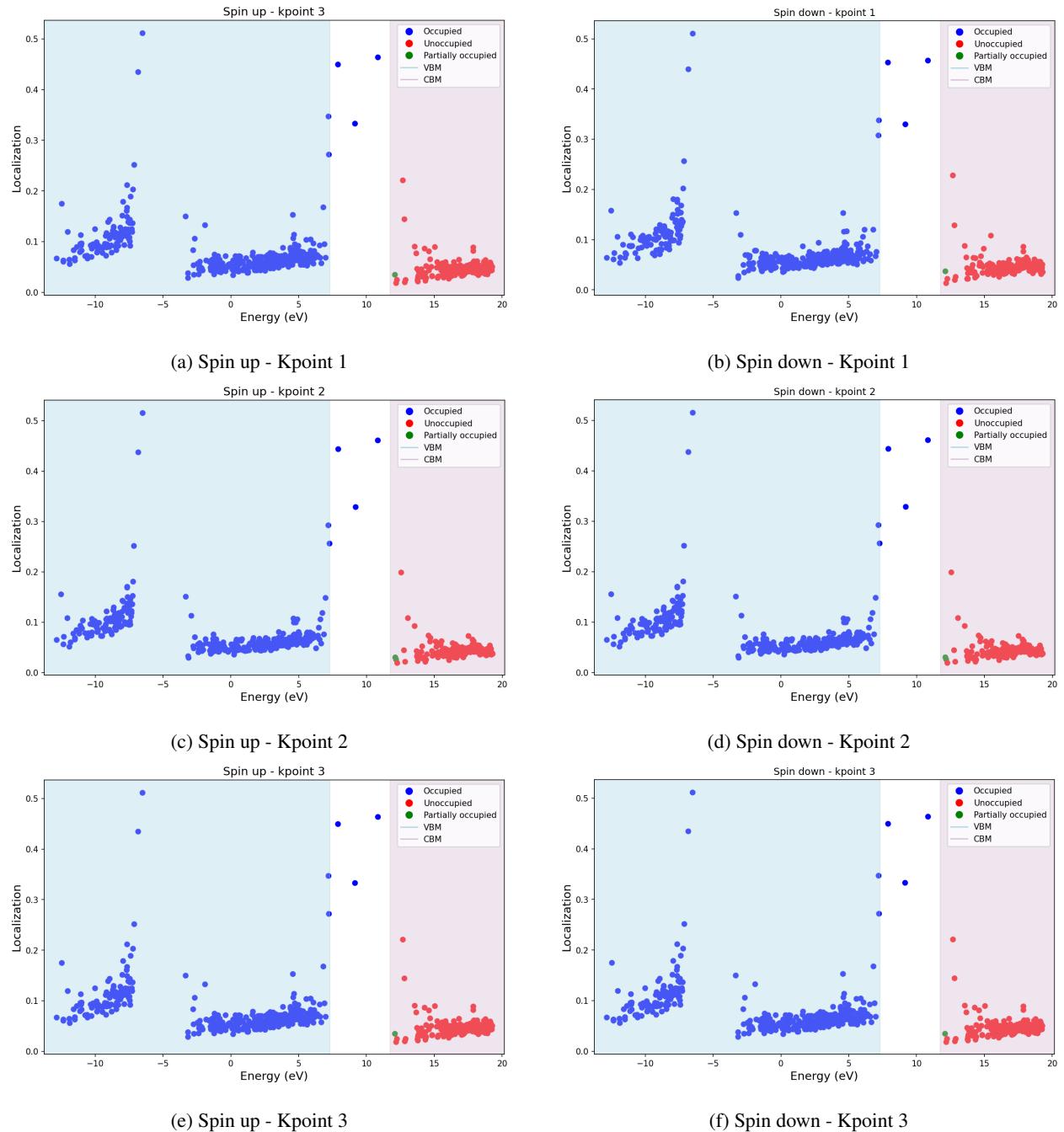


Figure 162: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

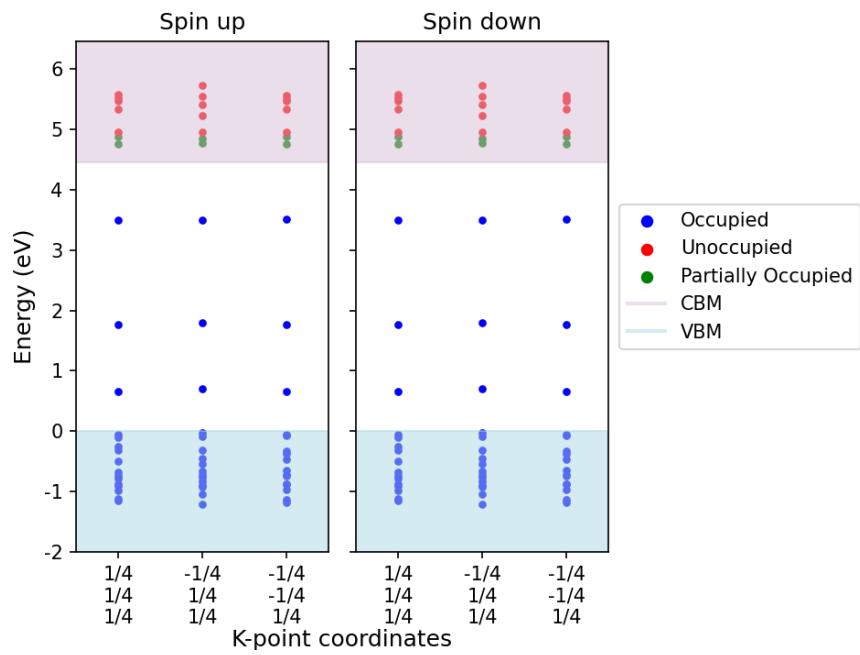


Figure 163: Kohn-Sham states.

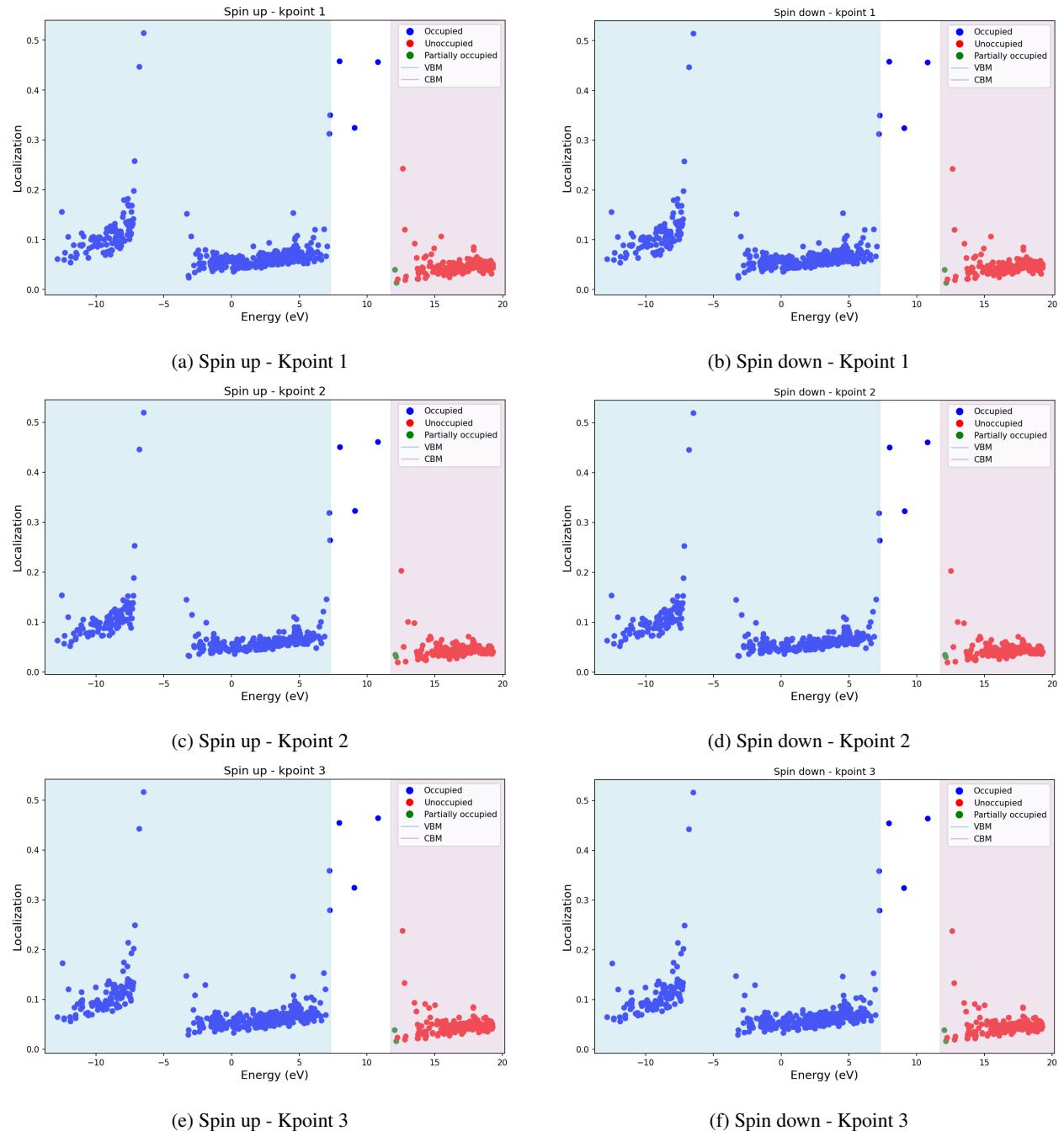


Figure 164: Localization factor using projected orbitals (s, p, and d).

### 1.83 Complex: $(C_N - V_B)^0$

[Go back to the Table 9](#)

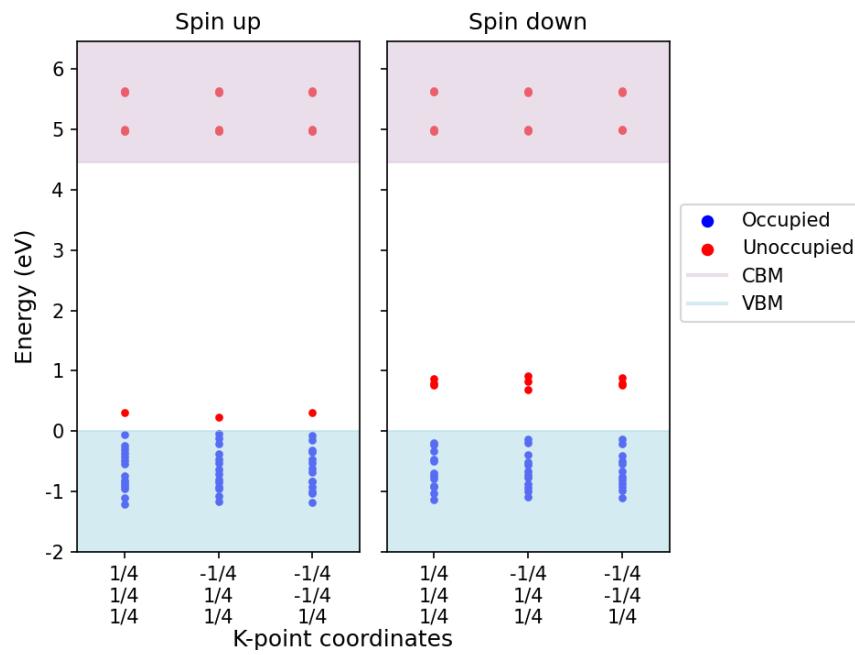


Figure 165: Kohn-Sham states.

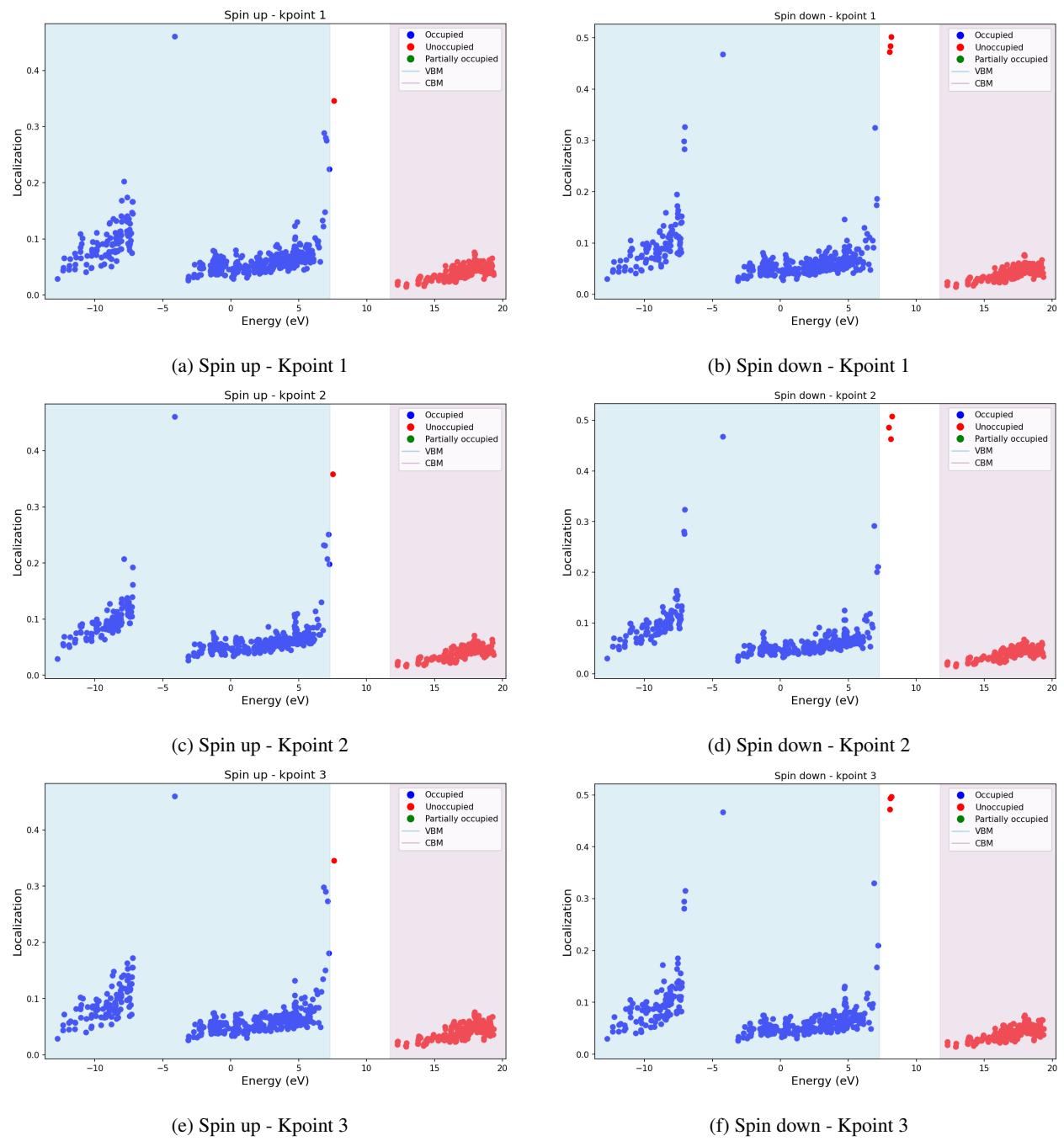


Figure 166: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

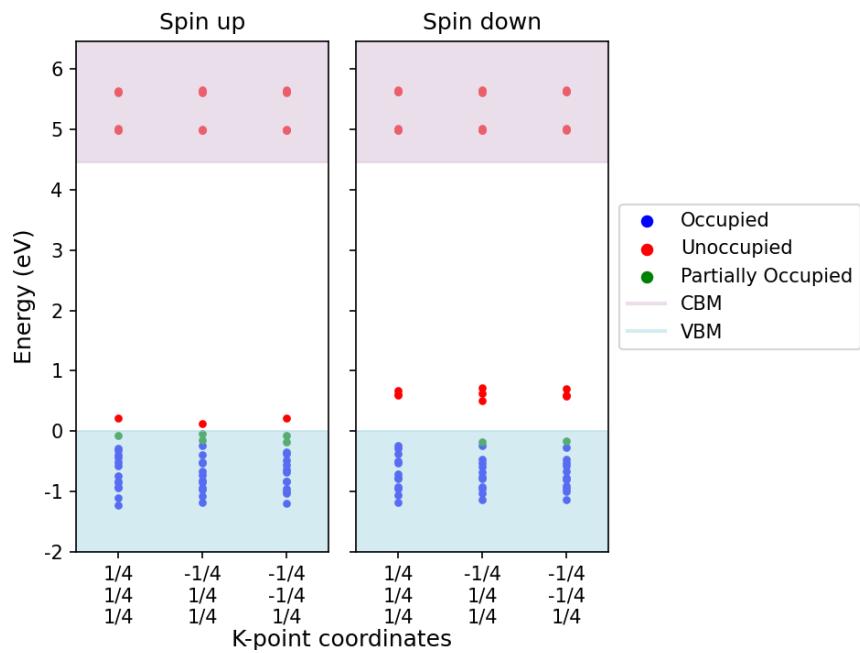


Figure 167: Kohn-Sham states.

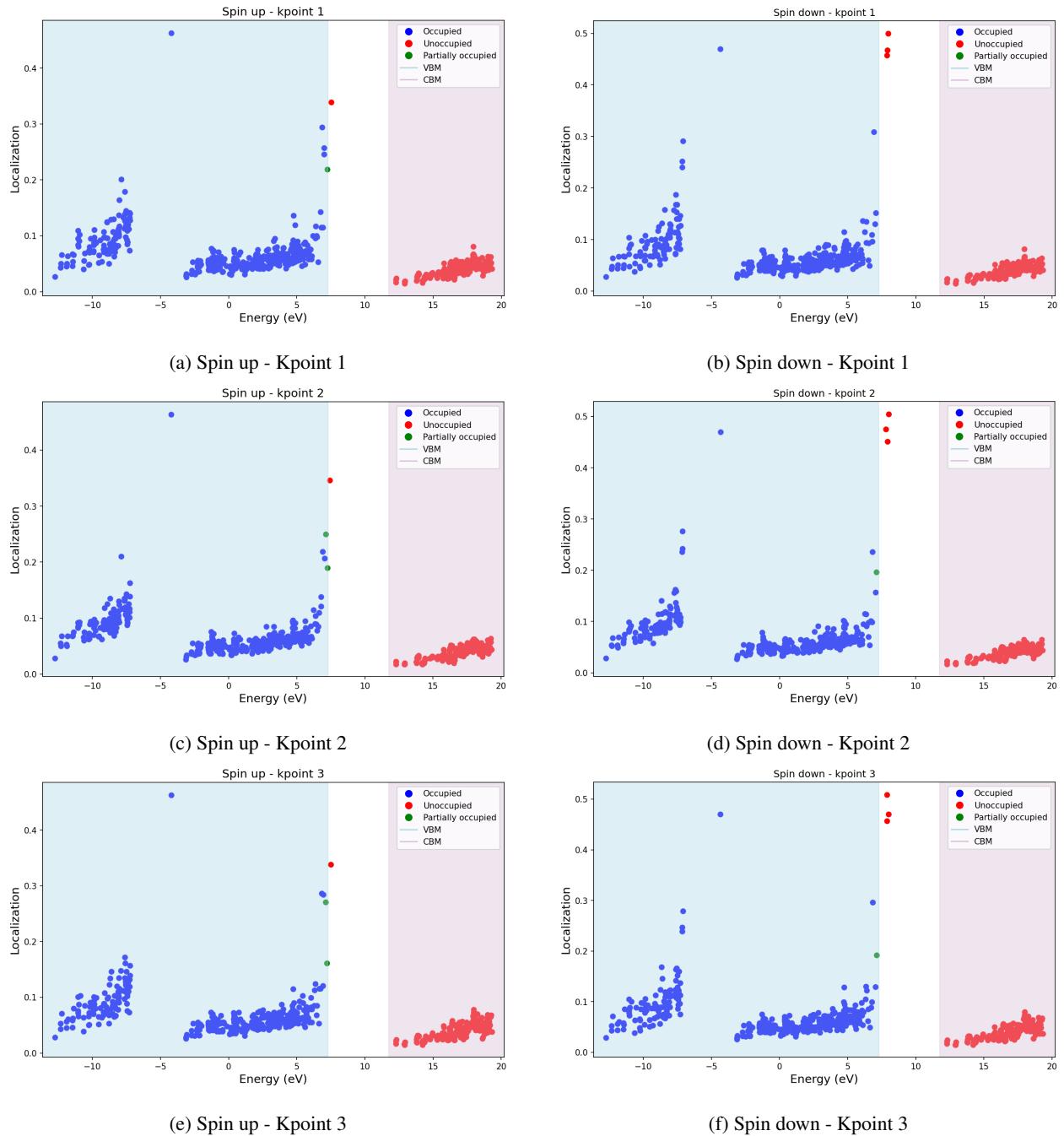


Figure 168: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

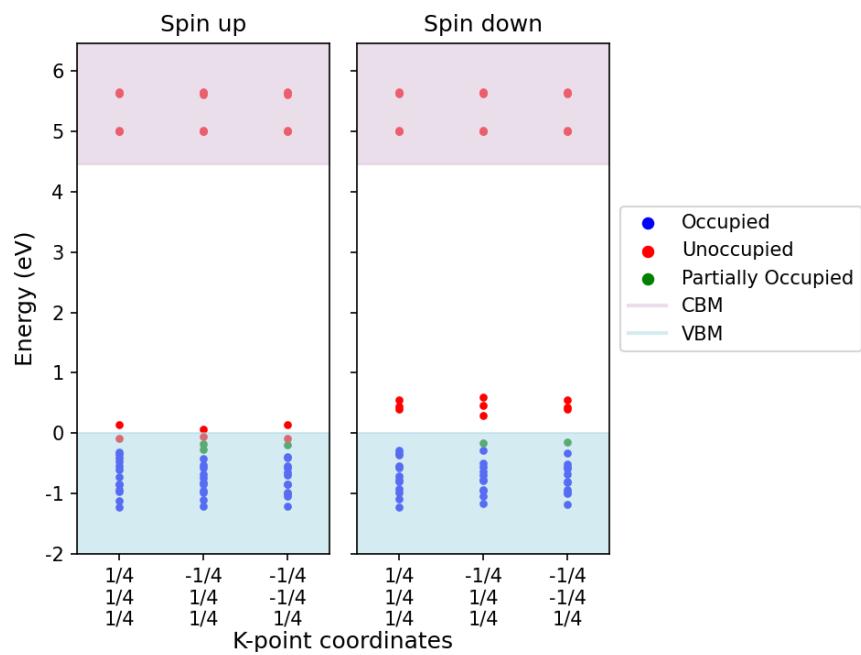


Figure 169: Kohn-Sham states.

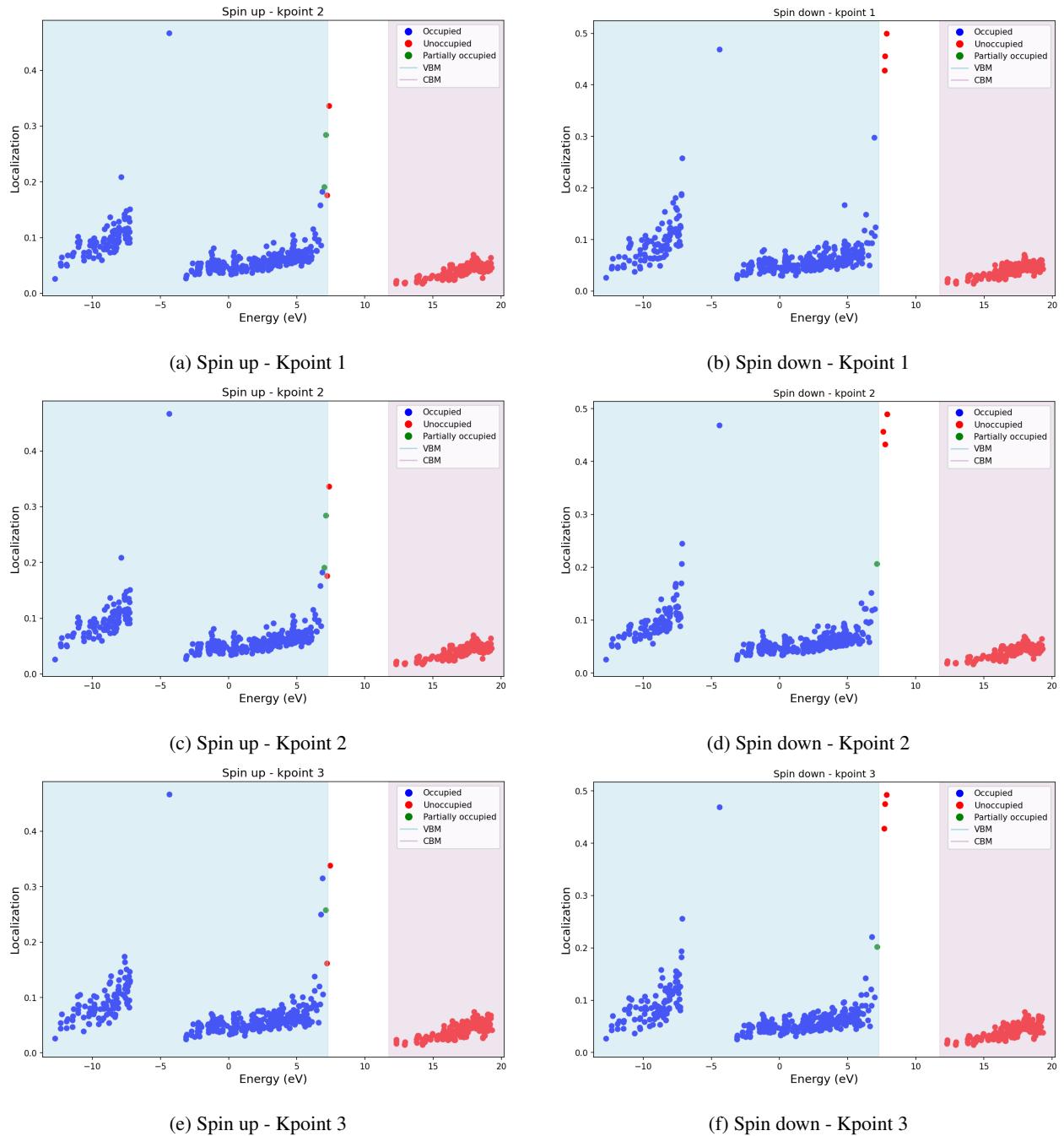


Figure 170: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

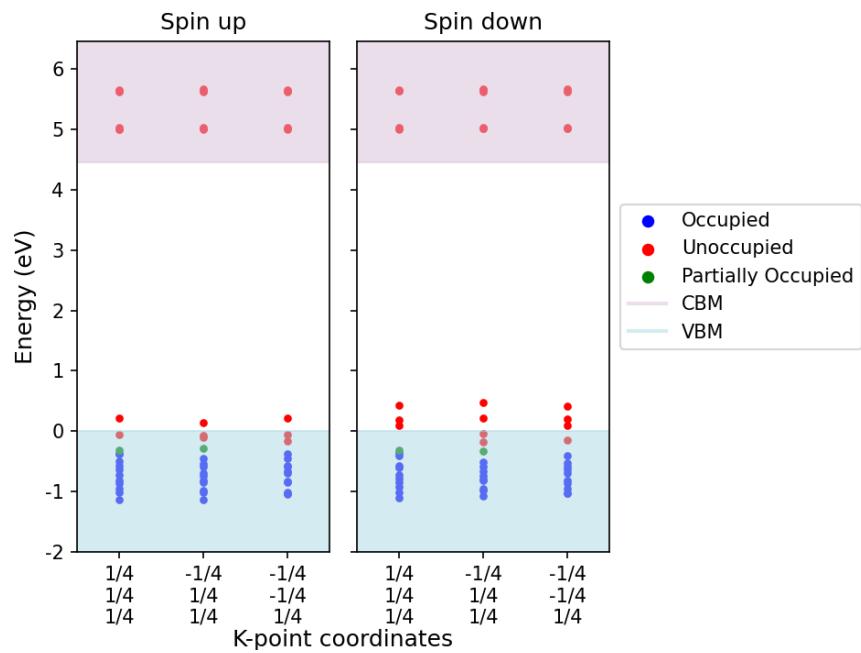


Figure 171: Kohn-Sham states.

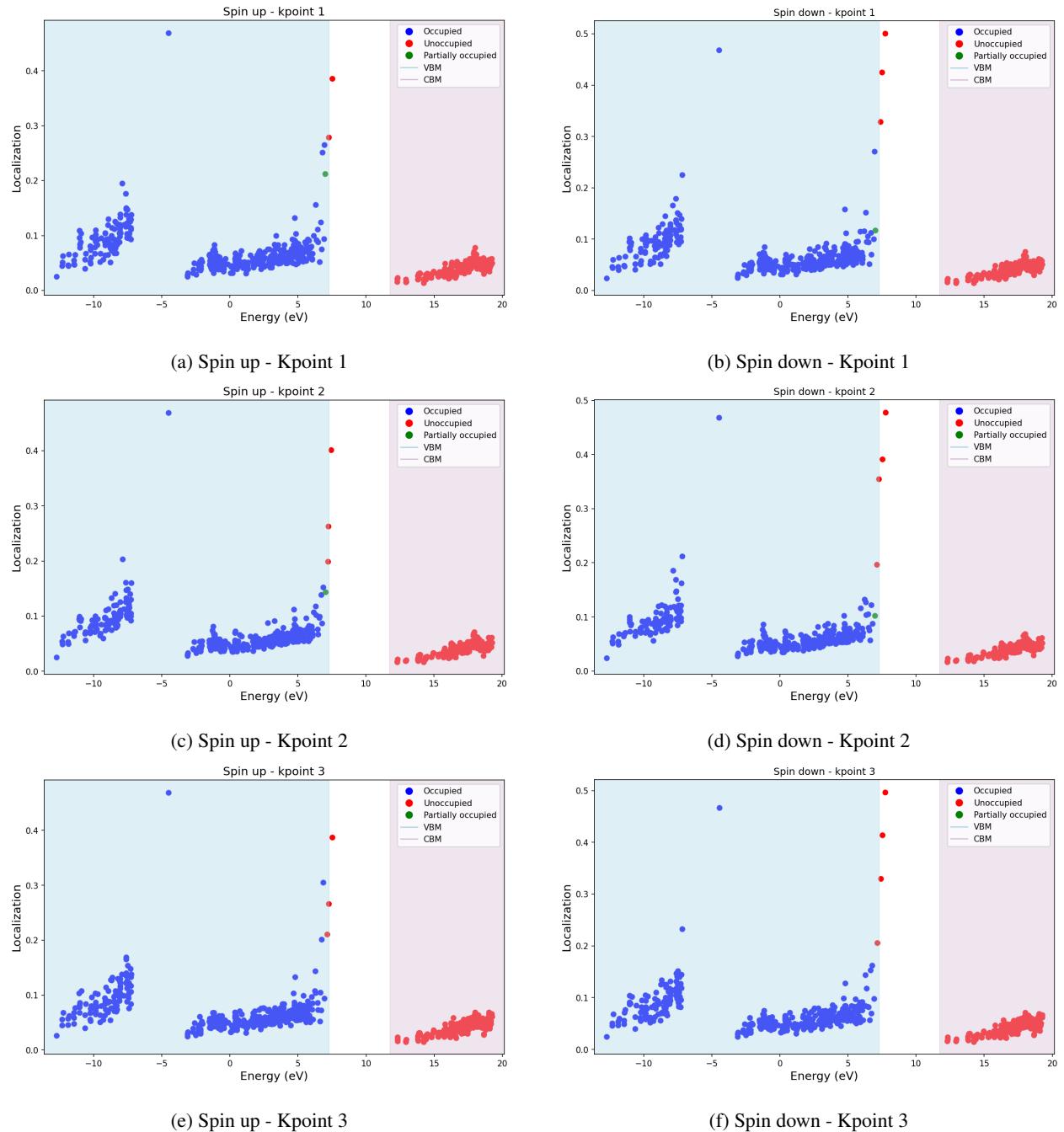


Figure 172: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

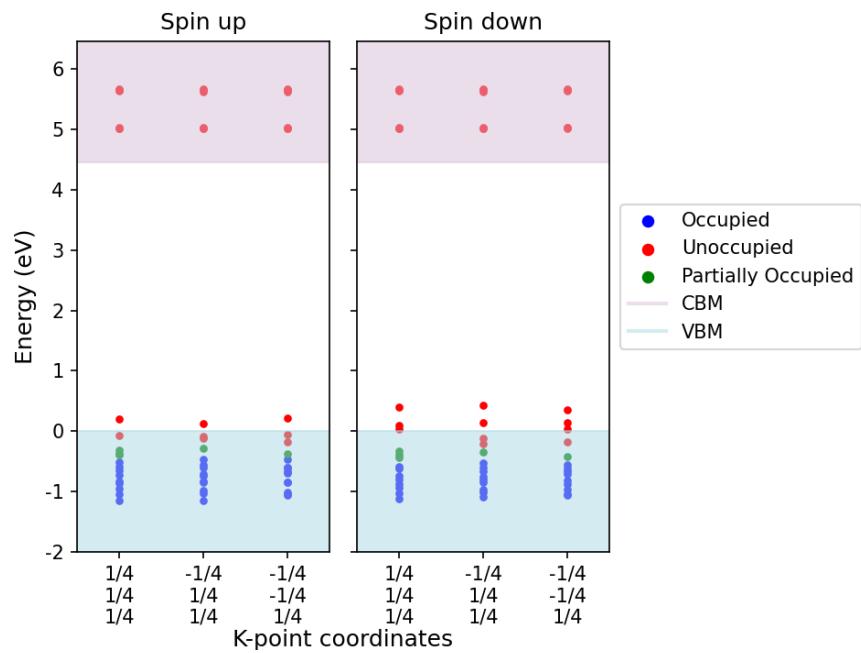


Figure 173: Kohn-Sham states.

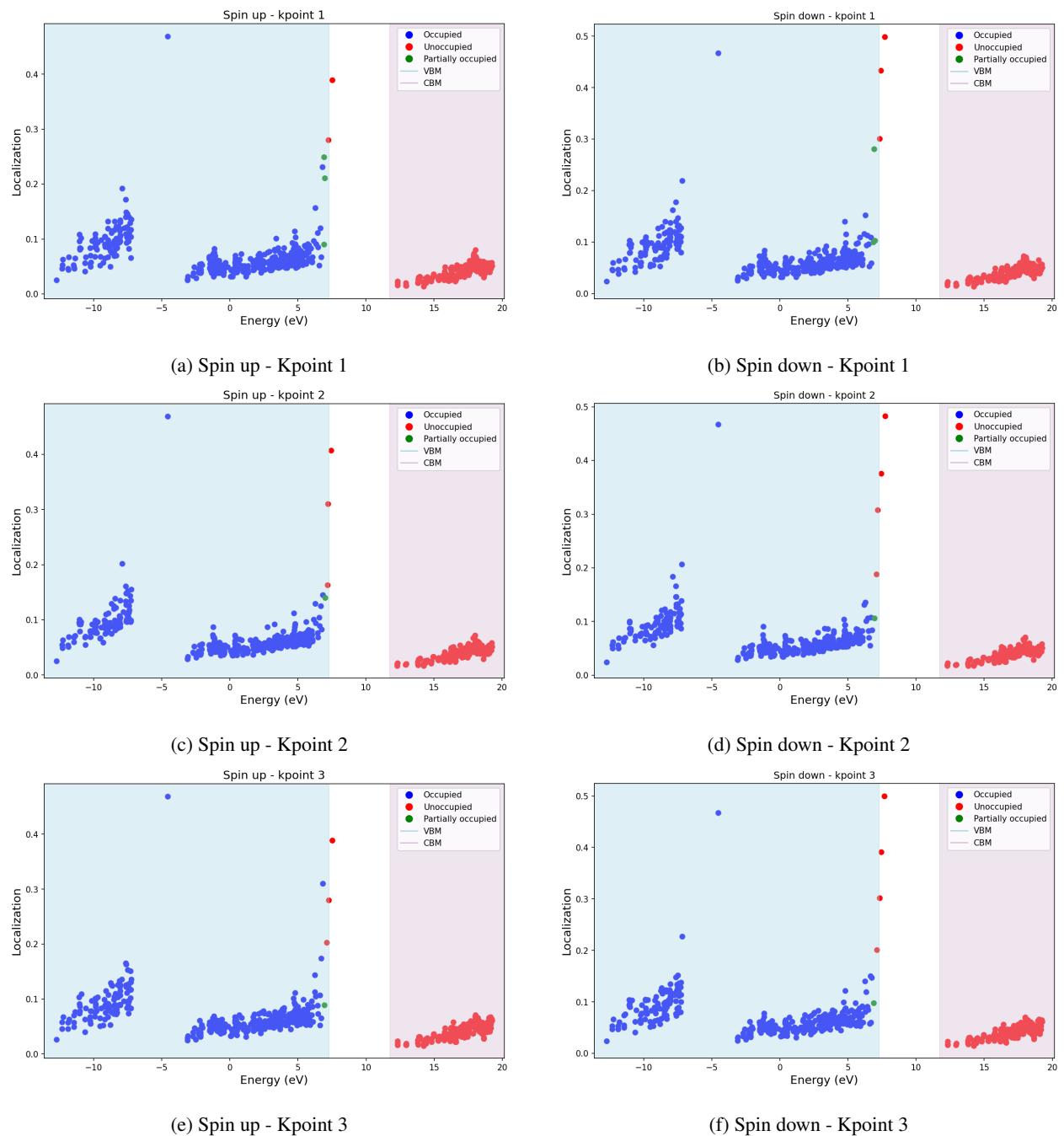


Figure 174: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

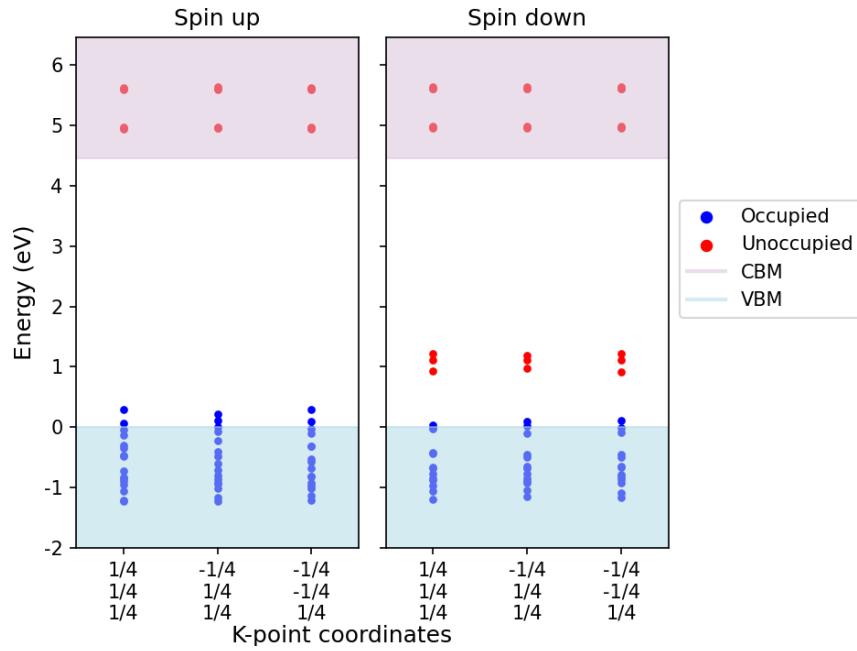


Figure 175: Kohn-Sham states.

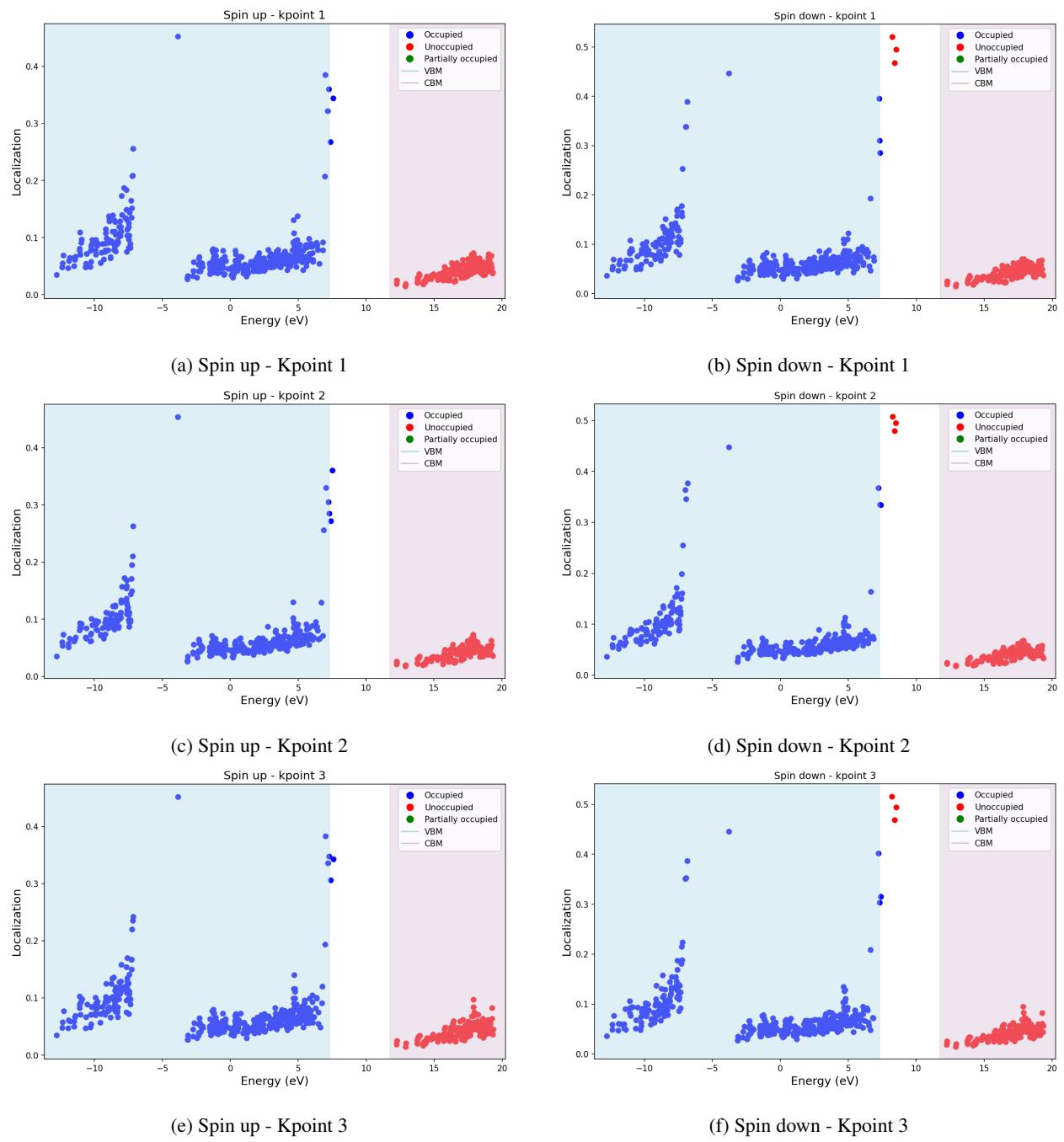


Figure 176: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

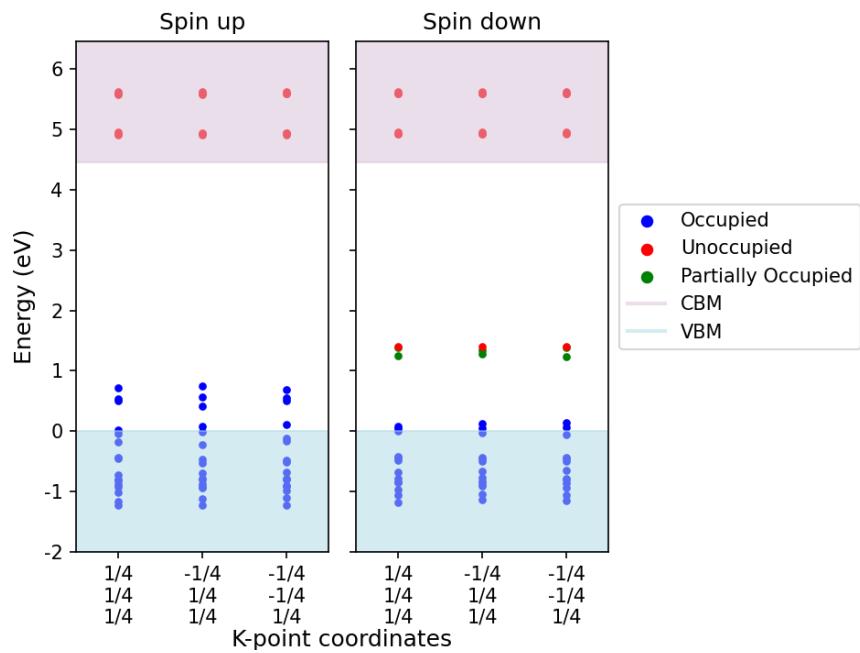


Figure 177: Kohn-Sham states.

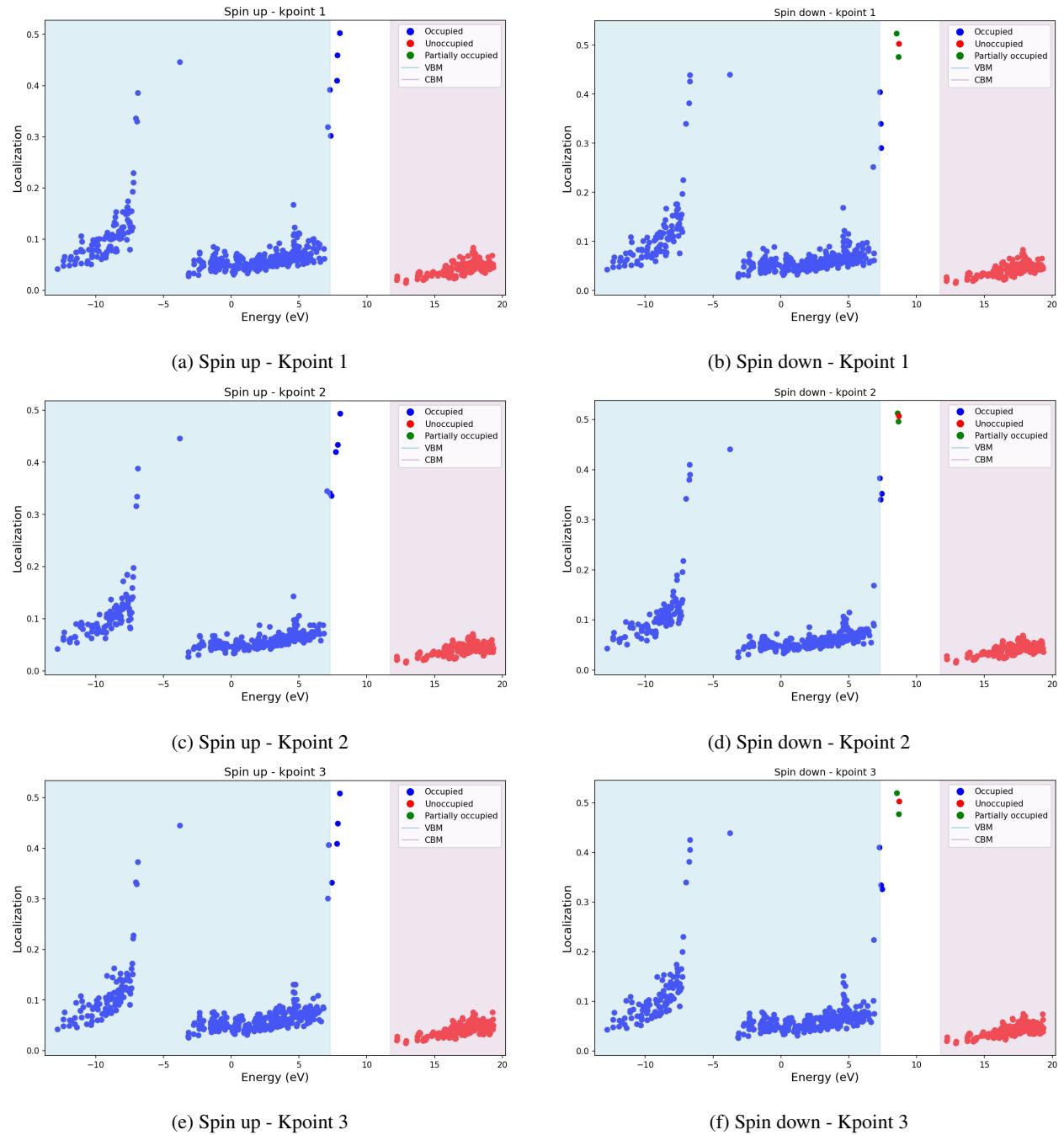


Figure 178: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

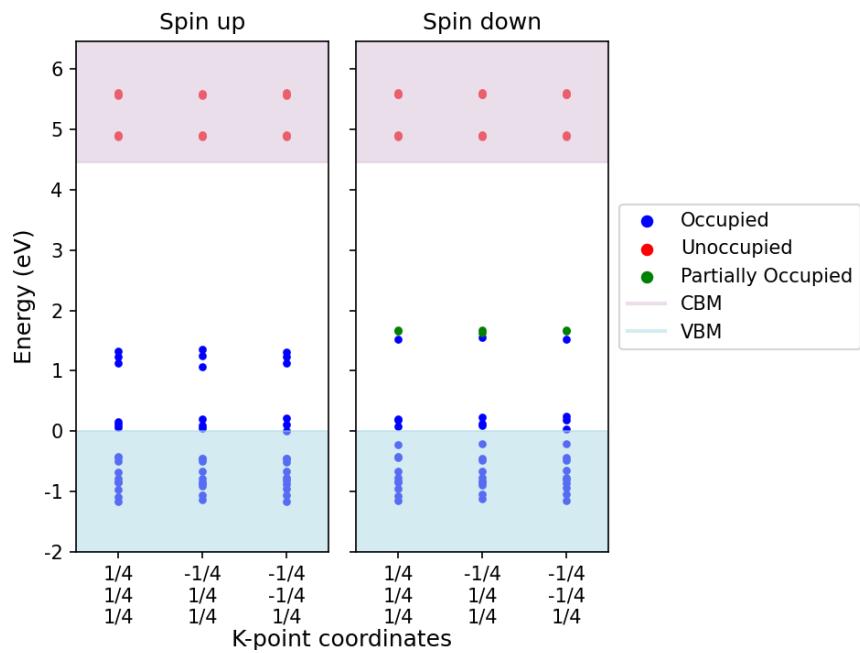


Figure 179: Kohn-Sham states.

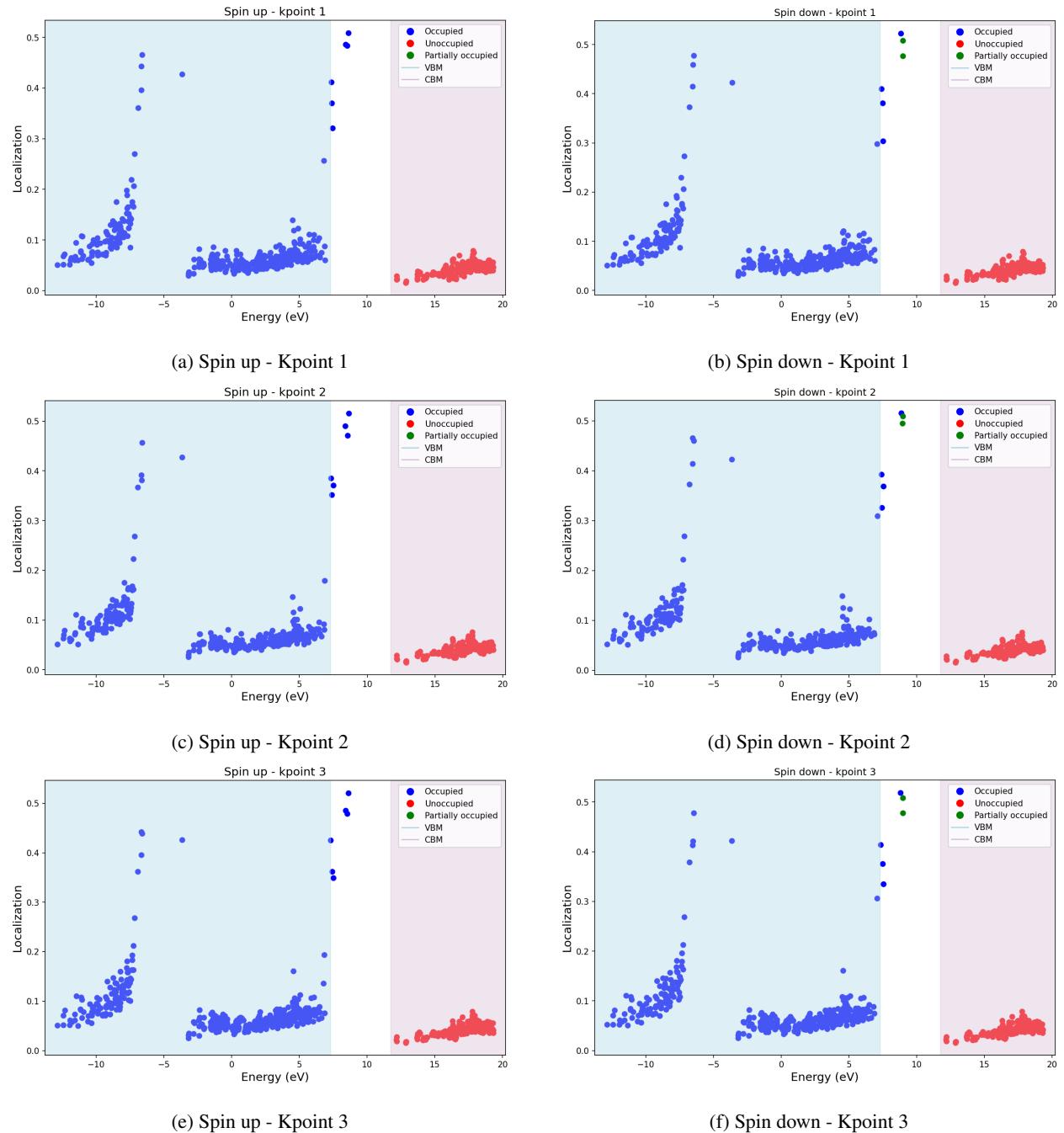


Figure 180: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

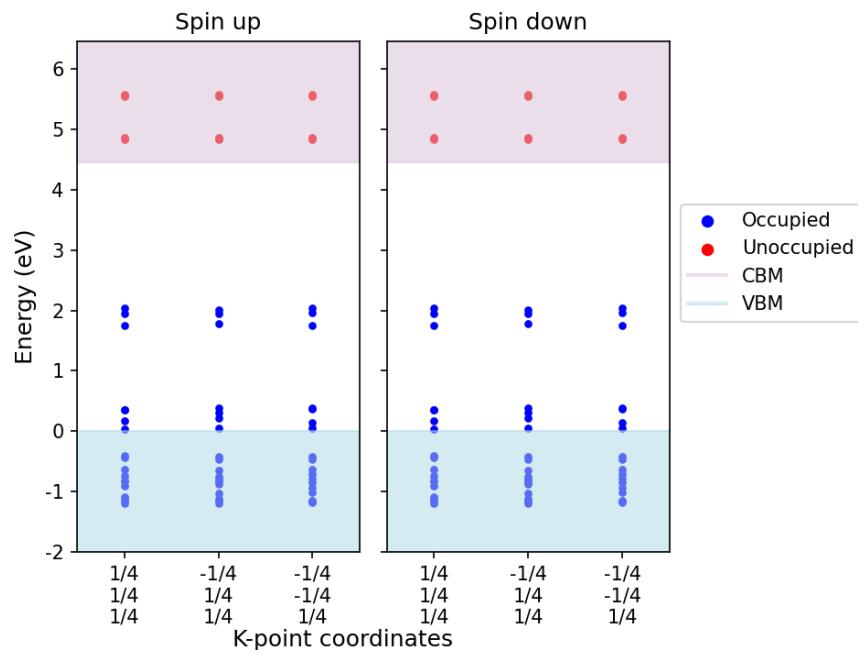


Figure 181: Kohn-Sham states.

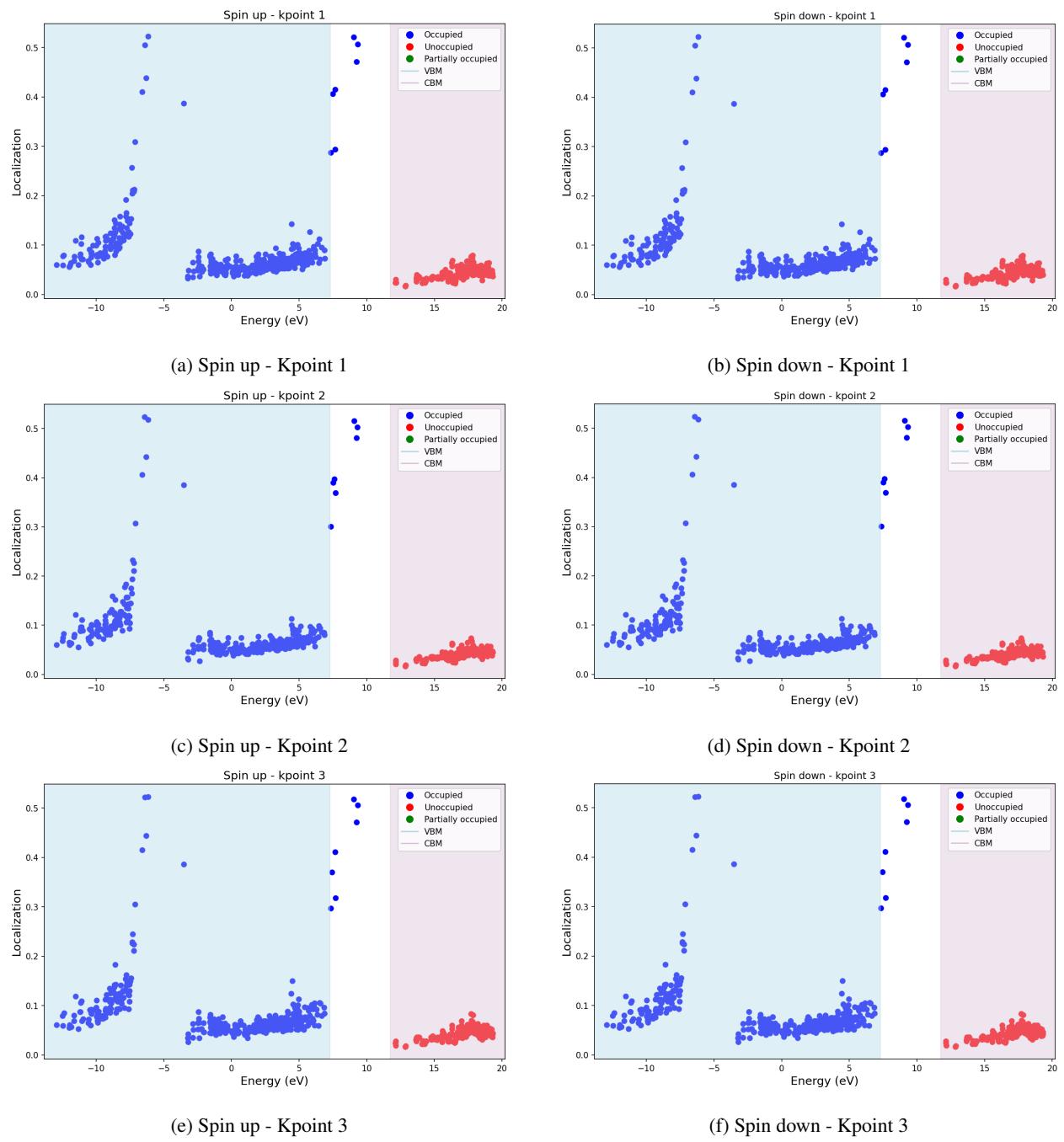


Figure 182: Localization factor using projected orbitals (s, p, and d).

## 1.92 Substitutional: $C_B^0$

[Go back to the Table 9](#)

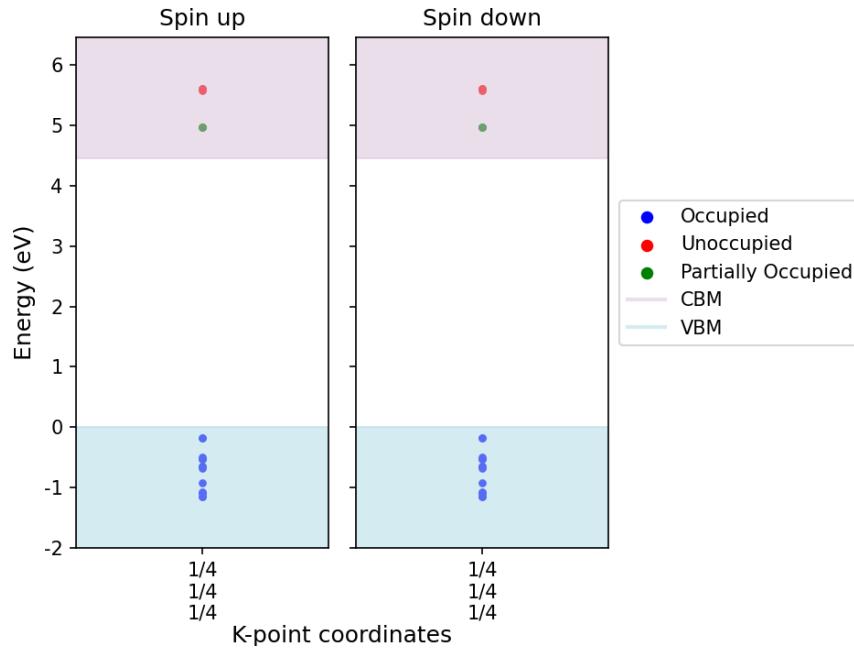


Figure 183: Kohn-Sham states.

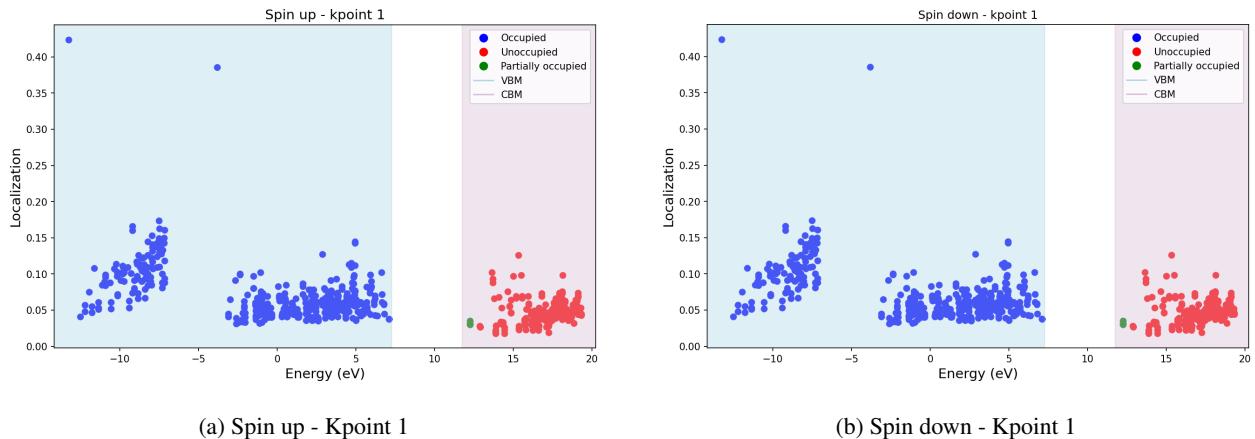


Figure 184: Localization factor using projected orbitals (s, p and d).

### 1.93 Substitutional: $C_B^{+1}$

[Go back to the Table 9](#)

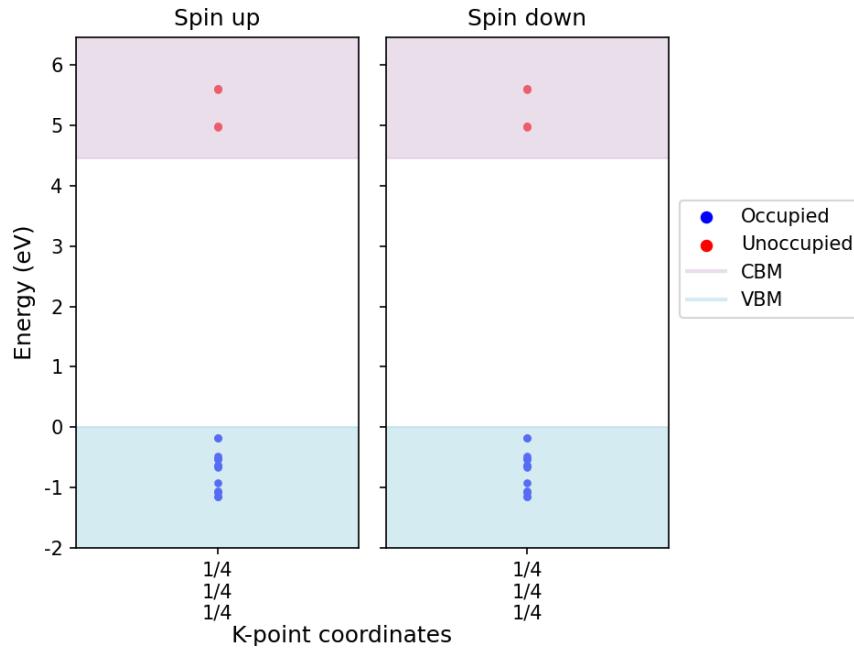


Figure 185: Kohn-Sham states.

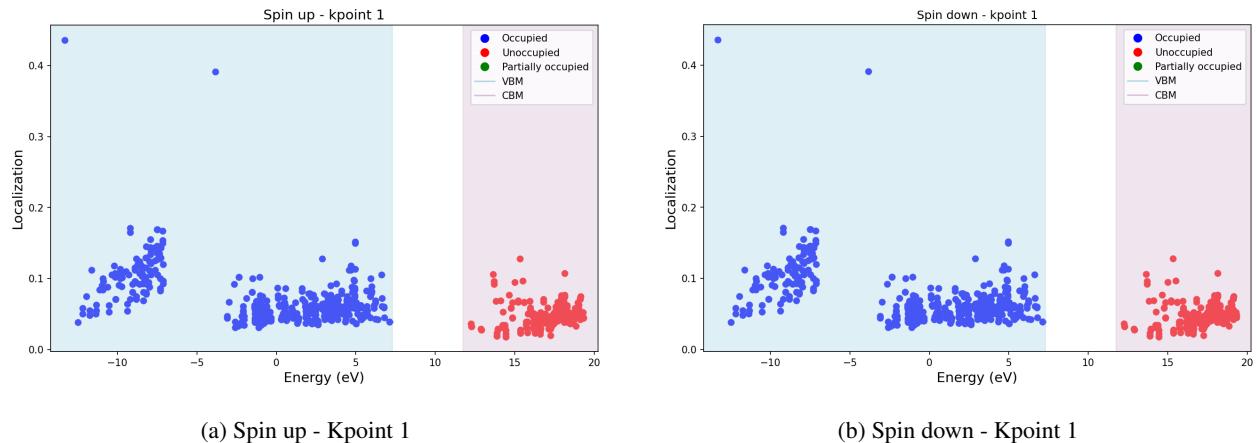


Figure 186: Localization factor using projected orbitals (s, p and d).

## 1.94 Substitutional: $C_B^{+2}$

[Go back to the Table 9](#)

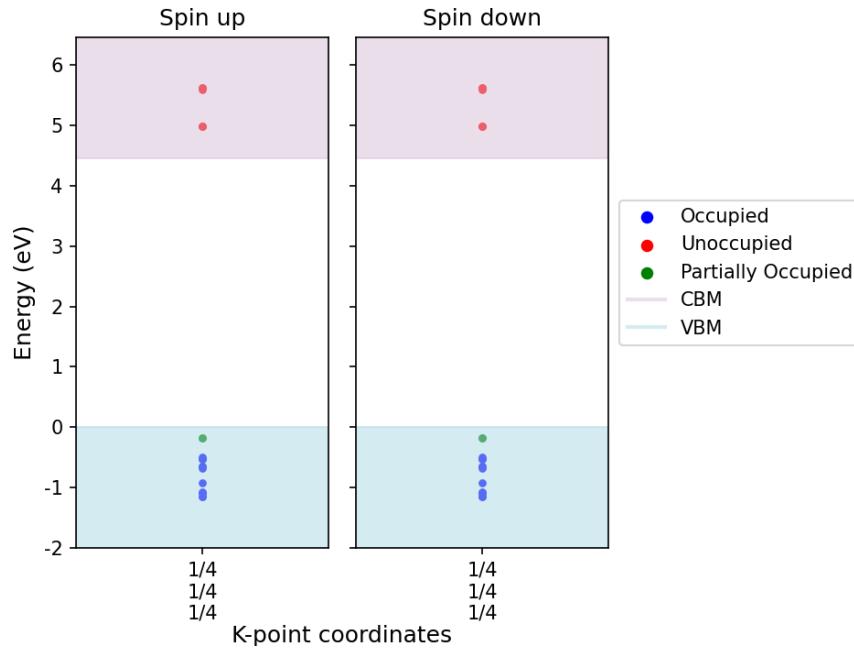


Figure 187: Kohn-Sham states.

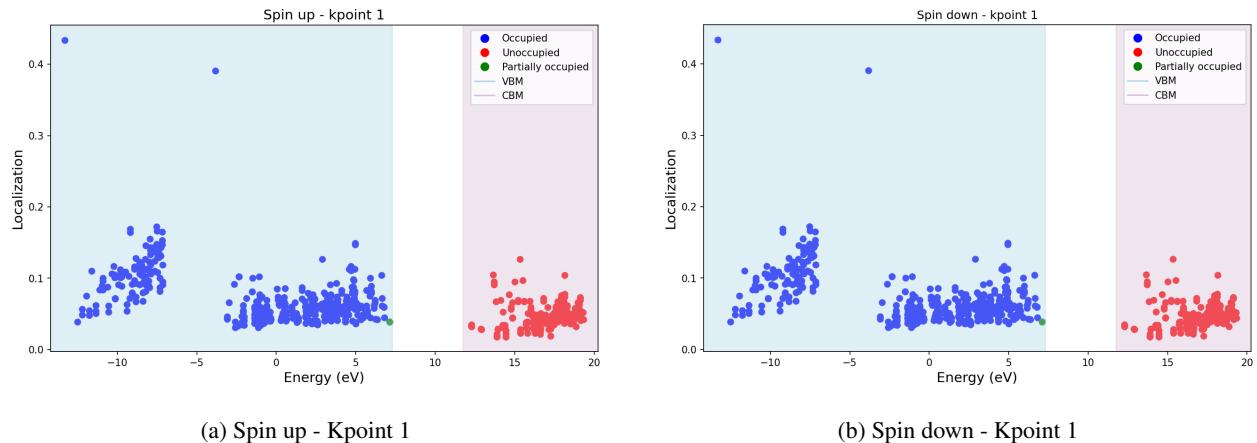


Figure 188: Localization factor using projected orbitals (s, p and d).

## 1.95 Substitutional: $C_B^{-1}$

[Go back to the Table 9](#)

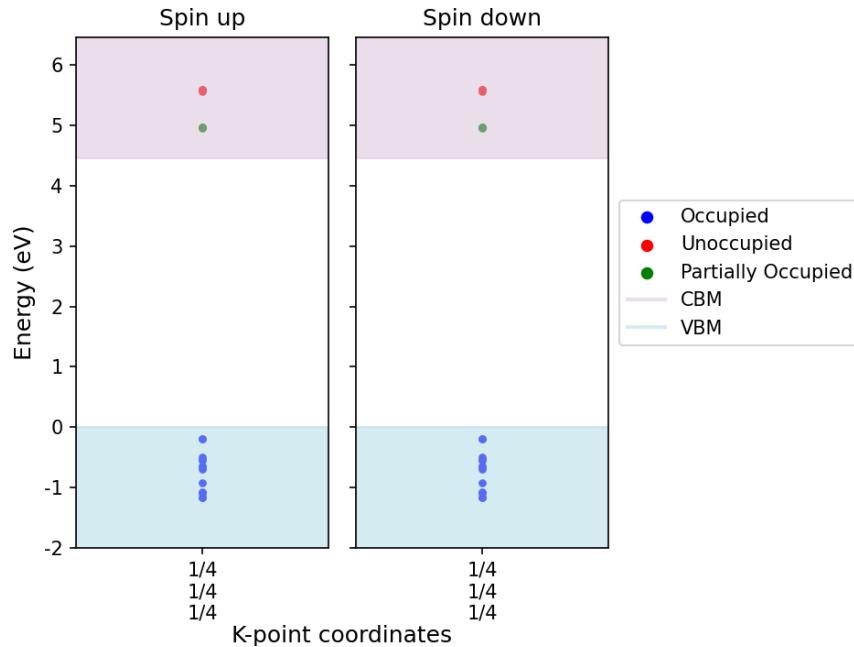


Figure 189: Kohn-Sham states.

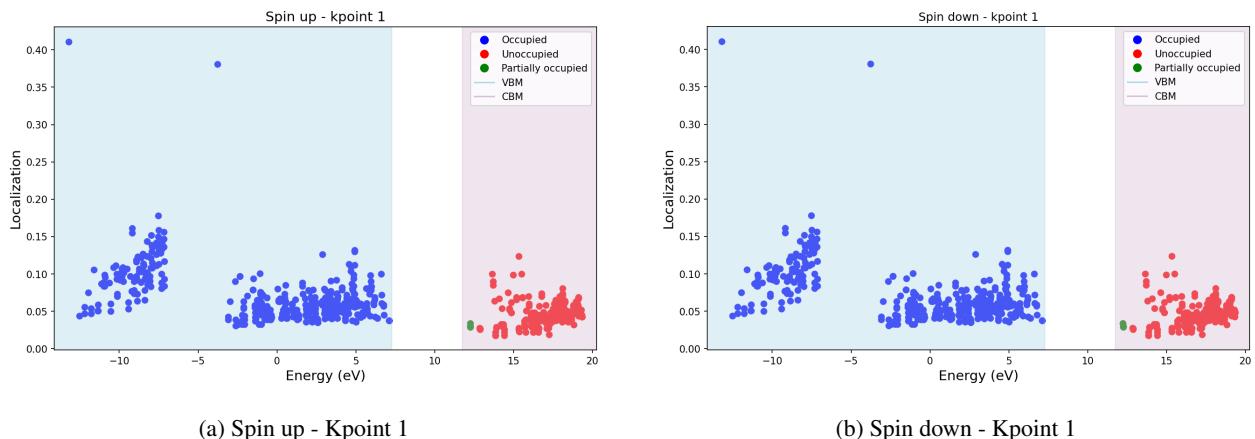


Figure 190: Localization factor using projected orbitals (s, p and d).

## 1.96 Substitutional: $C_B^{-2}$

[Go back to the Table 9](#)

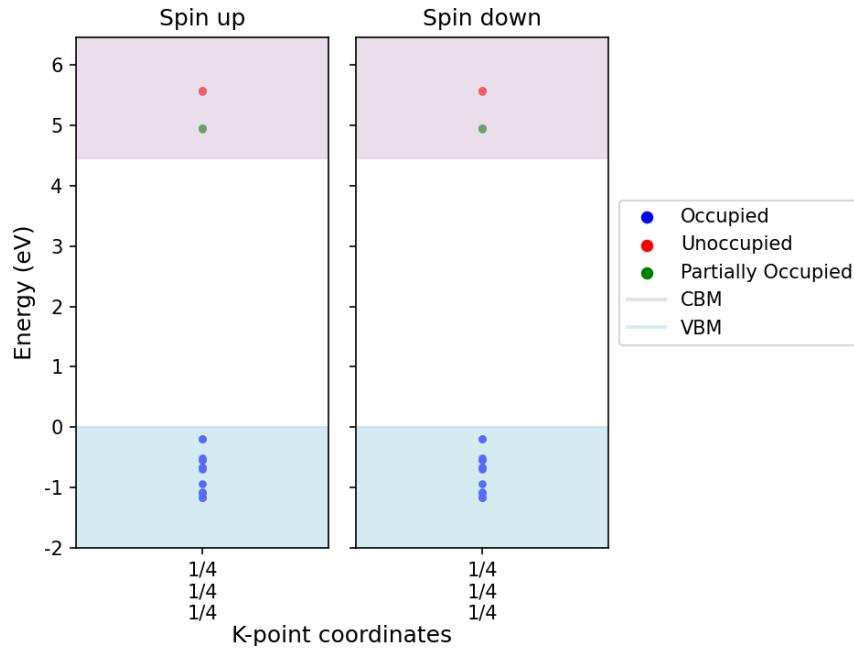


Figure 191: Kohn-Sham states.

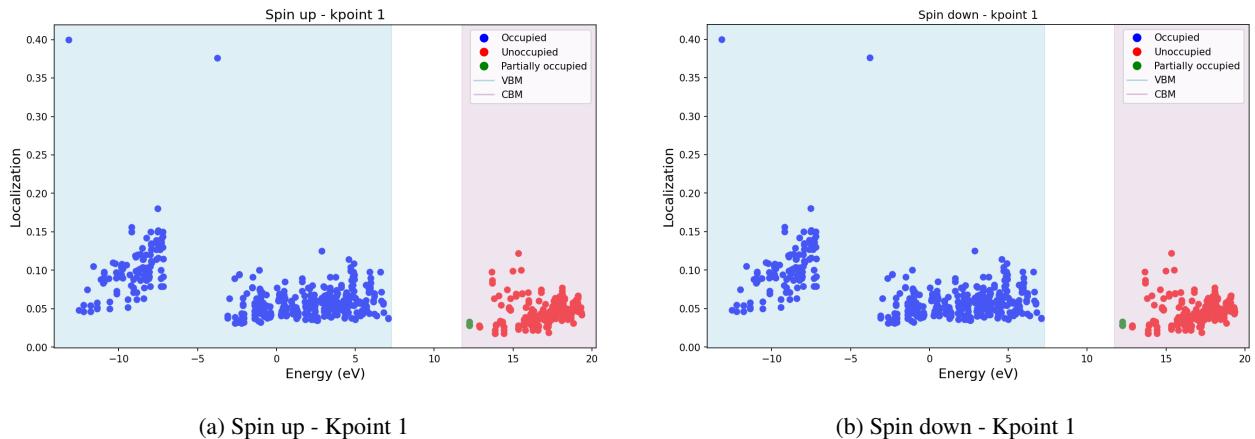


Figure 192: Localization factor using projected orbitals (s, p and d).

### 1.97 Substitutional: $C_N^0$

[Go back to the Table 9](#)

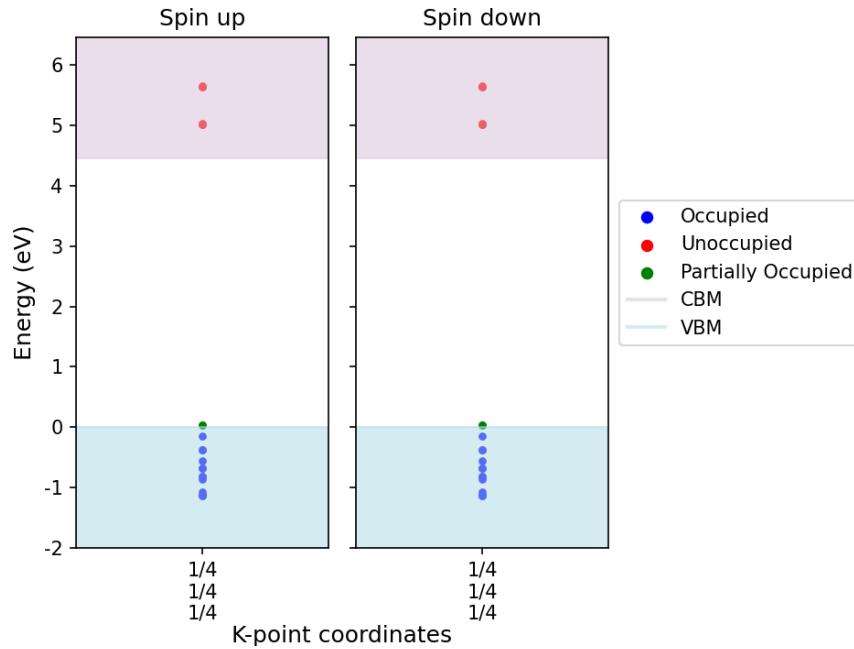


Figure 193: Kohn-Sham states.

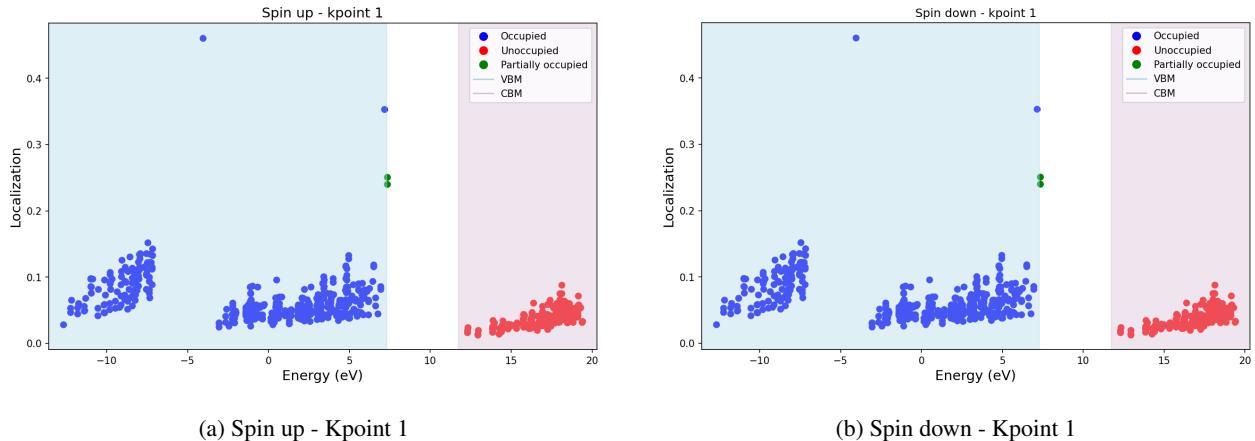


Figure 194: Localization factor using projected orbitals (s, p and d).

## 1.98 Substitutional: $C_N^{+1}$

[Go back to the Table 9](#)

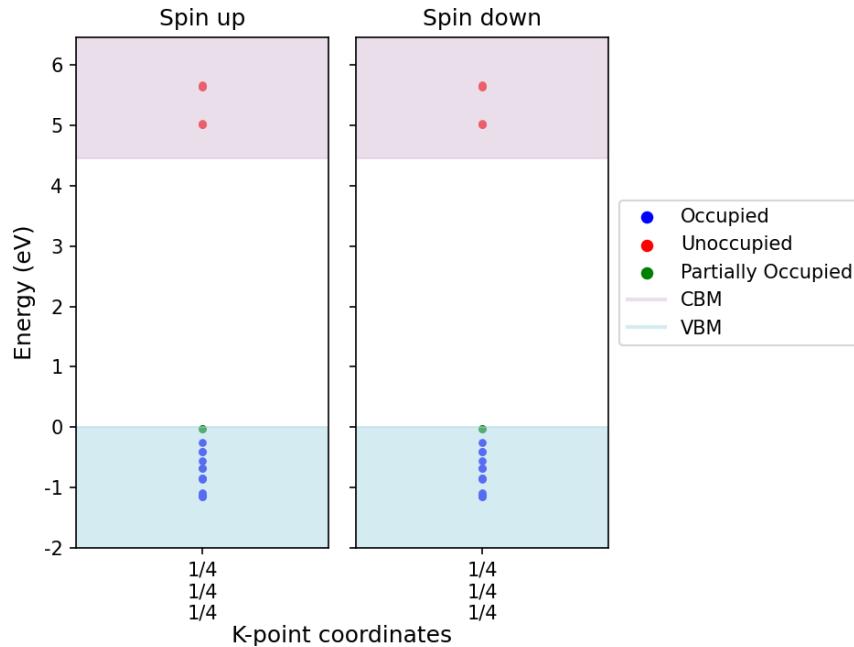


Figure 195: Kohn-Sham states.

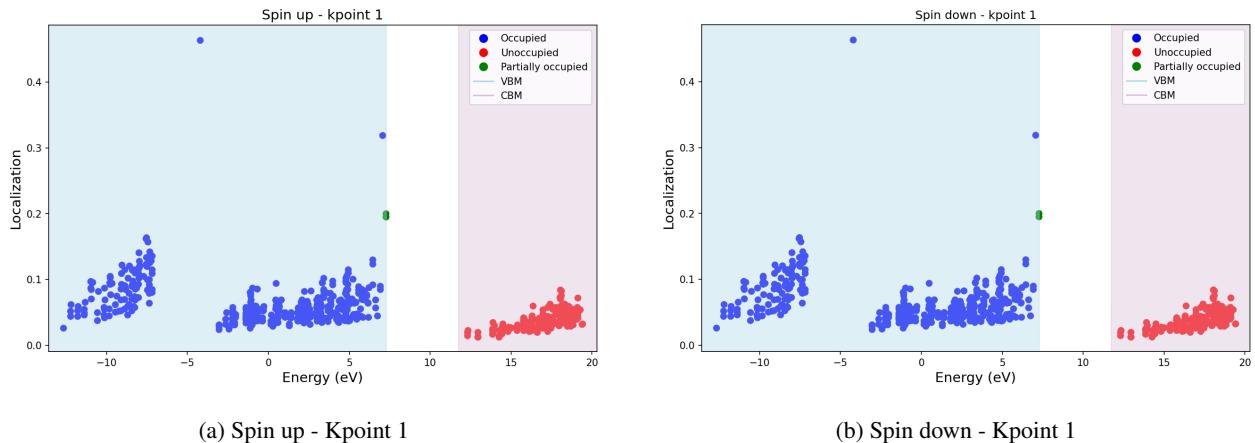


Figure 196: Localization factor using projected orbitals (s, p and d).

### 1.99 Substitutional: $C_N^{+2}$

[Go back to the Table 9](#)

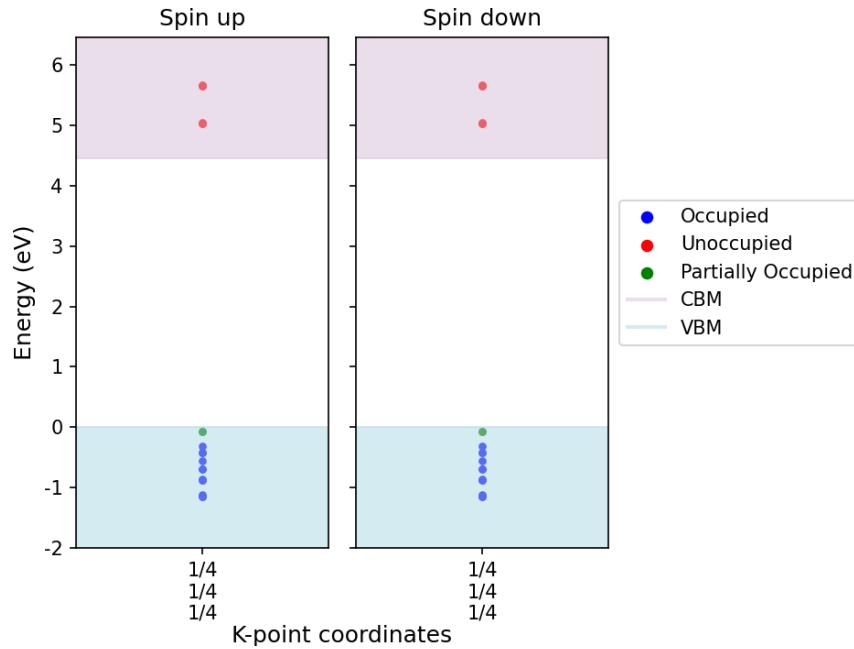


Figure 197: Kohn-Sham states.

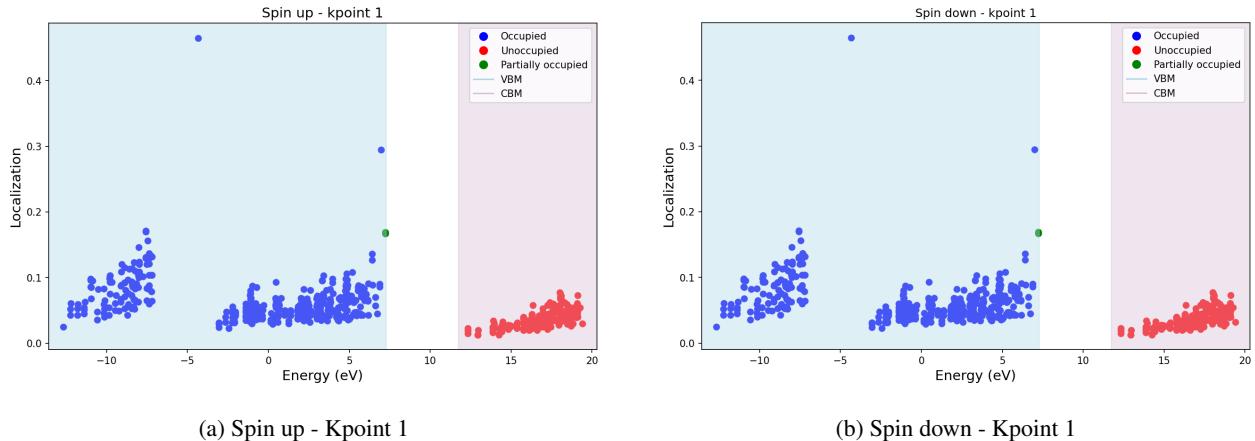


Figure 198: Localization factor using projected orbitals (s, p and d).

## 1.100 Substitutional: $C_N^{-1}$

[Go back to the Table 9](#)

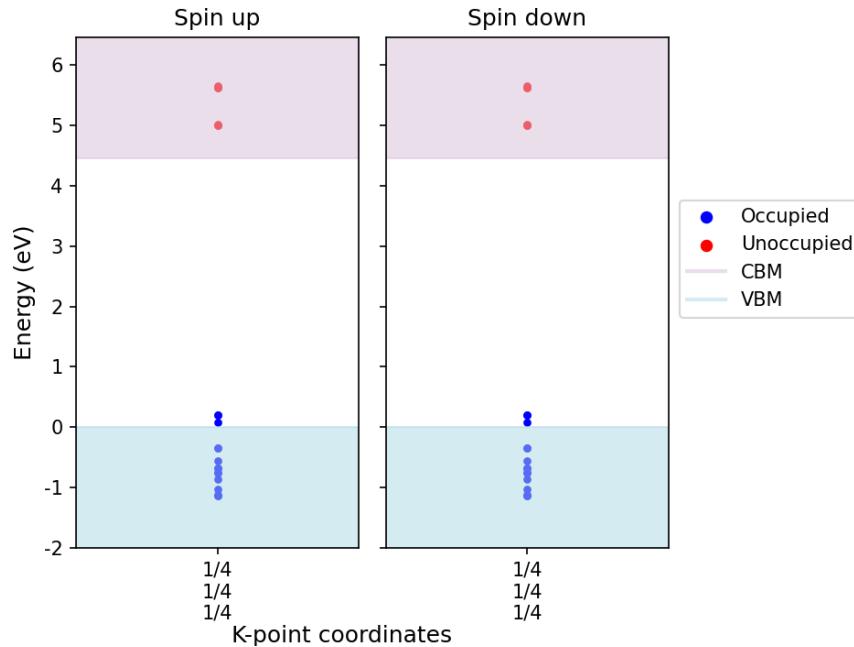


Figure 199: Kohn-Sham states.

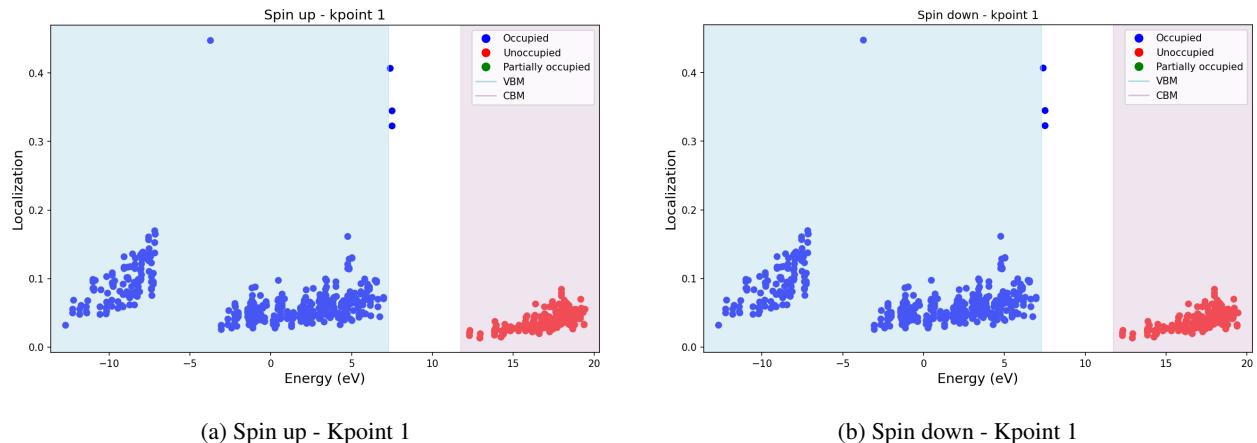


Figure 200: Localization factor using projected orbitals (s, p and d).

### 1.101 Substitutional: $C_N^{-2}$

[Go back to the Table 9](#)

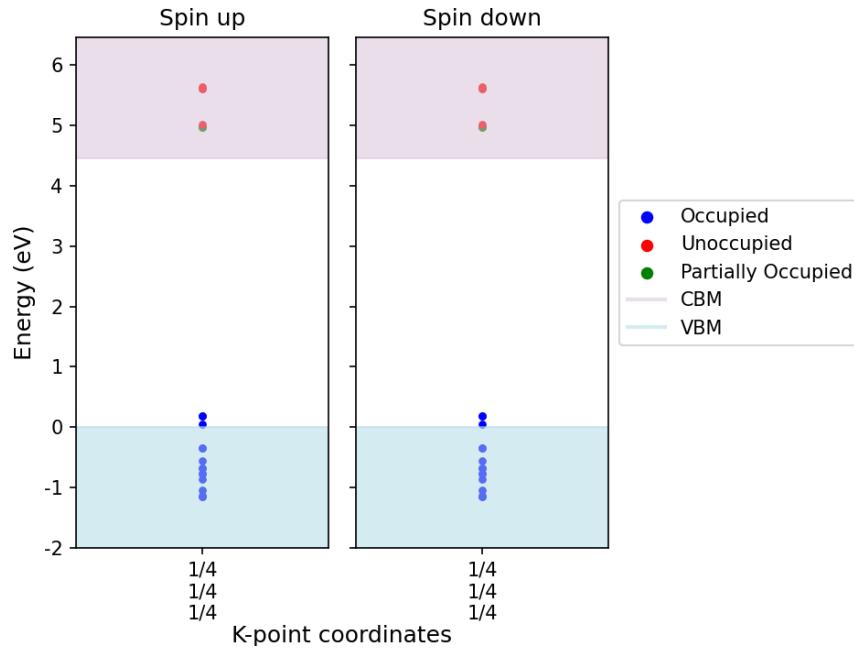


Figure 201: Kohn-Sham states.

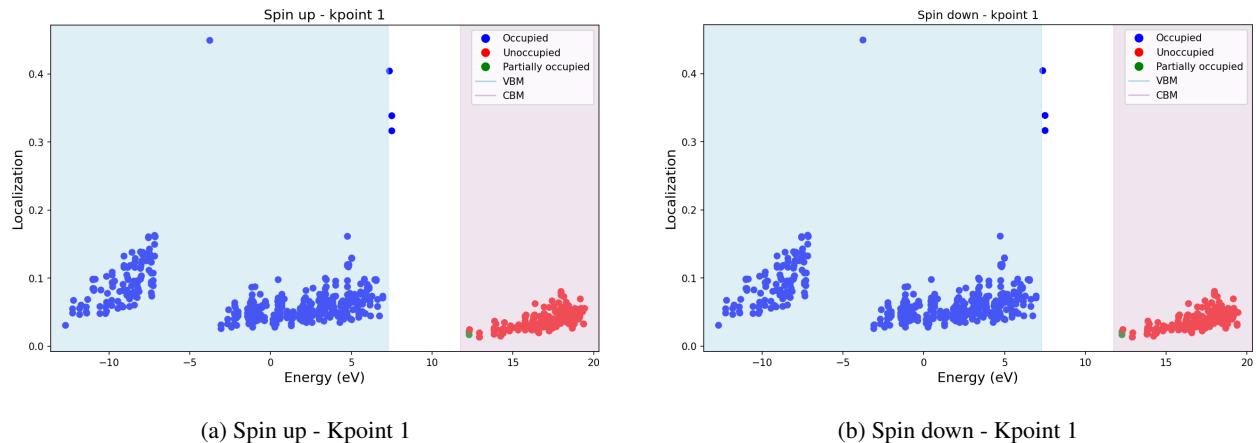


Figure 202: Localization factor using projected orbitals (s, p and d).

## 1.102 Substitutional: $O_B^0$

[Go back to the Table 9](#)

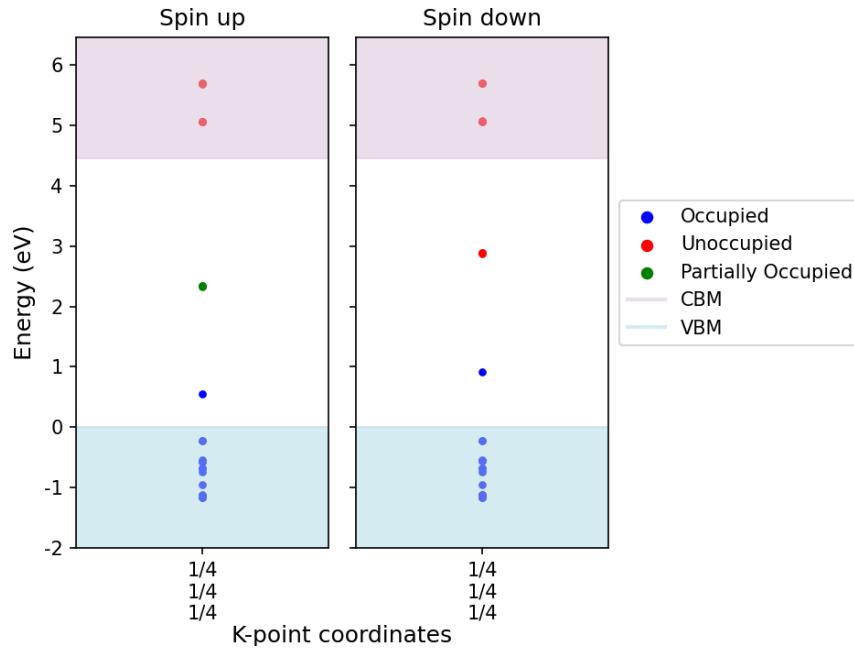


Figure 203: Kohn-Sham states.

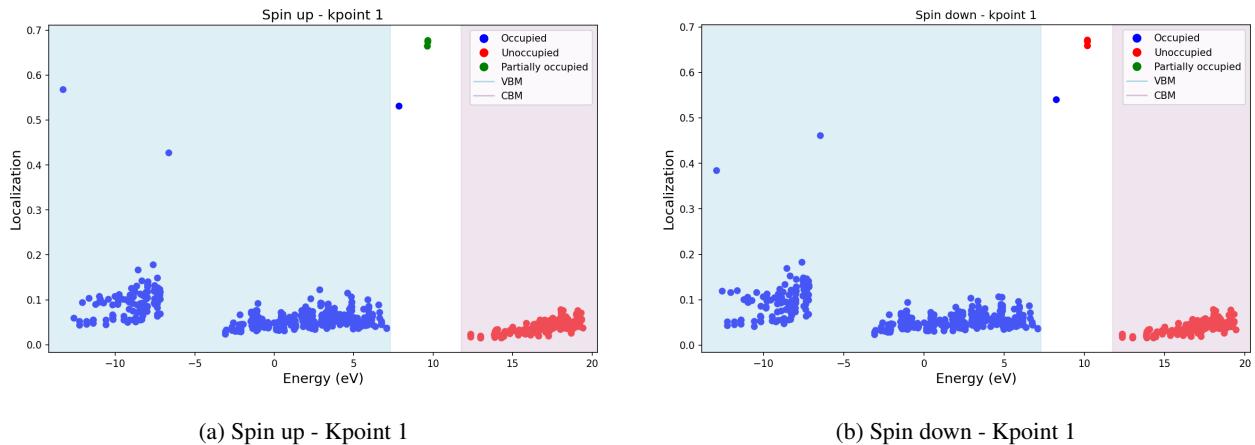


Figure 204: Localization factor using projected orbitals (s, p and d).

### 1.103 Substitutional: $O_B^{+1}$

[Go back to the Table 9](#)

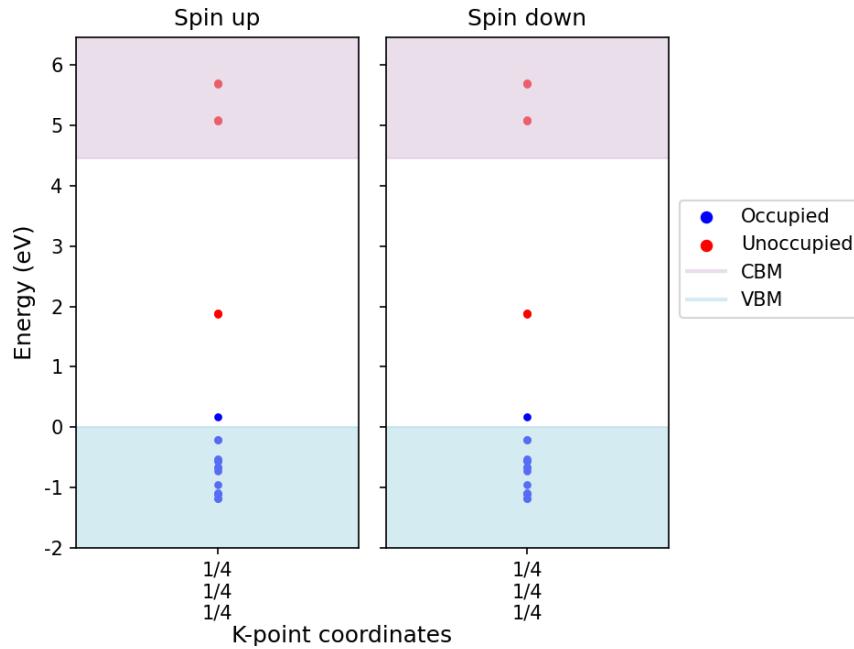


Figure 205: Kohn-Sham states.

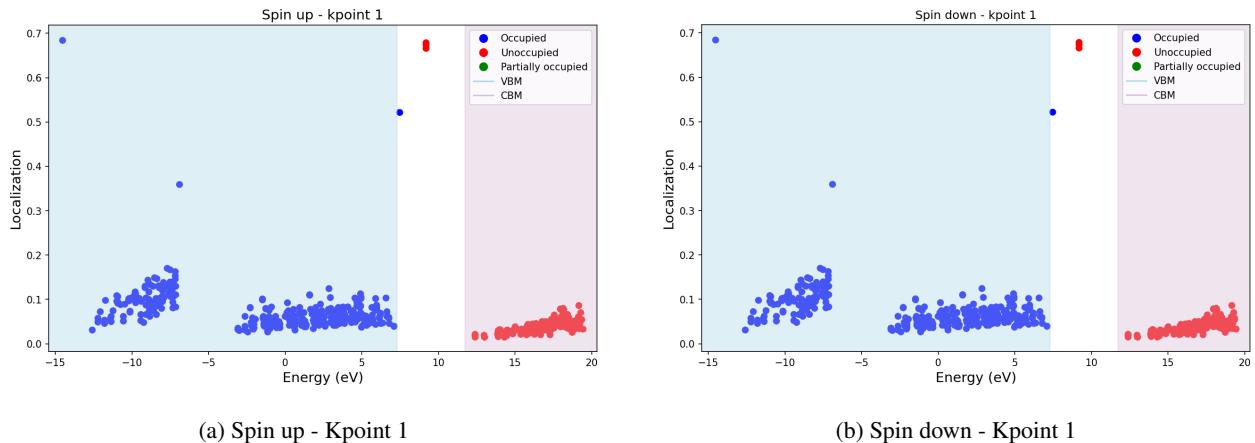


Figure 206: Localization factor using projected orbitals (s, p and d).

## 1.104 Substitutional: $O_B^{+2}$

[Go back to the Table 9](#)

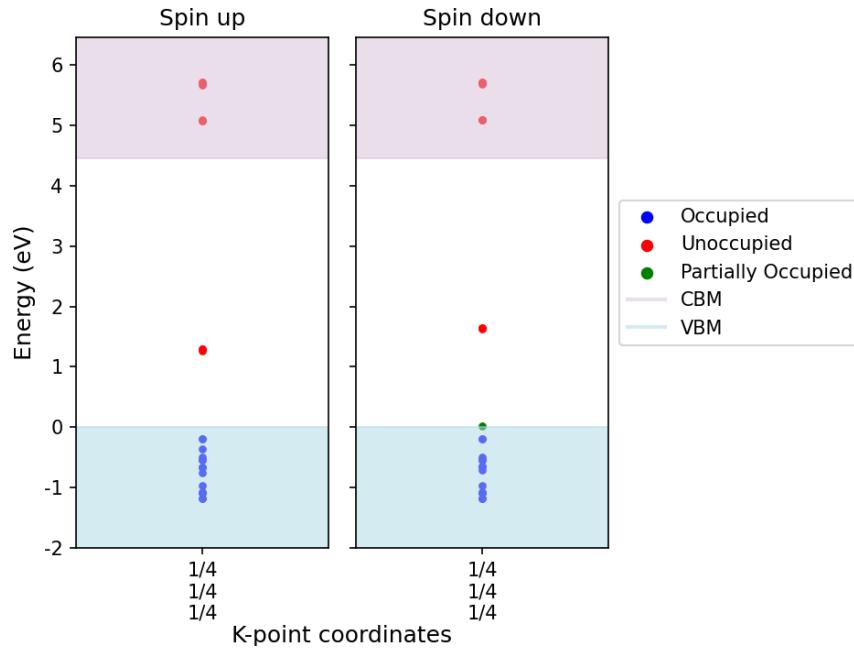


Figure 207: Kohn-Sham states.

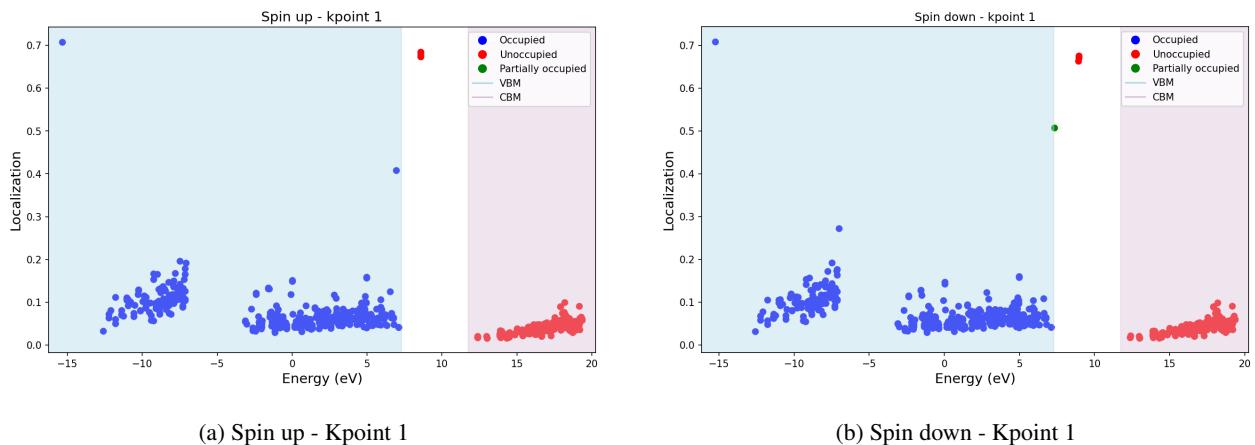


Figure 208: Localization factor using projected orbitals (s, p and d).

### 1.105 Substitutional: $O_B^{-1}$

[Go back to the Table 9](#)

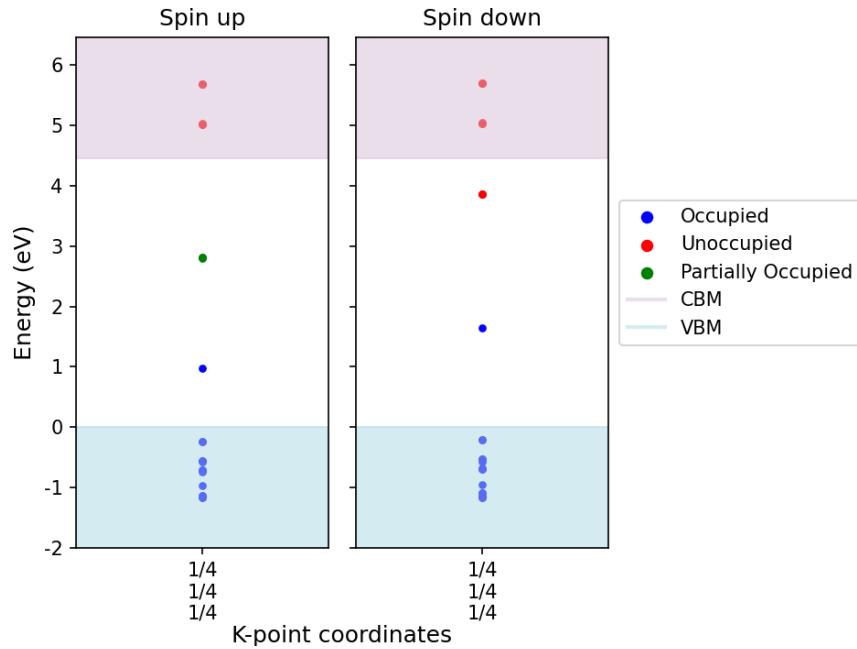


Figure 209: Kohn-Sham states.

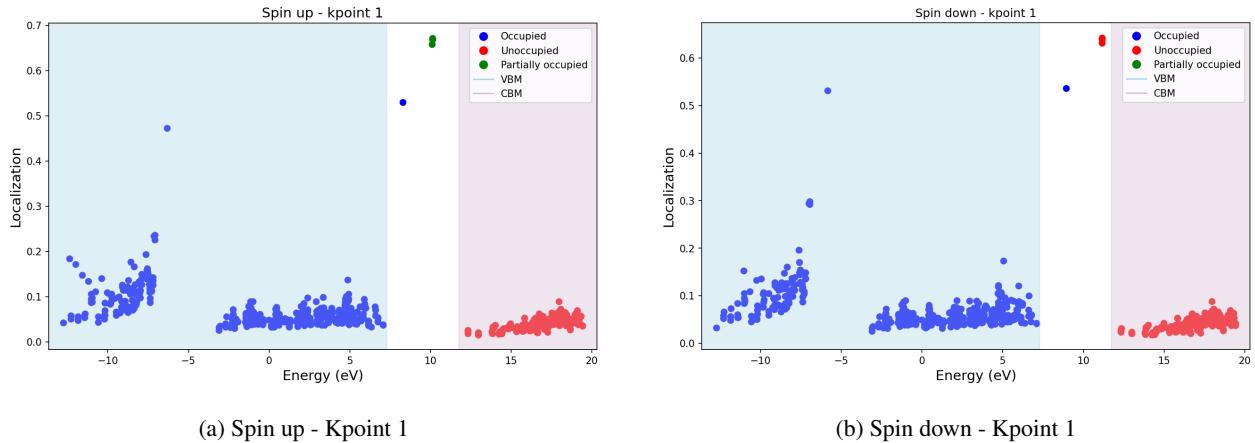


Figure 210: Localization factor using projected orbitals (s, p and d).

## 1.106 Substitutional: $O_B^{-2}$

[Go back to the Table 9](#)

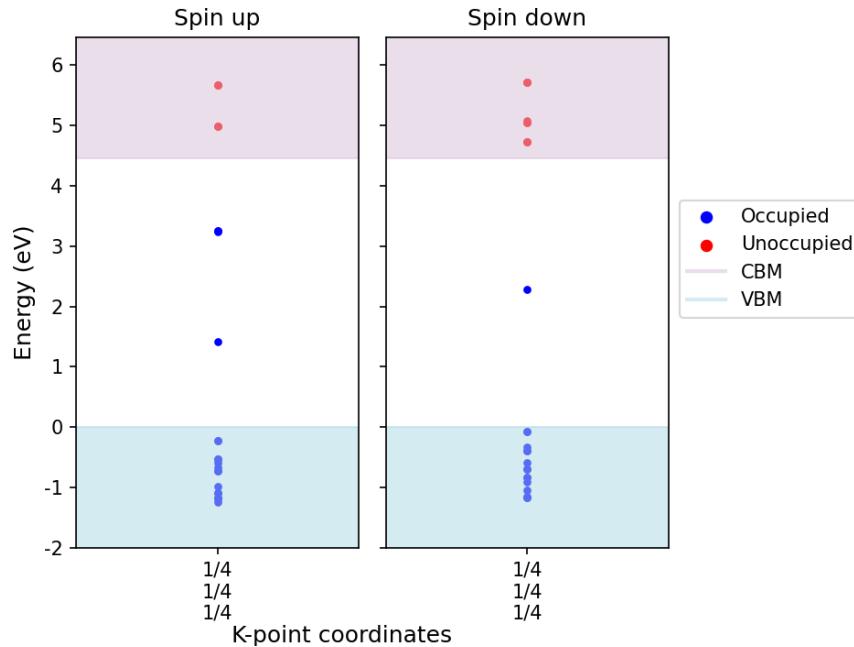


Figure 211: Kohn-Sham states.

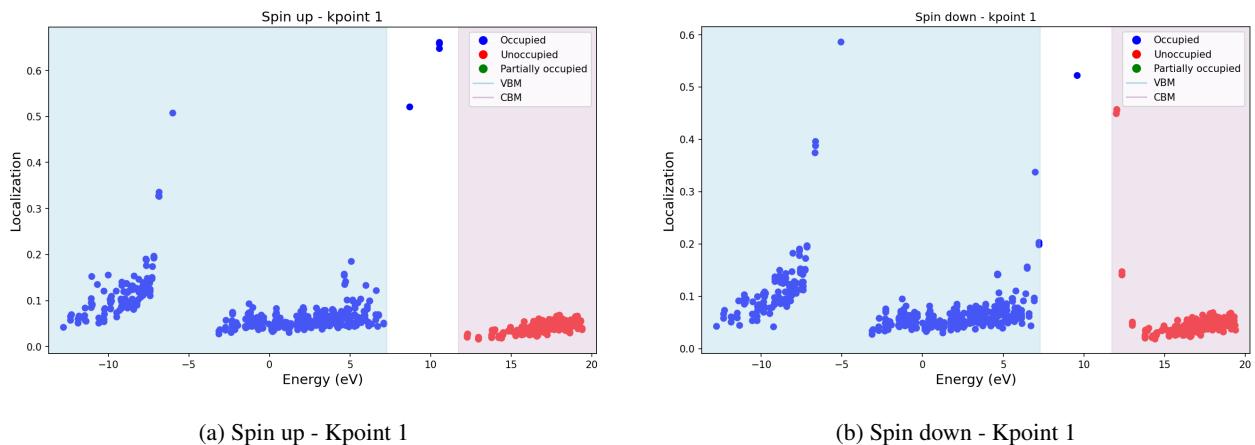


Figure 212: Localization factor using projected orbitals (s, p and d).

### 1.107 Substitutional: $O_N^0$

[Go back to the Table 9](#)

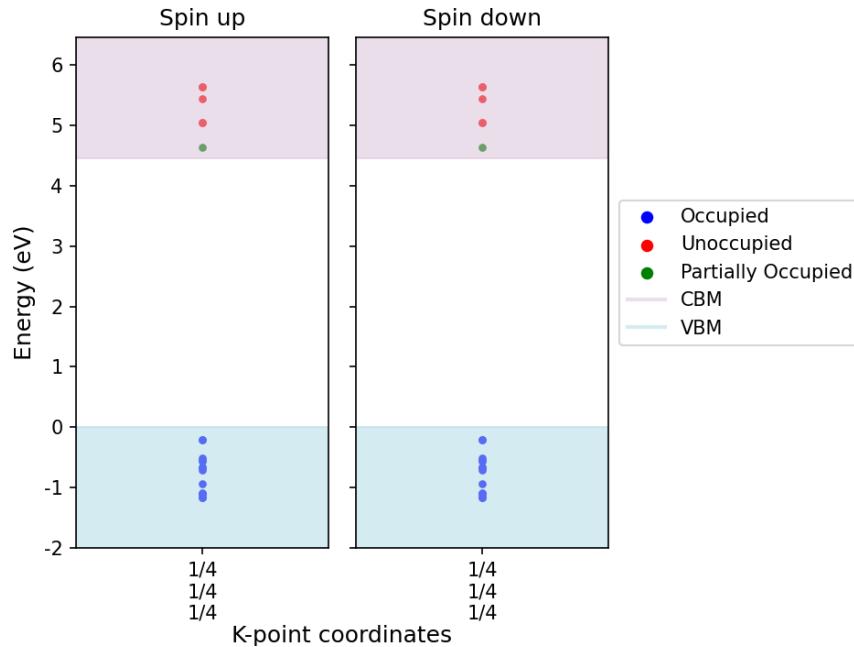


Figure 213: Kohn-Sham states.

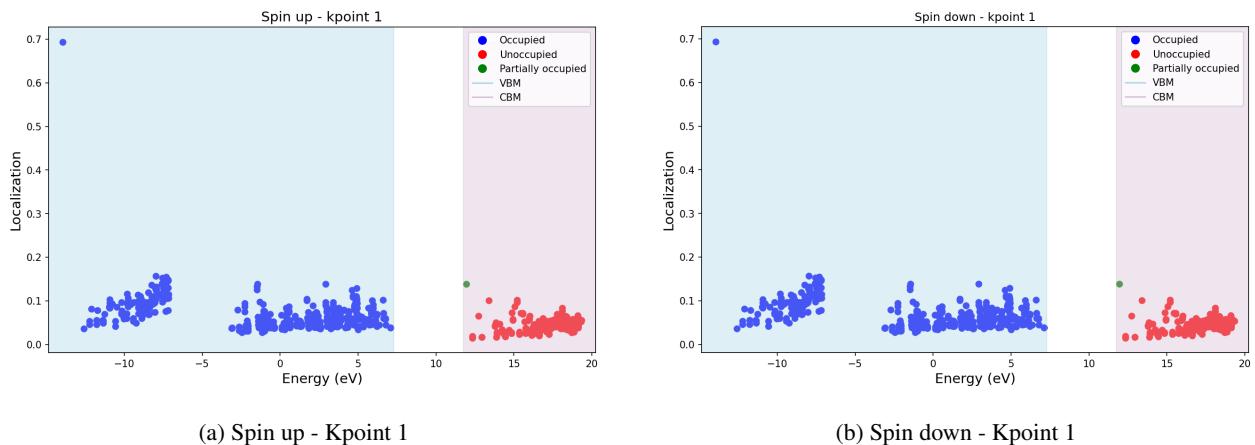


Figure 214: Localization factor using projected orbitals (s, p and d).

### 1.108 Substitutional: $O_N^{+1}$

[Go back to the Table 9](#)

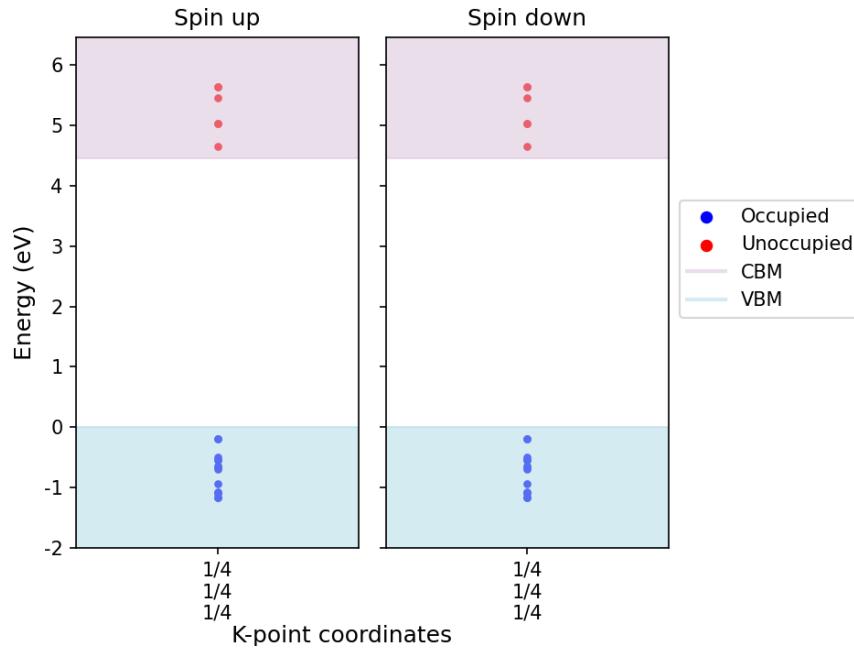


Figure 215: Kohn-Sham states.

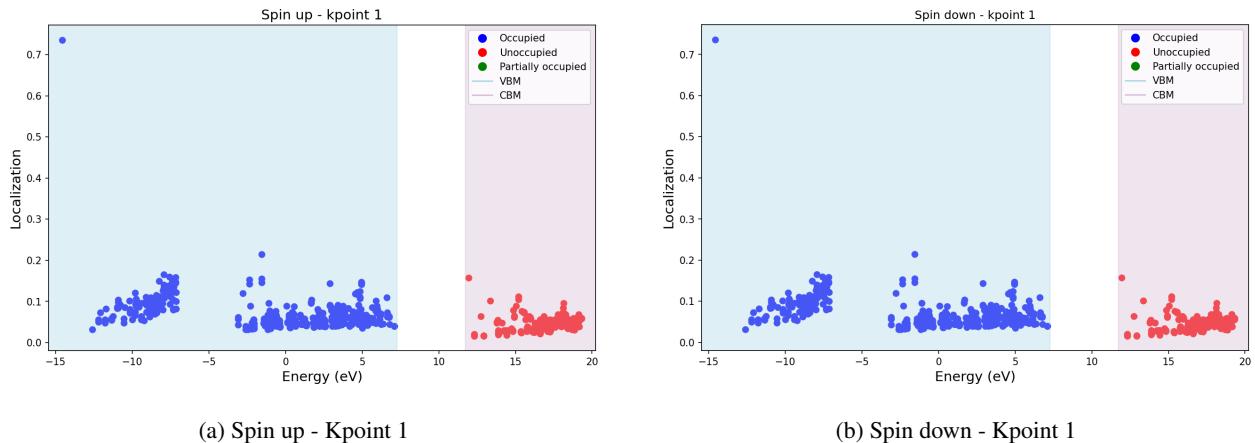


Figure 216: Localization factor using projected orbitals (s, p and d).

## 1.109 Substitutional: $O_N^{+2}$

[Go back to the Table 9](#)

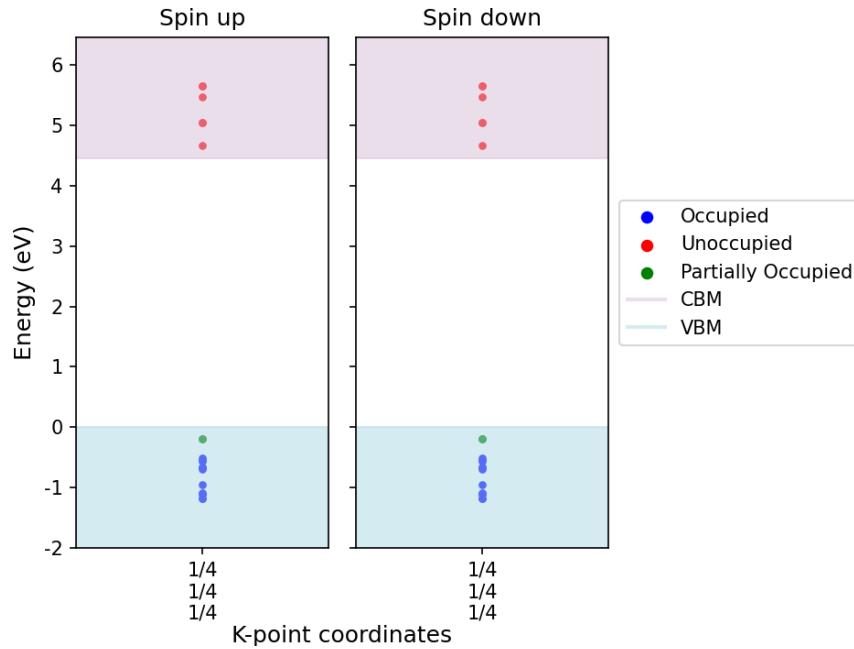


Figure 217: Kohn-Sham states.

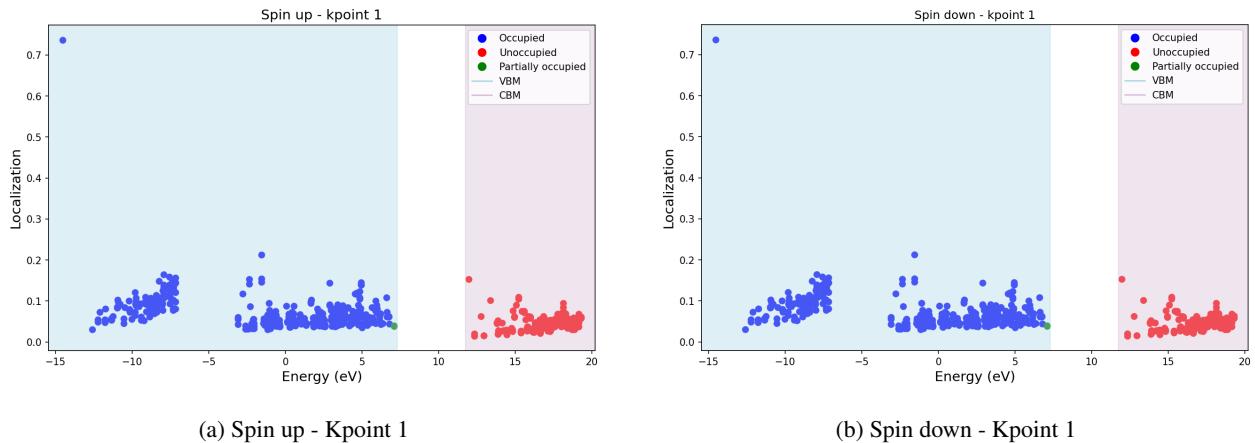


Figure 218: Localization factor using projected orbitals (s, p and d).

### 1.110 Substitutional: $O_N^{-1}$

[Go back to the Table 9](#)

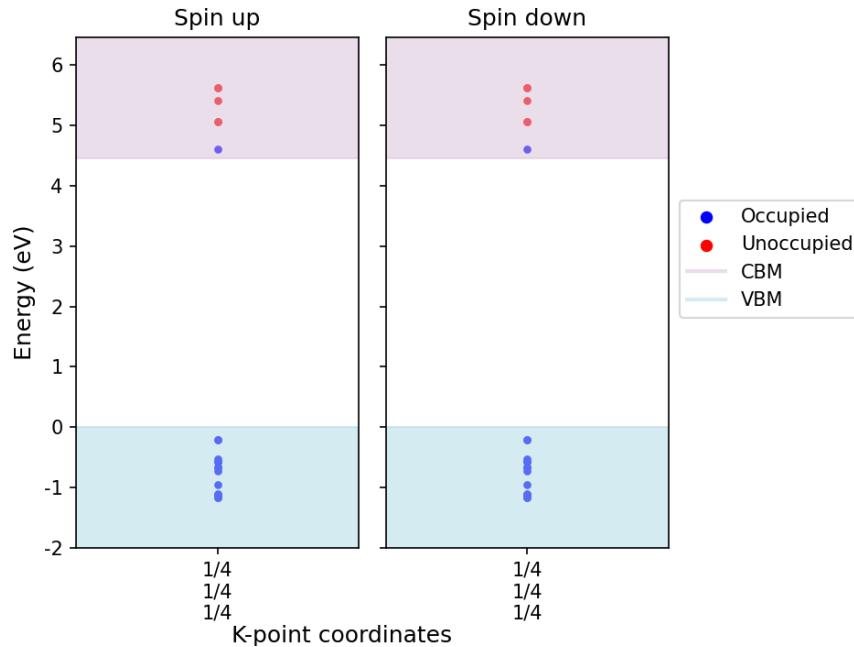


Figure 219: Kohn-Sham states.

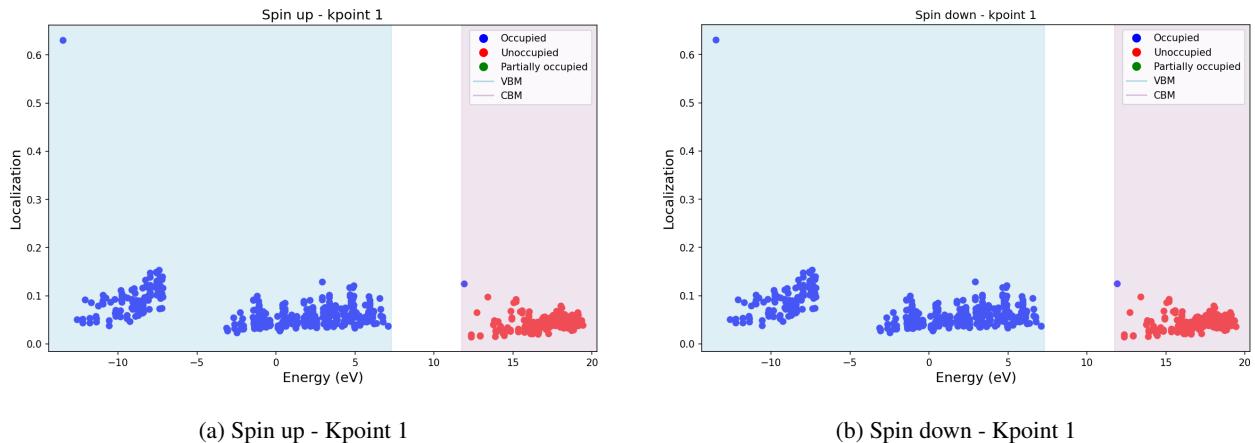


Figure 220: Localization factor using projected orbitals (s, p and d).

### 1.111 Substitutional: $O_N^{-2}$

[Go back to the Table 9](#)

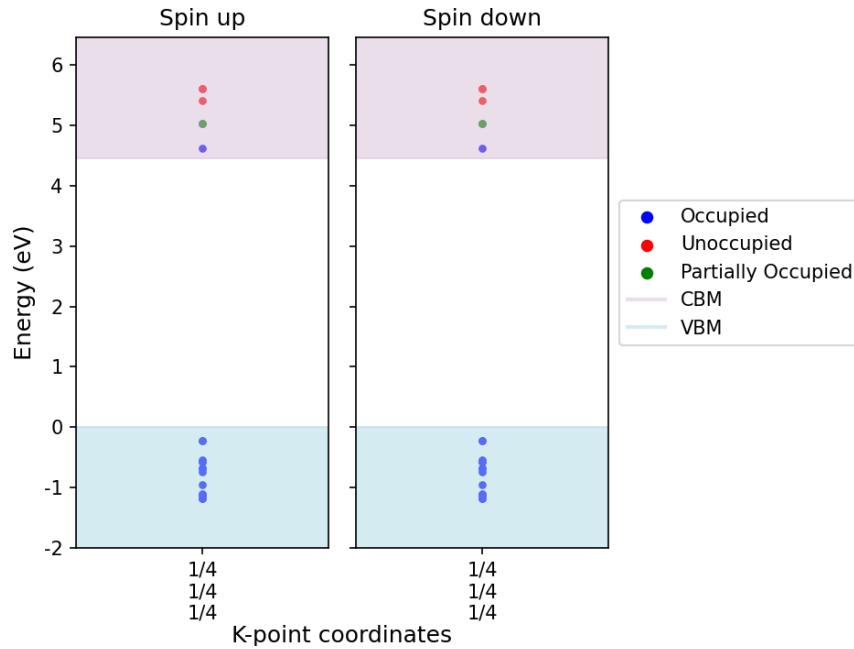


Figure 221: Kohn-Sham states.

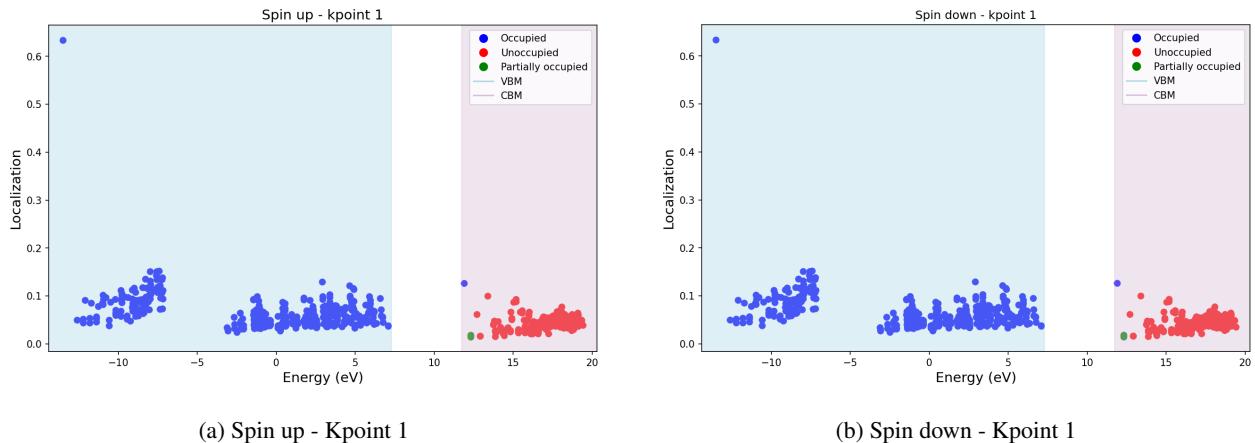


Figure 222: Localization factor using projected orbitals (s, p and d).

### 1.112 Complex: $(V_B - O_N)^0$

[Go back to the Table 9](#)

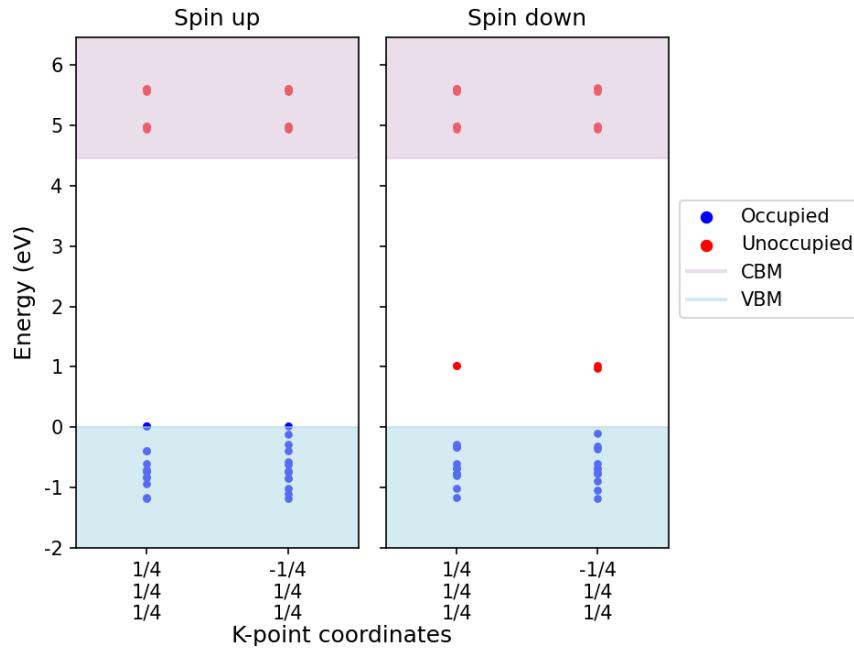


Figure 223: Kohn-Sham states.

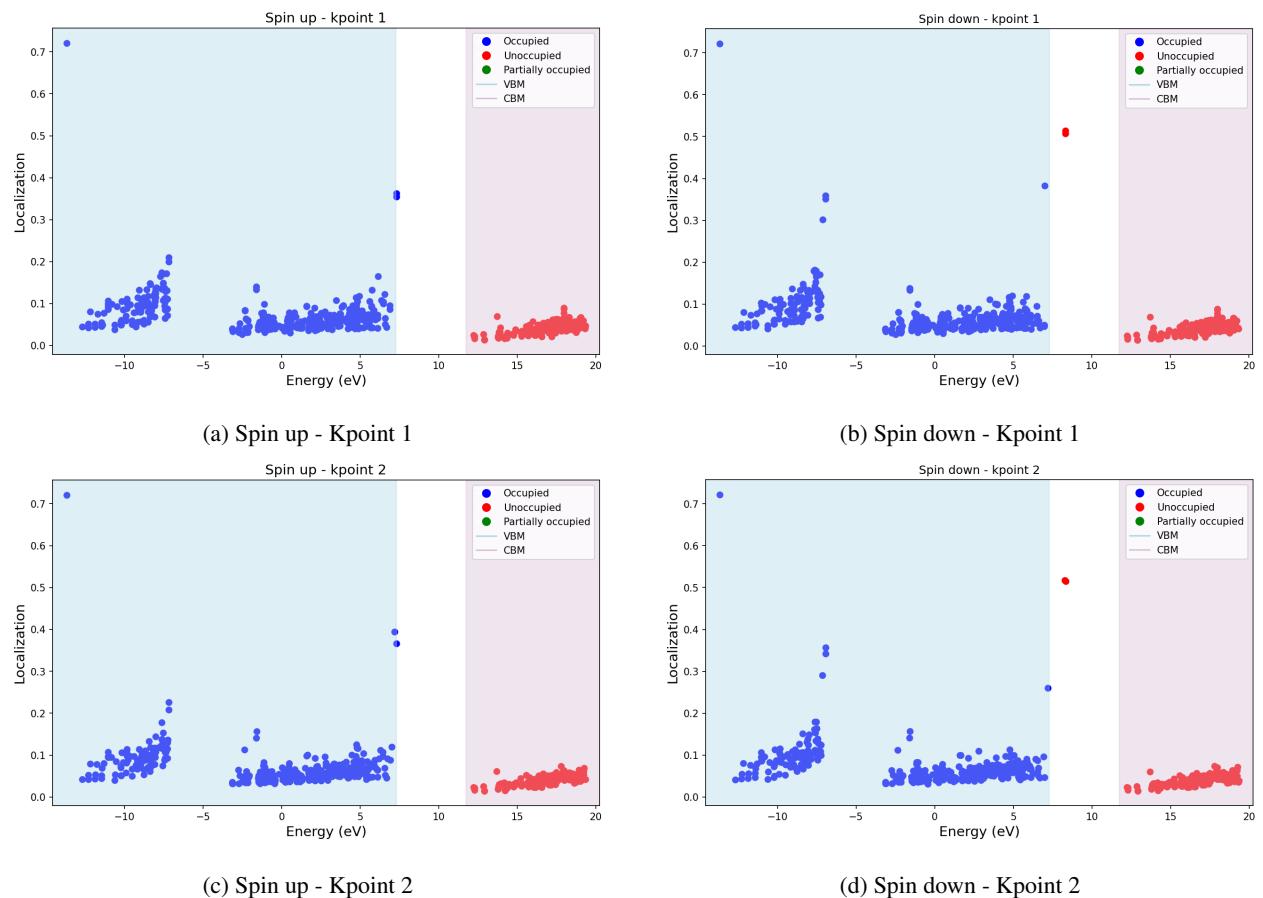


Figure 224: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

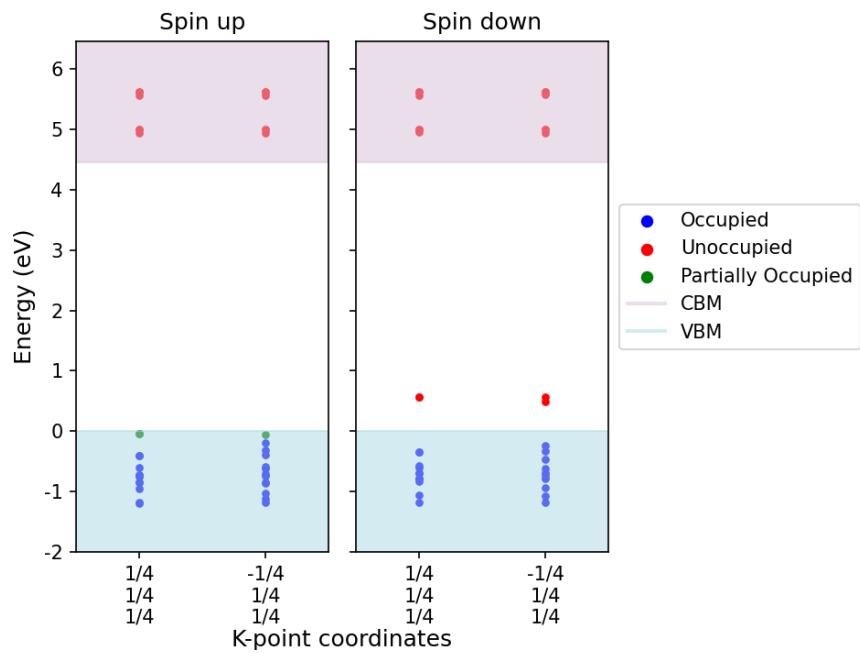


Figure 225: Kohn-Sham states.

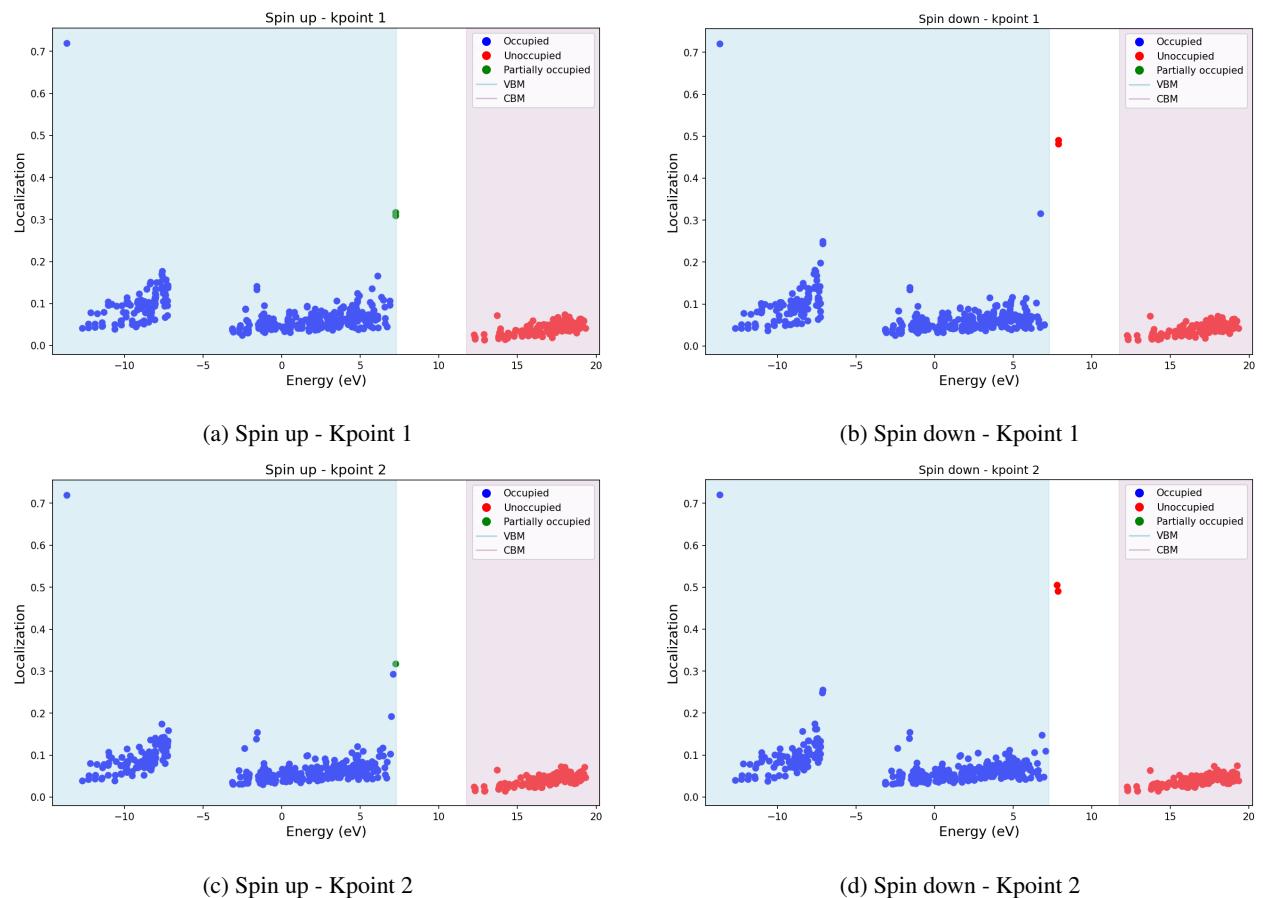


Figure 226: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

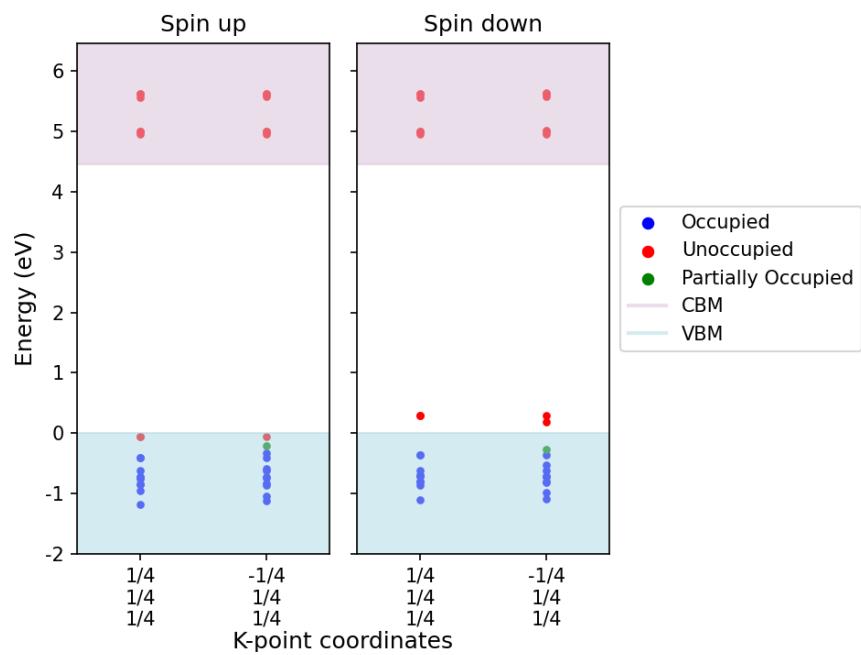


Figure 227: Kohn-Sham states.

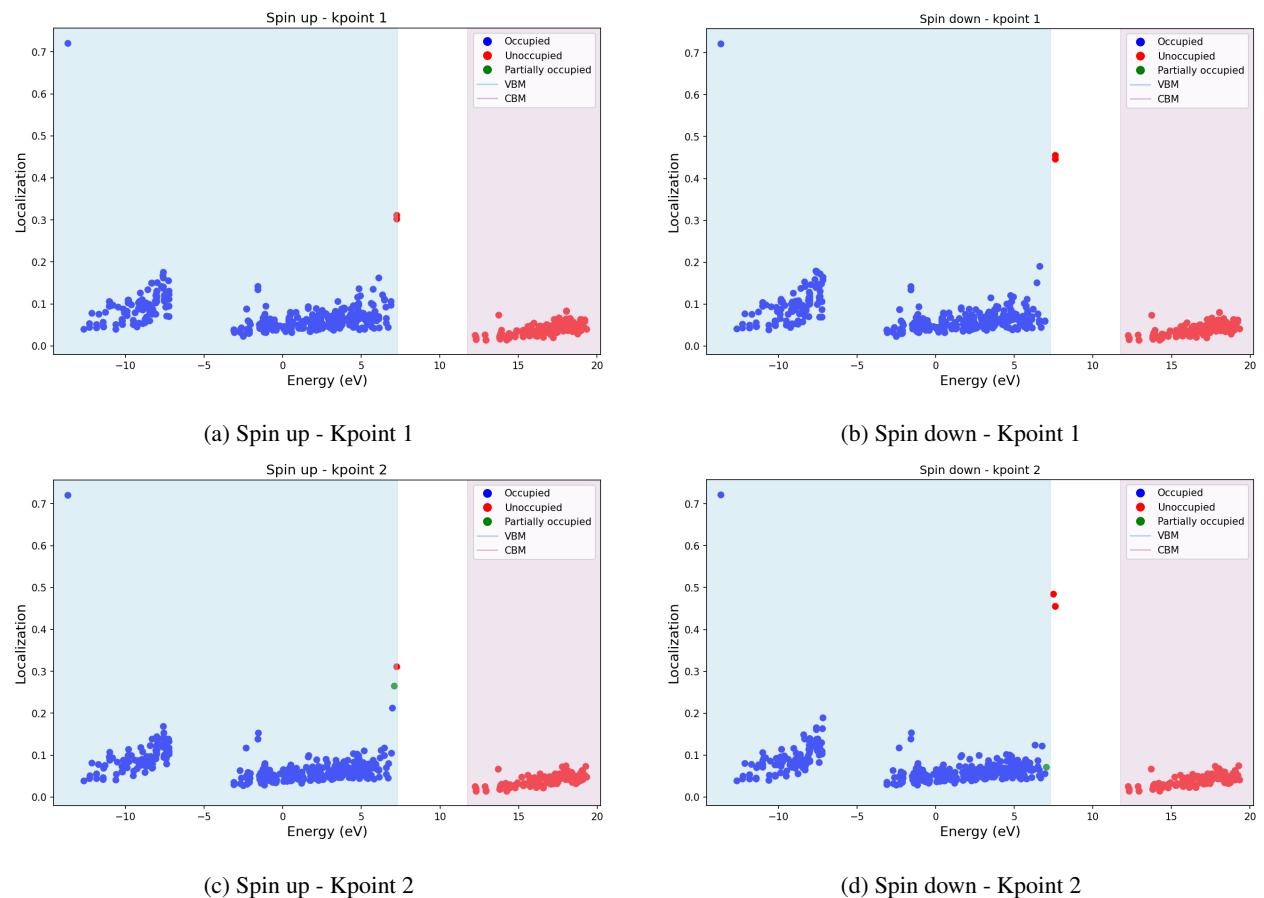


Figure 228: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

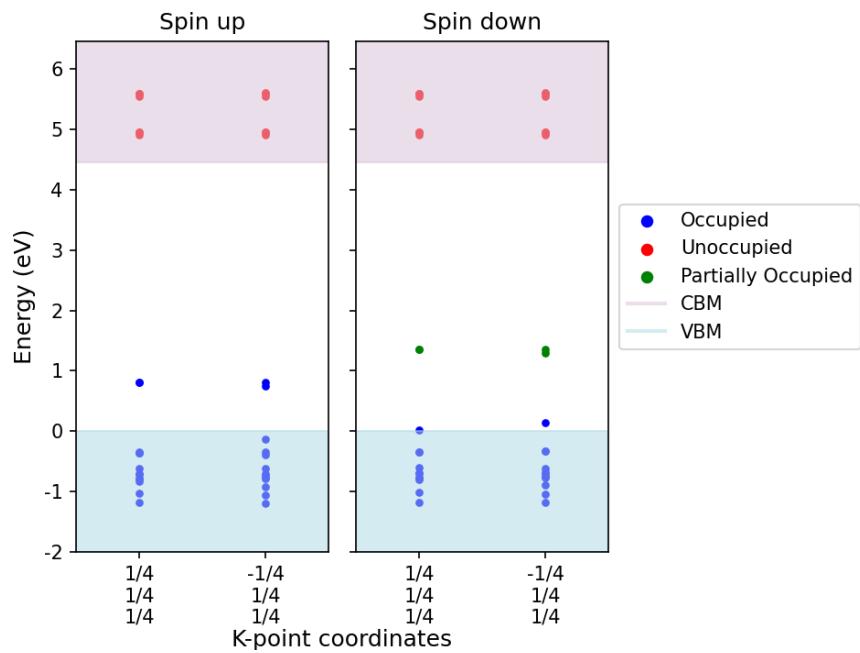


Figure 229: Kohn-Sham states.

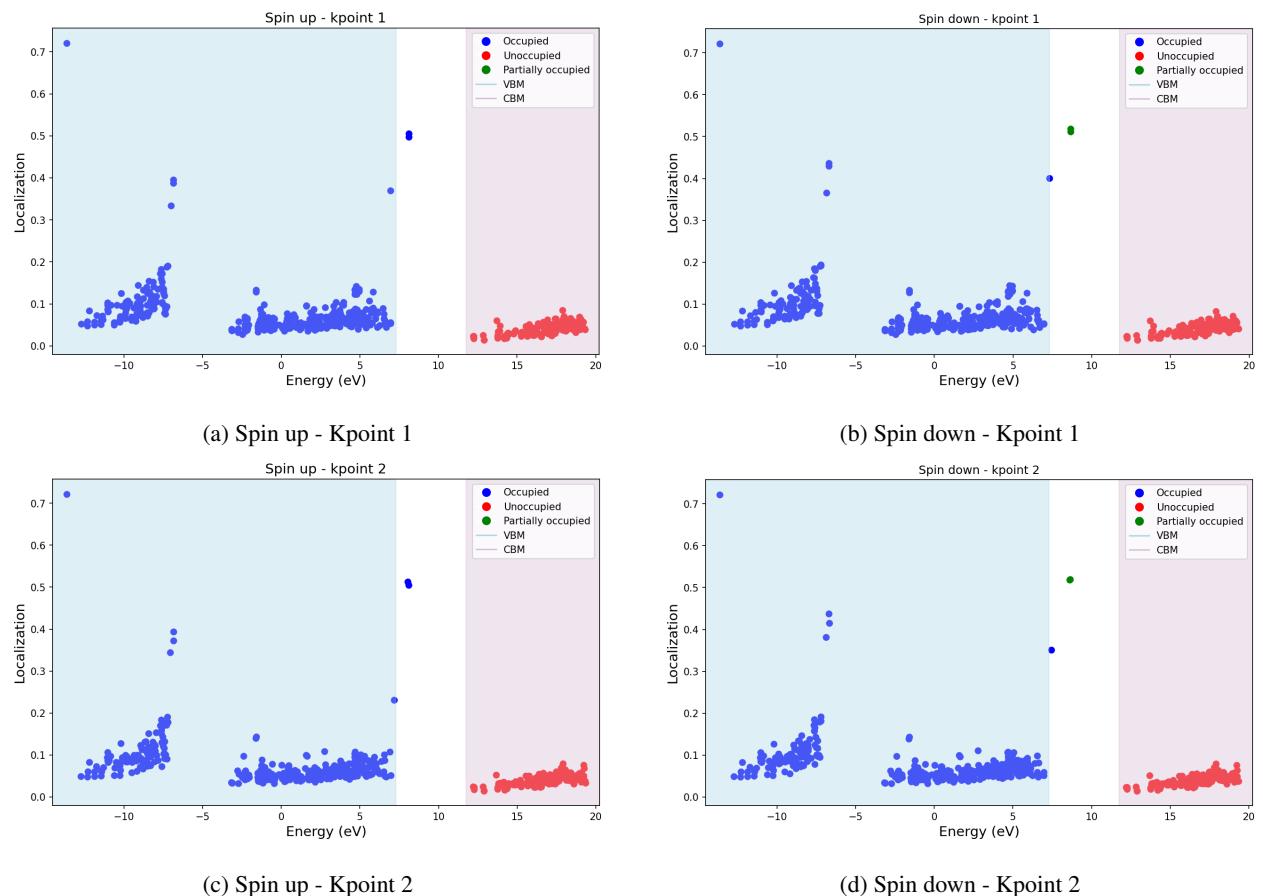


Figure 230: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

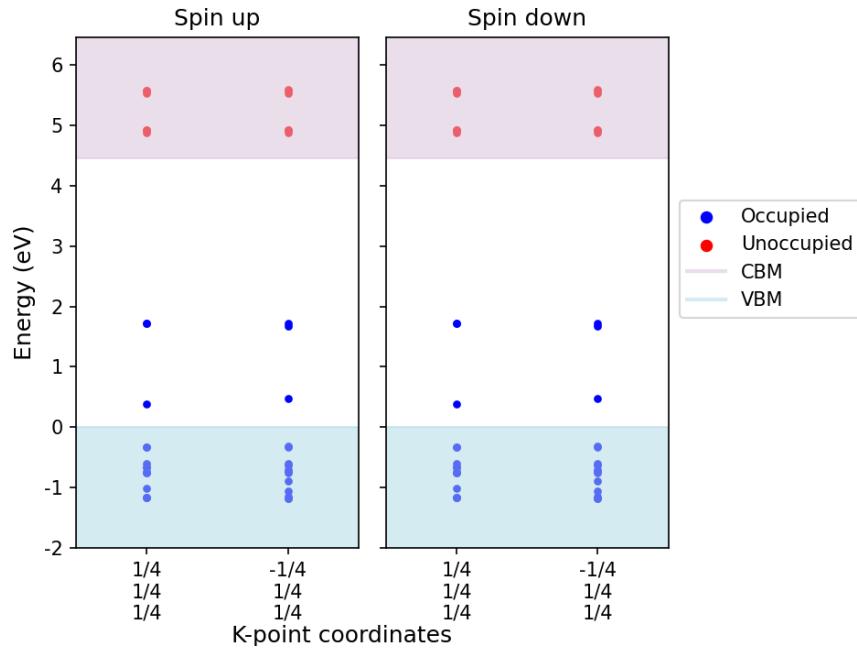


Figure 231: Kohn-Sham states.

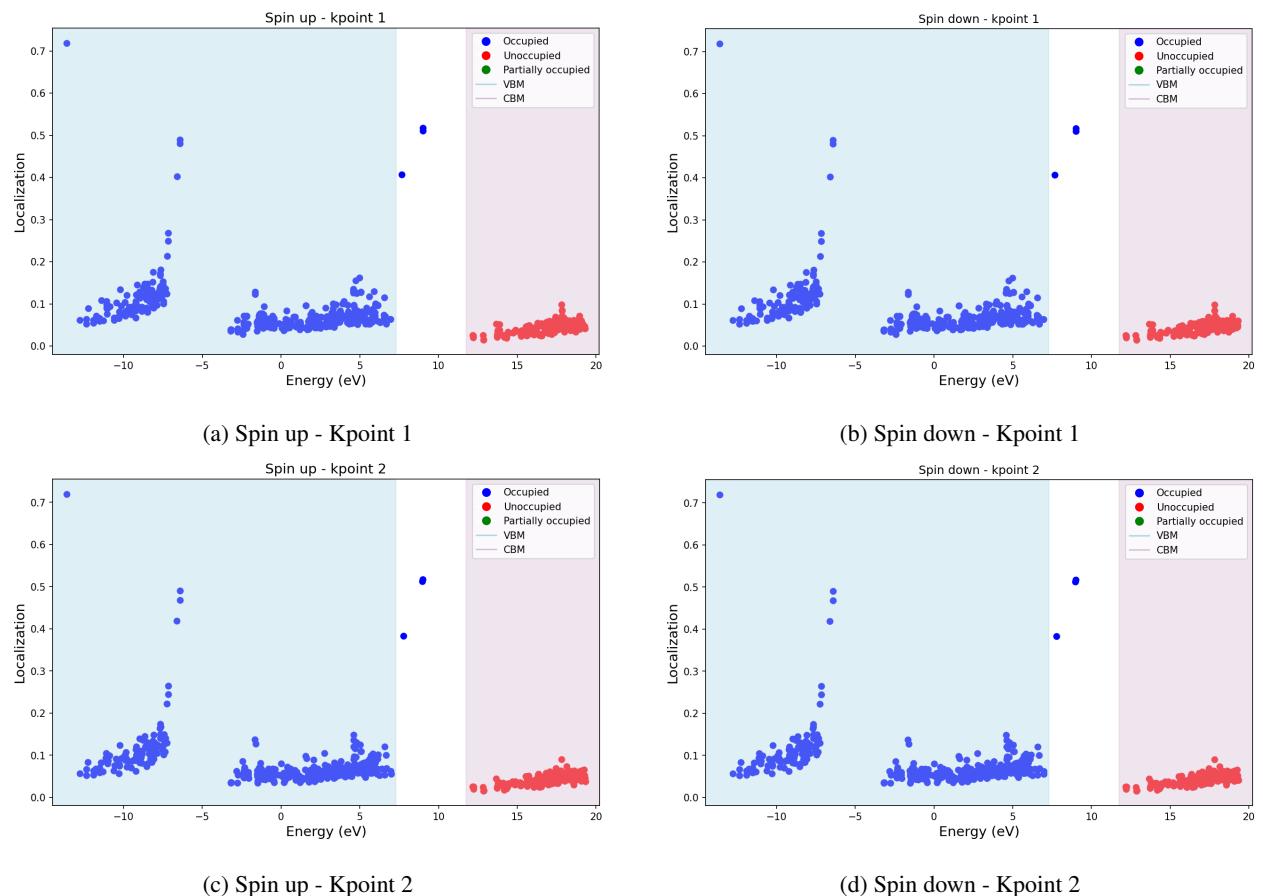


Figure 232: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

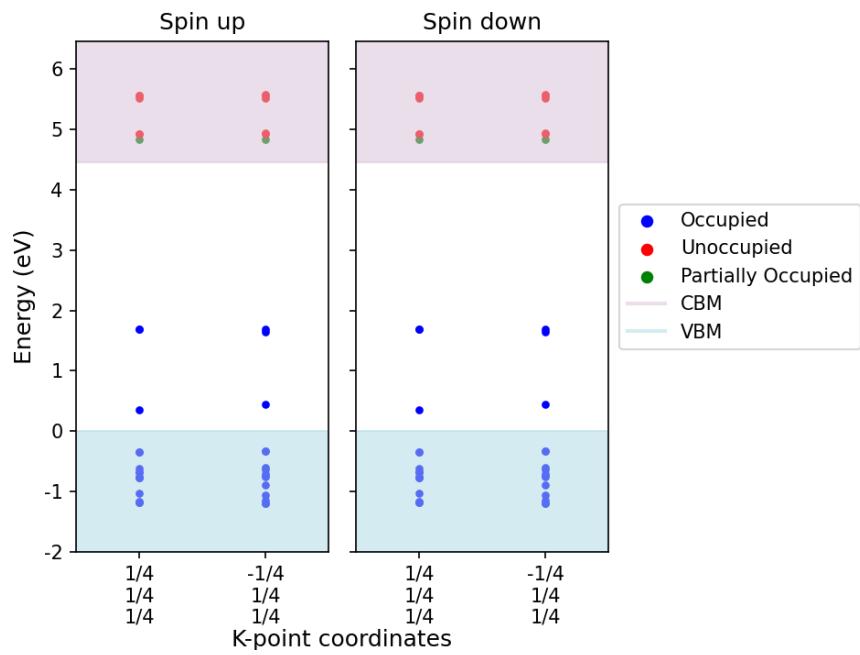


Figure 233: Kohn-Sham states.

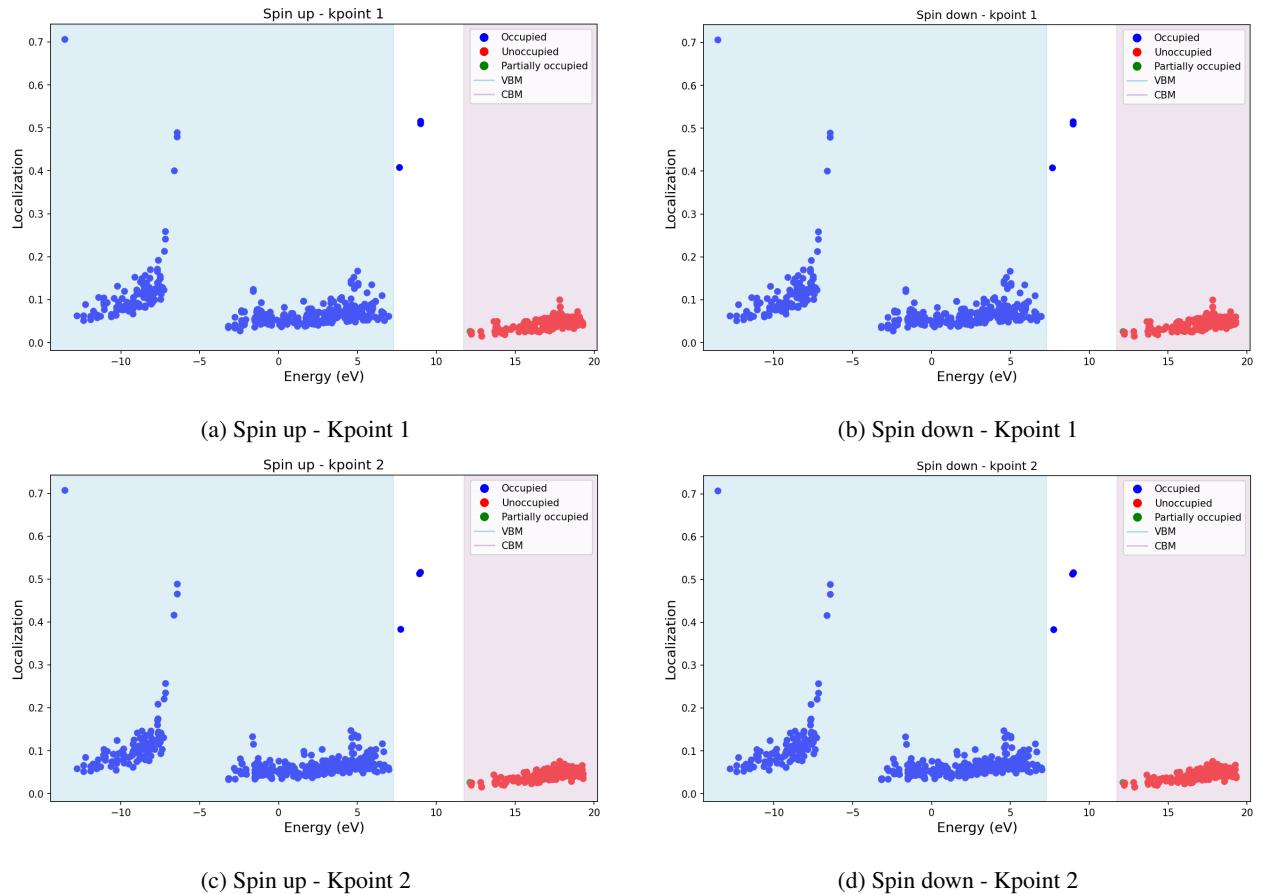


Figure 234: Localization factor using projected orbitals (s, p, and d).

### 1.118 Complex: $(V_B - Si_B)^0$

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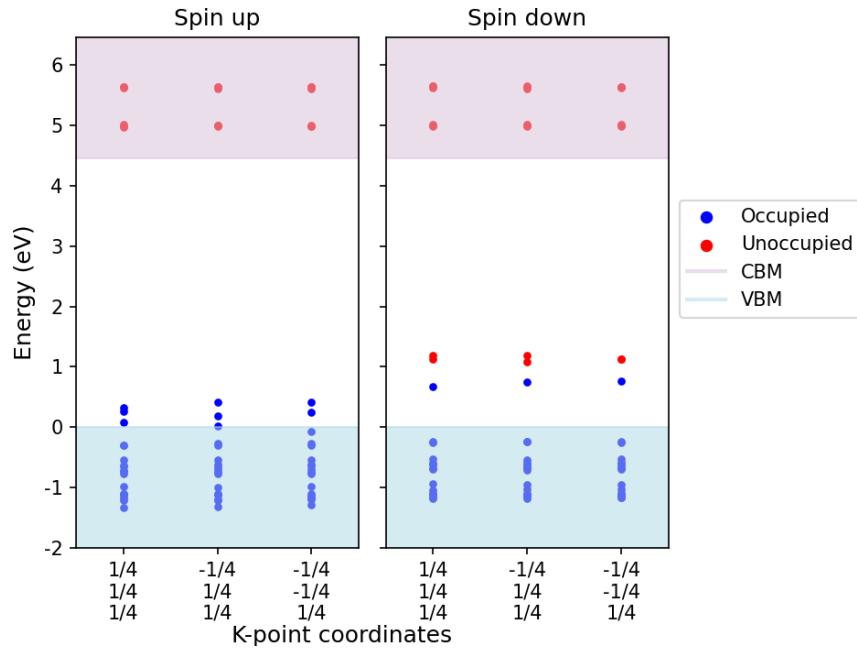


Figure 235: Kohn-Sham states.

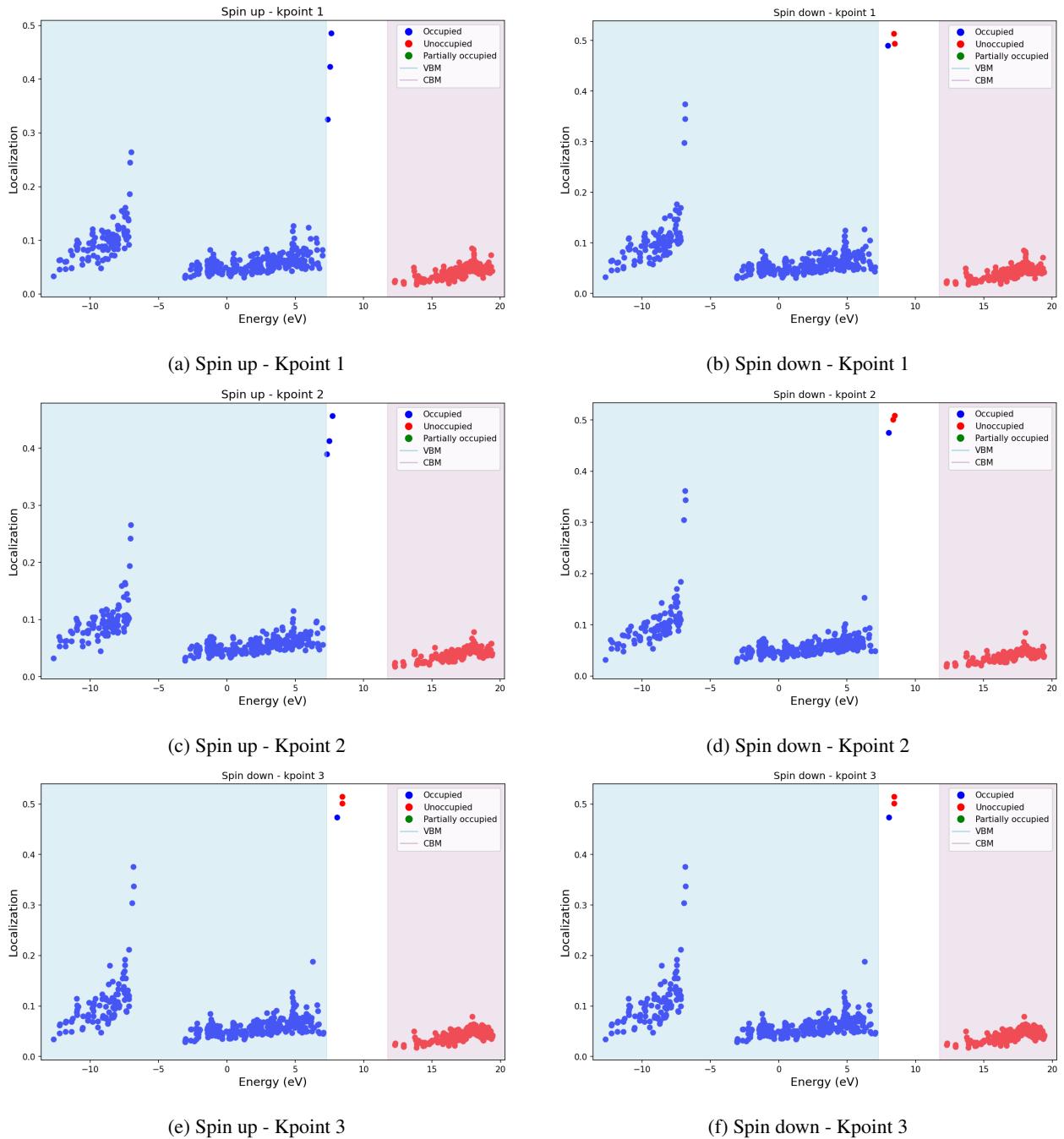


Figure 236: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

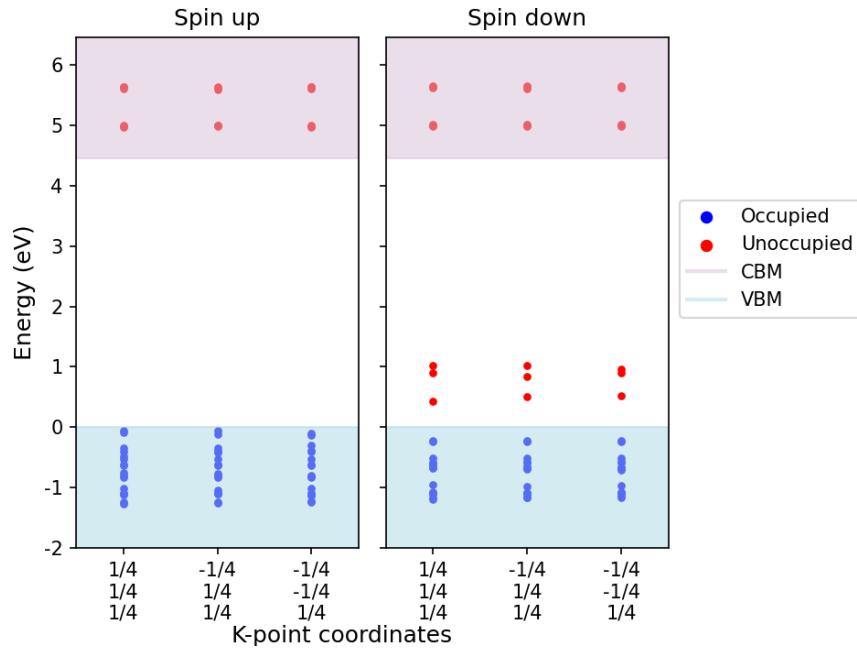


Figure 237: Kohn-Sham states.

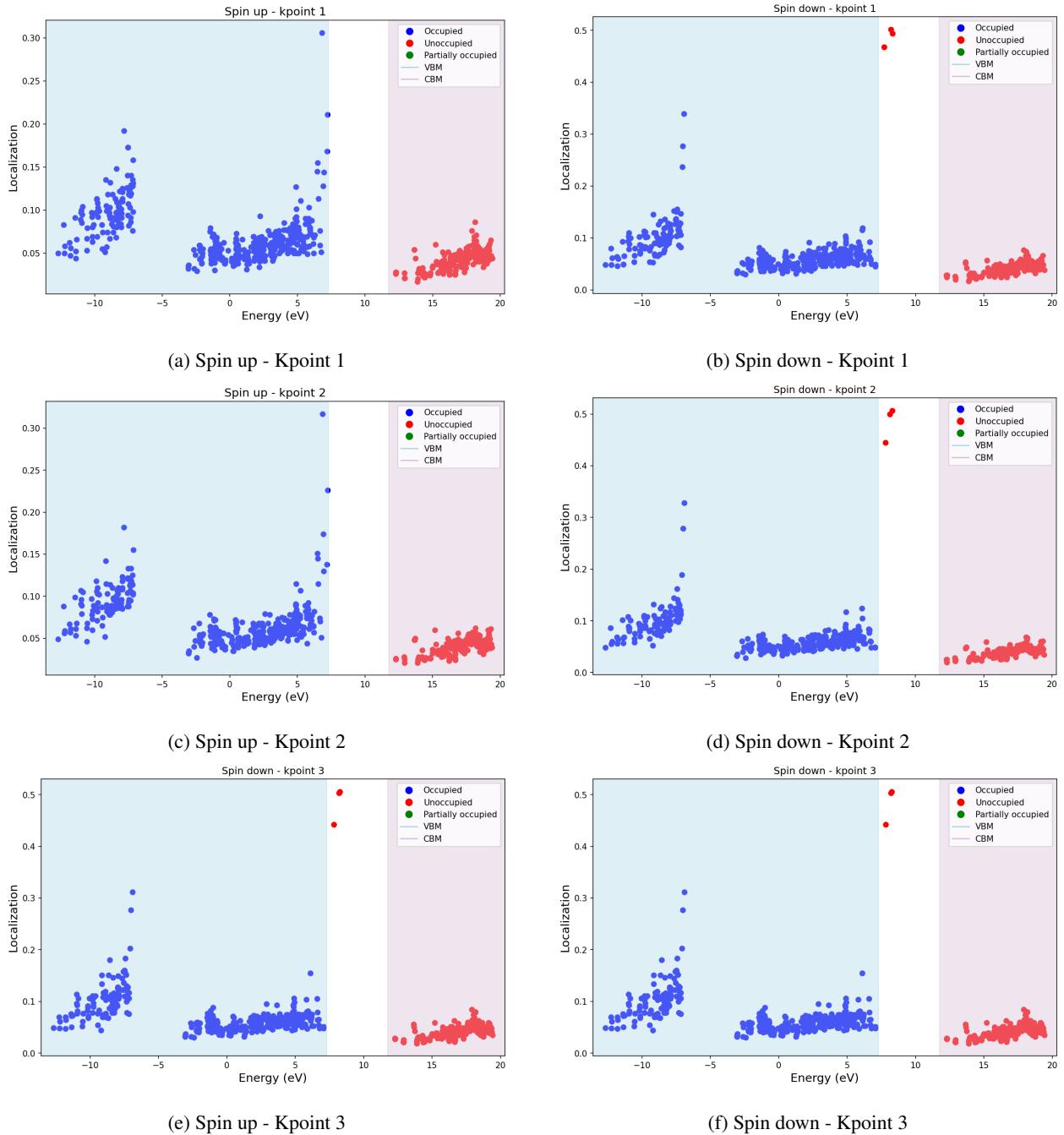


Figure 238: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

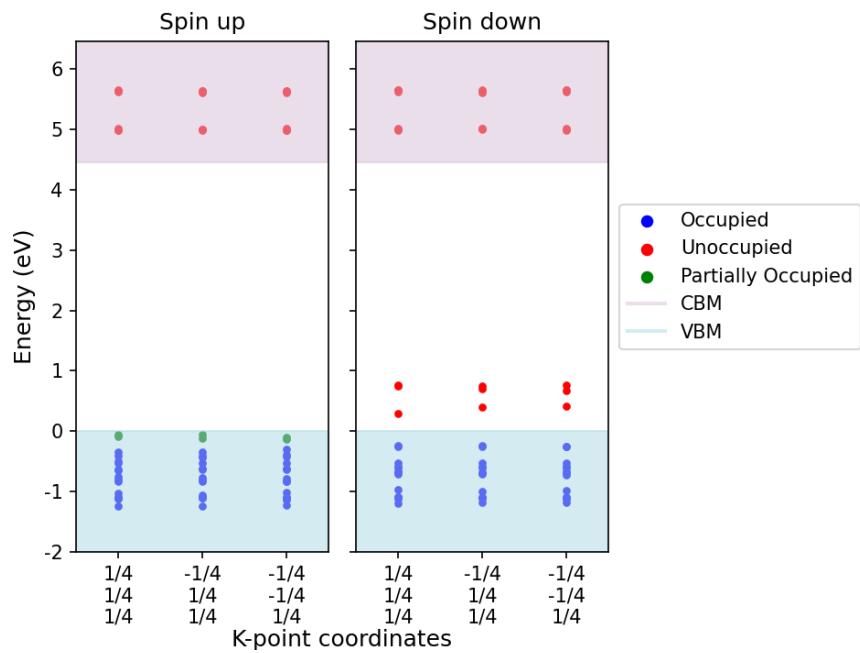


Figure 239: Kohn-Sham states.

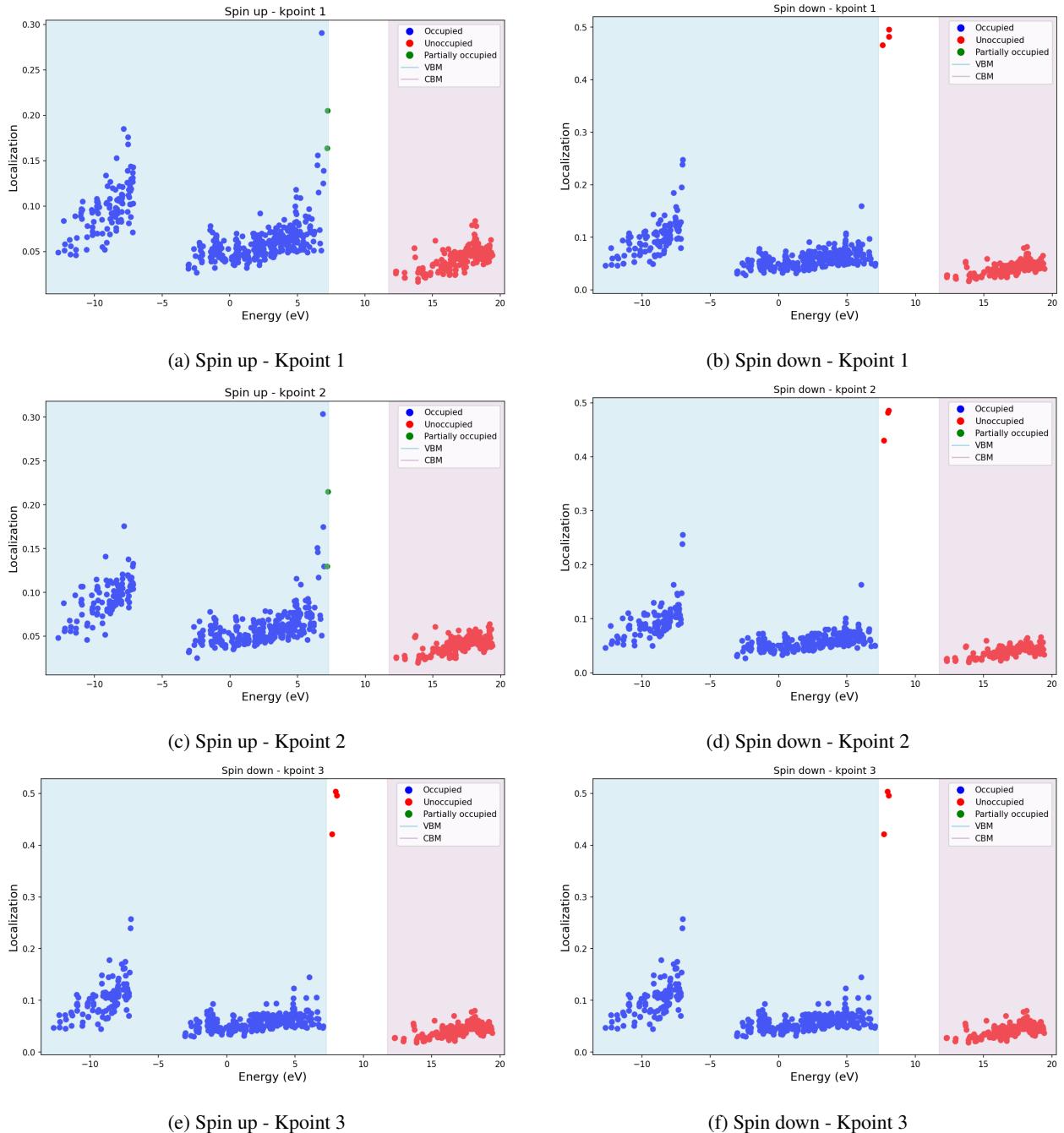


Figure 240: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

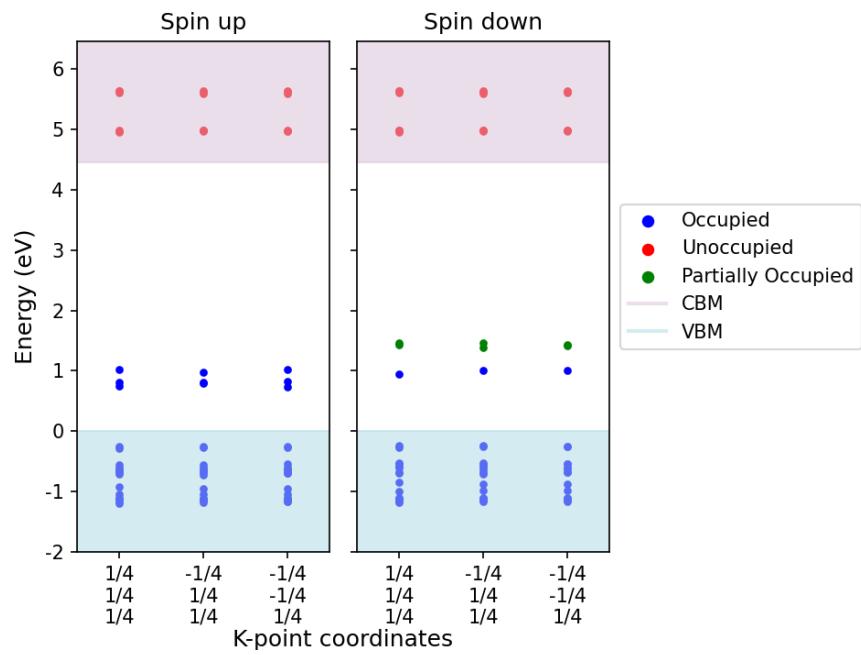


Figure 241: Kohn-Sham states.

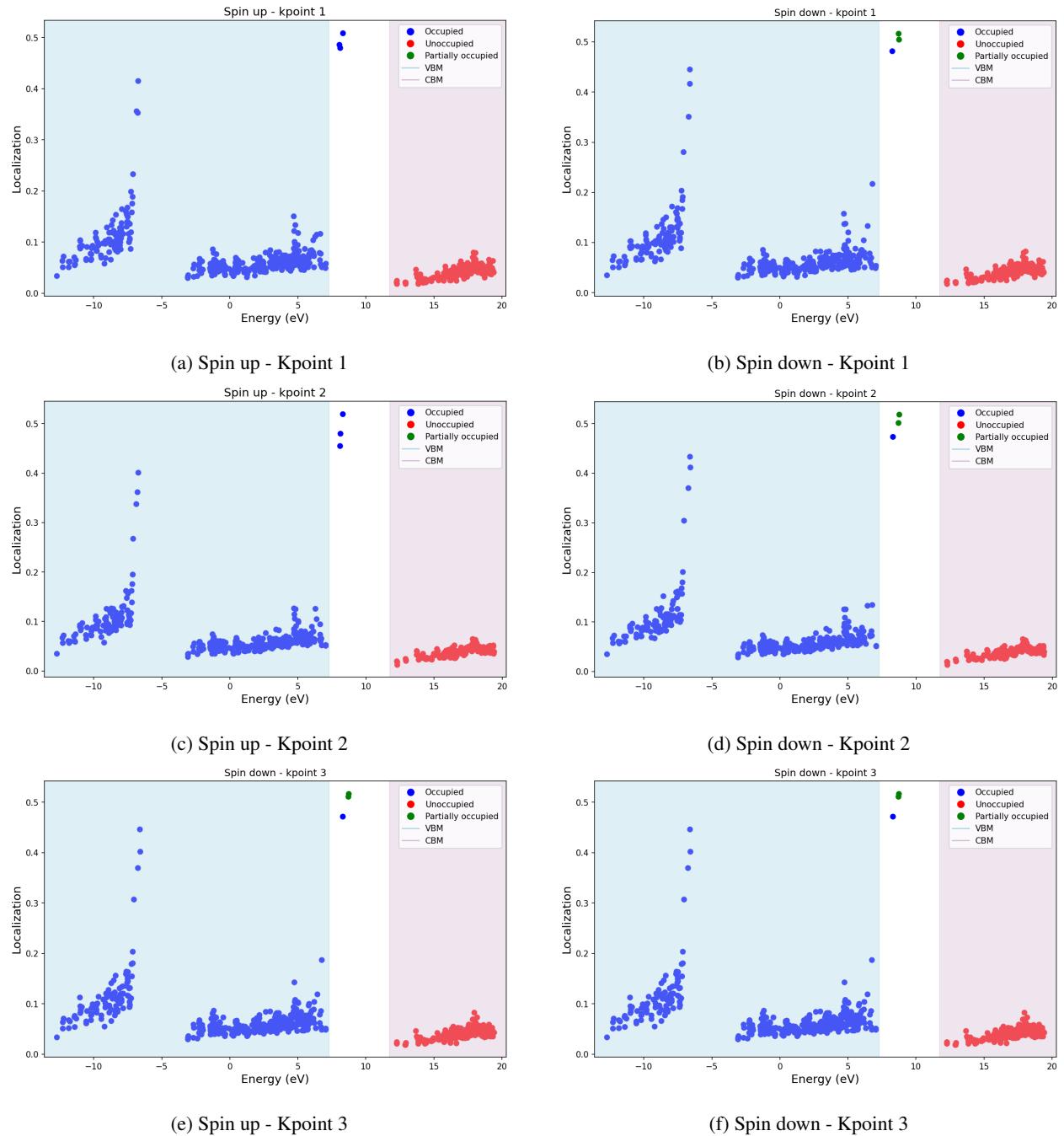


Figure 242: Localization factor using projected orbitals (s, p, and d).

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

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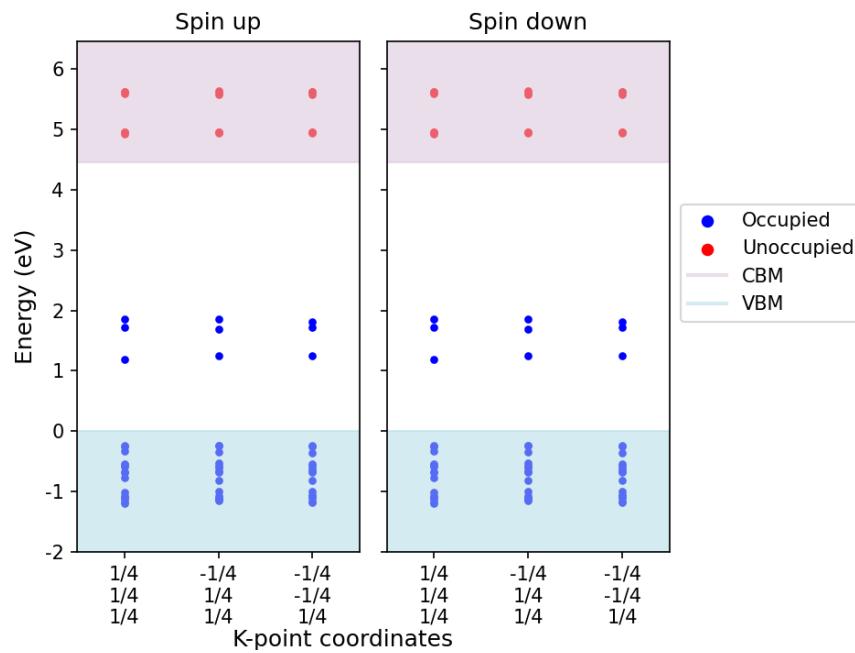


Figure 243: Kohn-Sham states.

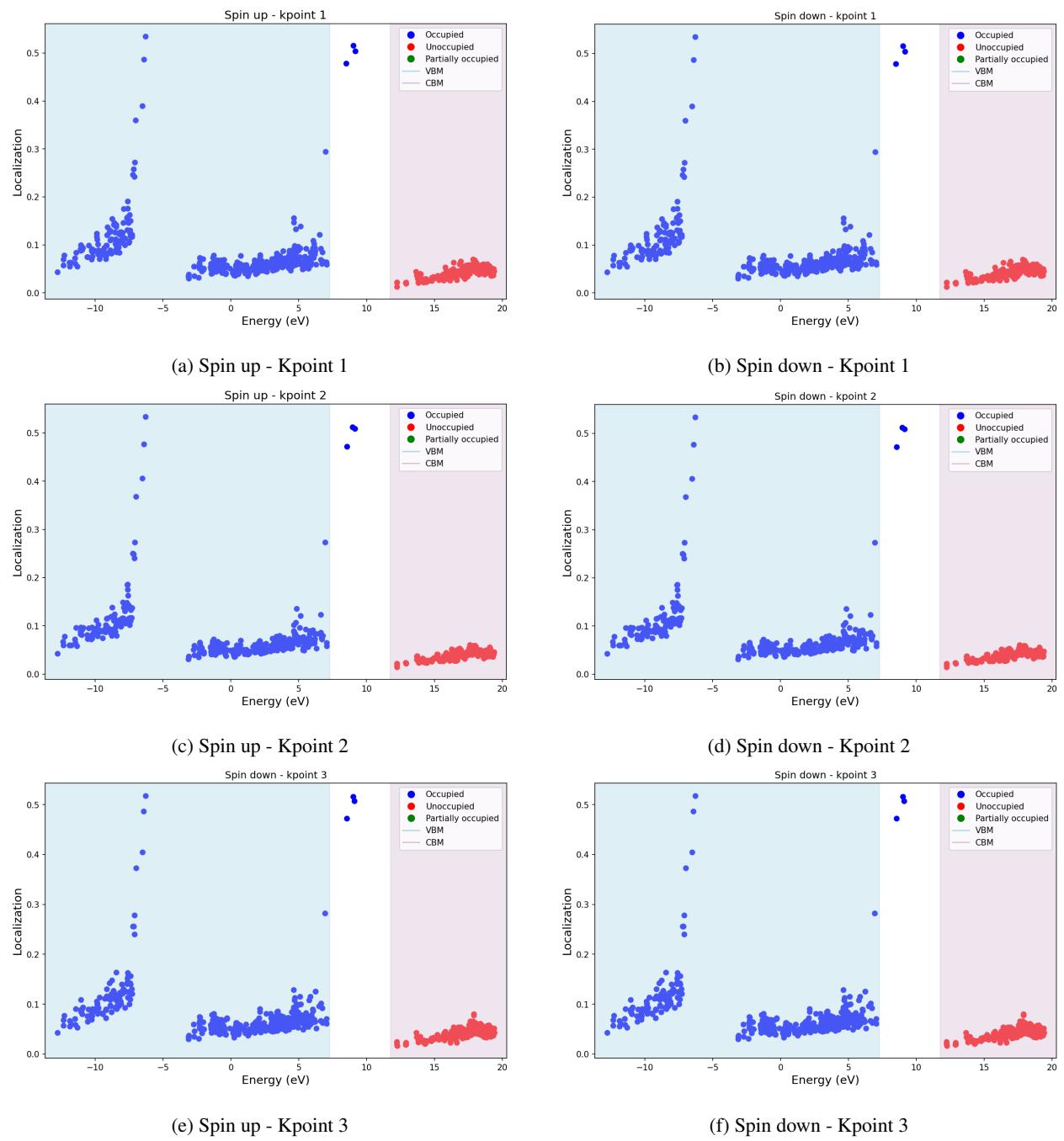


Figure 244: Localization factor using projected orbitals (s, p, and d).

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

[Go back to the Table 9](#)

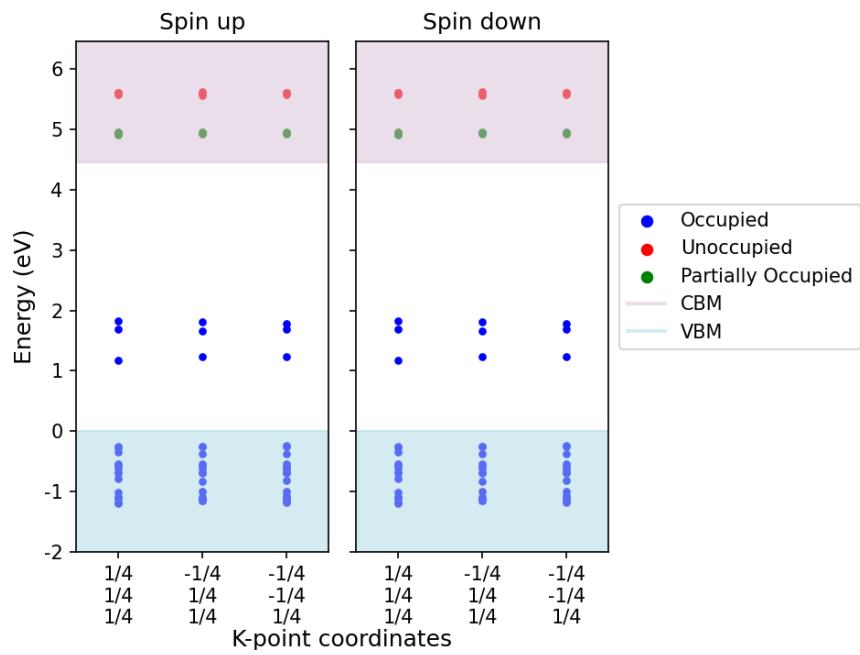


Figure 245: Kohn-Sham states.

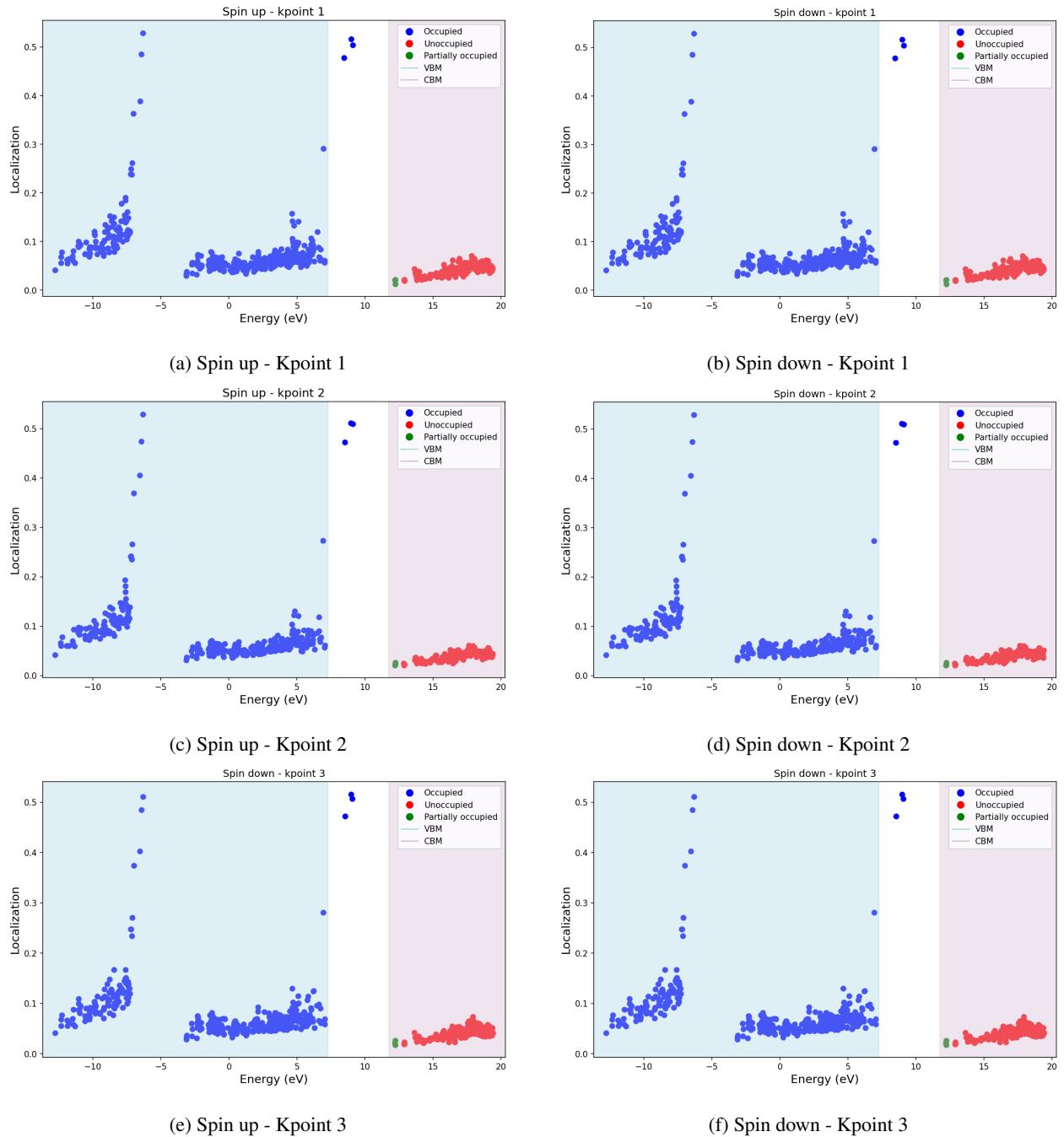


Figure 246: Localization factor using projected orbitals (s, p, and d).

## 2 Formation energy diagrams

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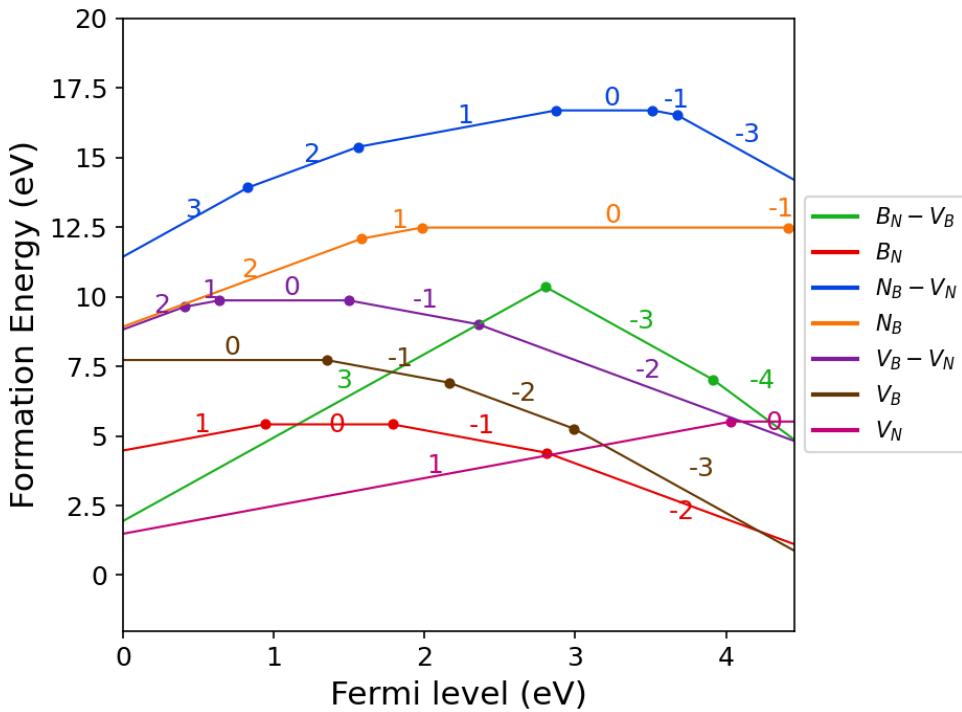


Figure 247: Boron rich condition. Also includes correction energies.

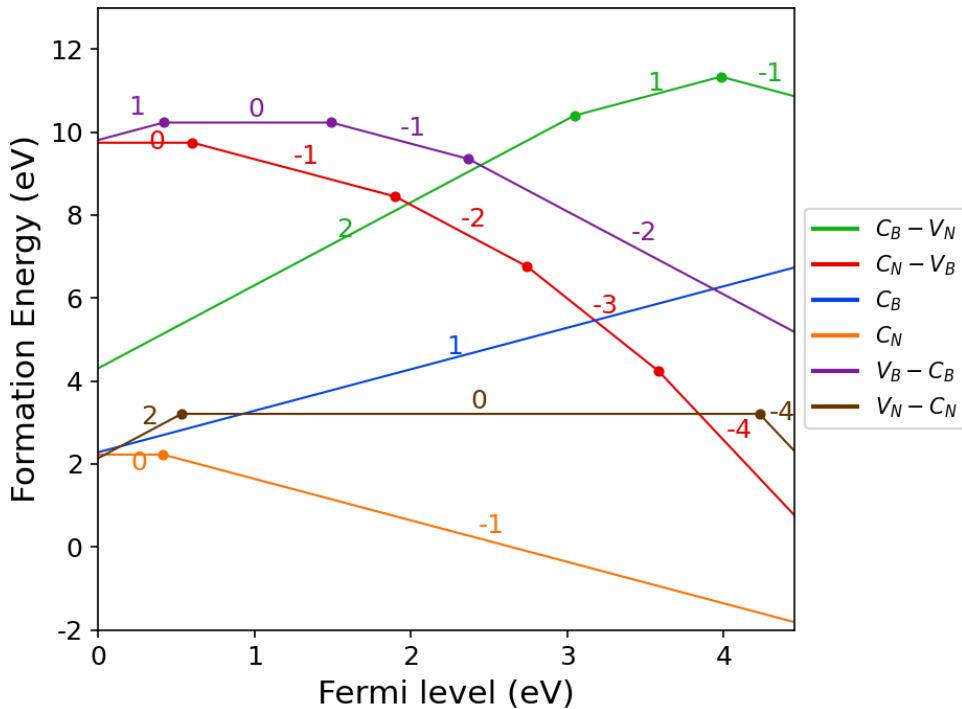


Figure 248: Boron rich condition. Also includes correction energies.

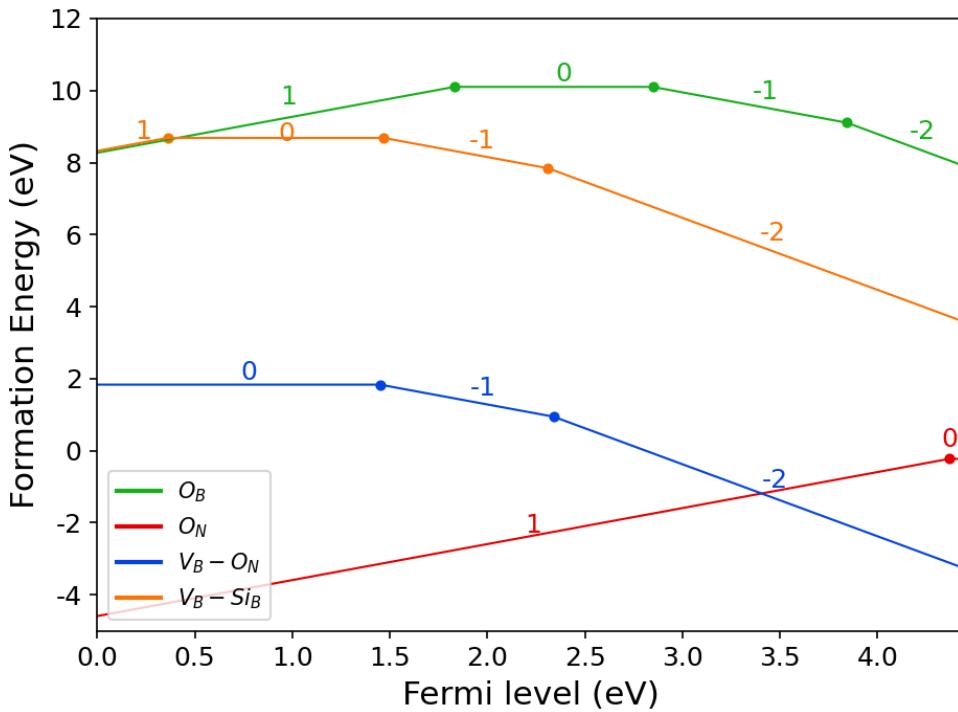


Figure 249: Boron rich condition. Also includes correction energies.

### 3 Defects

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Table 54: Selected defects.

Defect	Charge	Spin	Application	Channel
$V_B$	-1	1	Spin qubit	Down
$N_B$	0	0	SPE	
$N_B$	+1	1/2	Spin qubit	Up
$V_B - C_B$	0	1	Spin qubit	
$V_B - C_B$	-1	1/2	Spin qubit	
$V_B - V_N$	0	1	Spin qubit	Down
$V_B - V_N$	-1	1/2	Spin qubit	Down