1 Selected defects - PBE functional

Table 1: Selected defects. Calculations were performed with PBE functional.

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

2 Selected defects - HSE06 functional

The post-analysis was performed using LSPD.

Table 2: Selected defects. Calculations were performed with HSE06 functional.

Defect	Charge	Magnetization (μ_B)	Spin
V_B	-1	2	1
N_B	0	0	0
	+1	1	1/2
$V_B - C_B$	0	2	1
	-1	1	1/2
$V_B - V_N$	0	2	1
	-1	1	1/2

2.1 Vacancy: V_B^{-1}

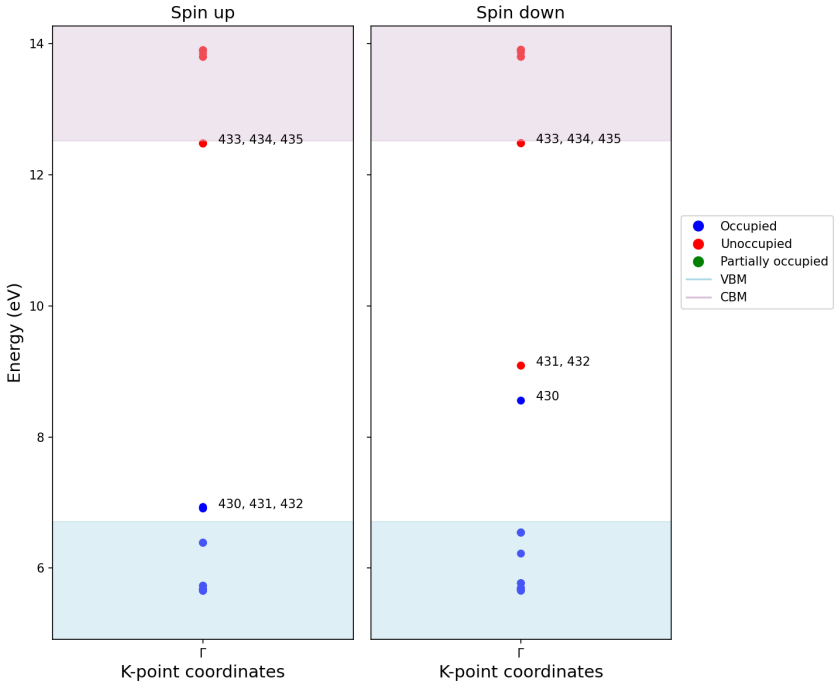
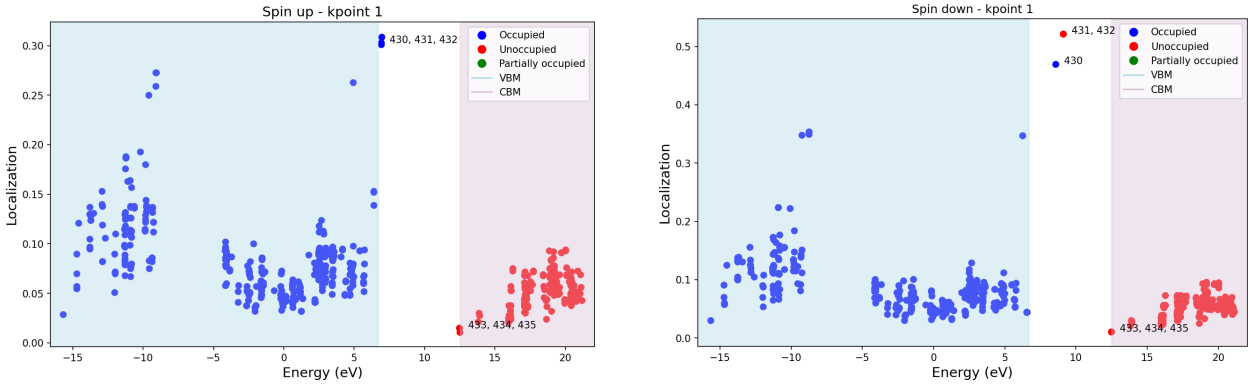


Figure 1: Kohn-Sham states.



(a) Spin up - Kpoint 1

(b) Spin down - Kpoint 1

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

2.2 Antisite: N_B^0

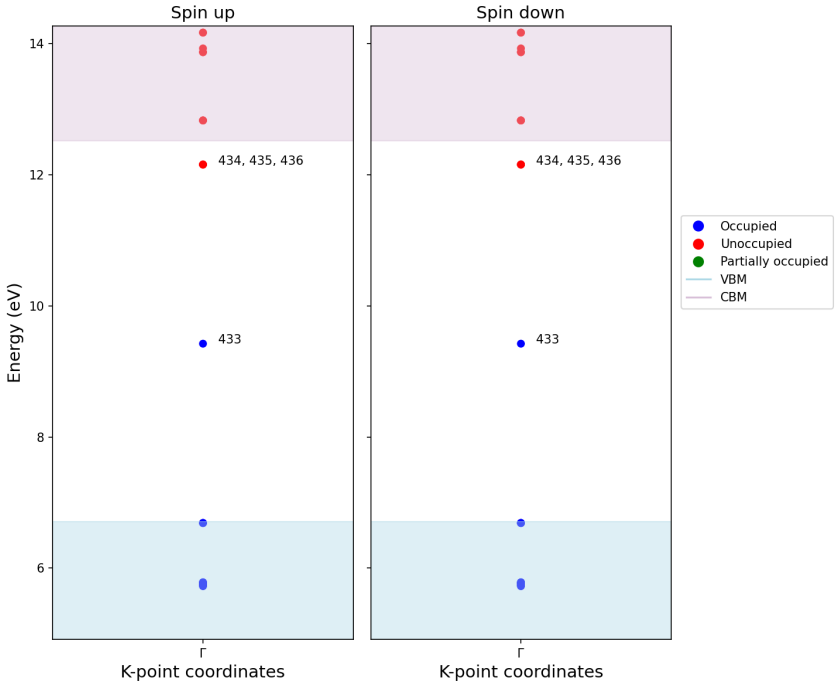
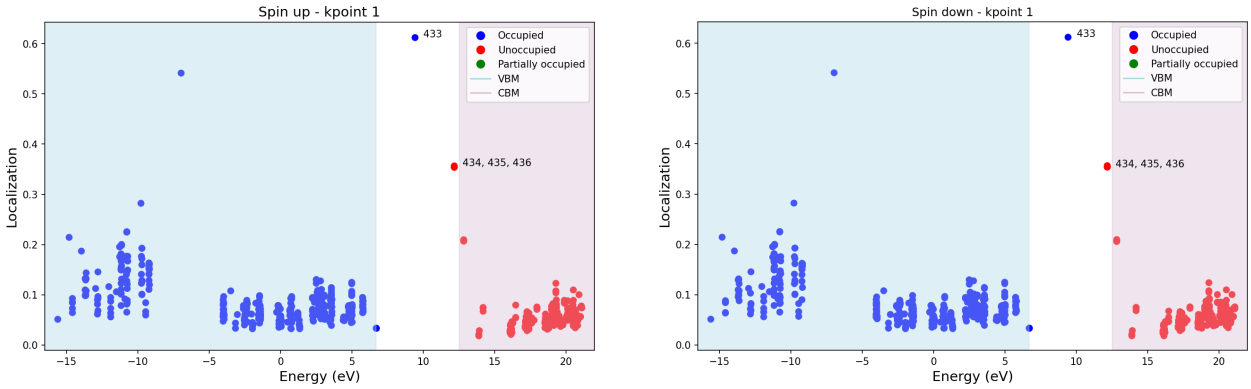


Figure 3: Kohn-Sham states.



(a) Spin up - Kpoint 1

(b) Spin down - Kpoint 1

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

2.3 Antisite: N_B^{+1}

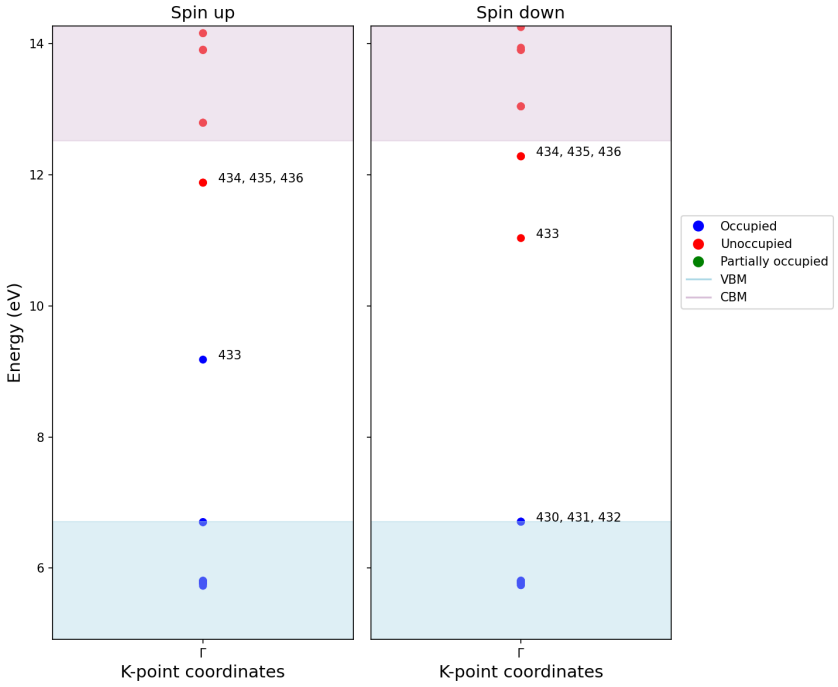
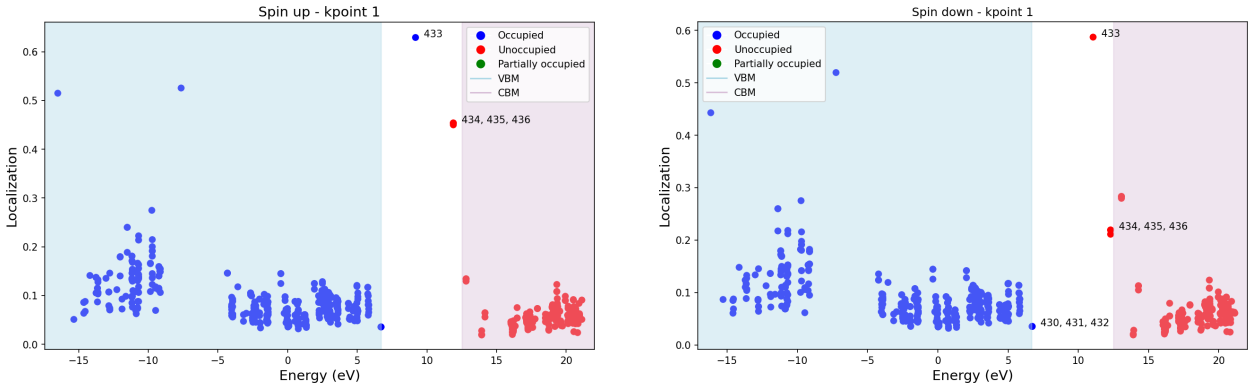


Figure 5: Kohn-Sham states.



(a) Spin up - Kpoint 1

(b) Spin down - Kpoint 1

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

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

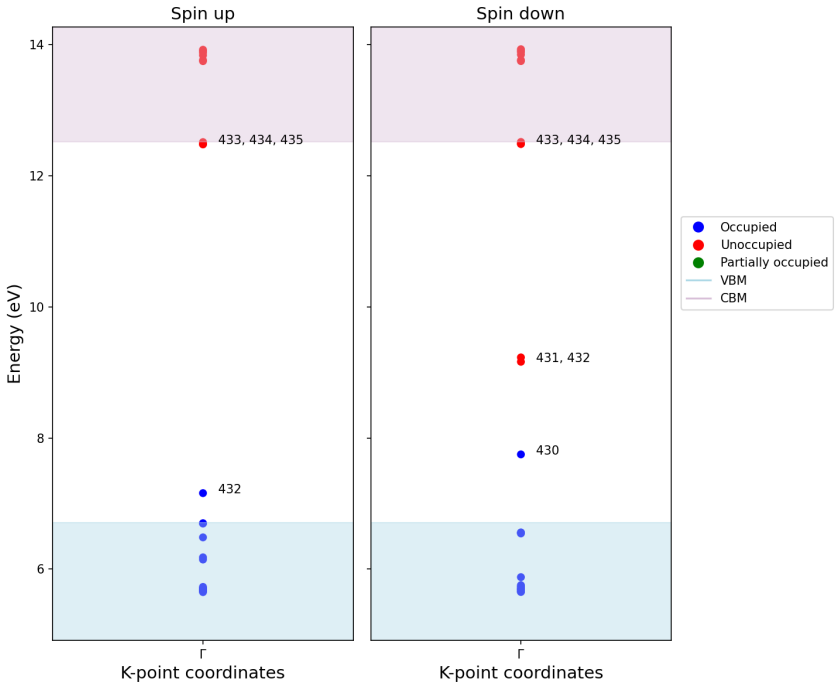
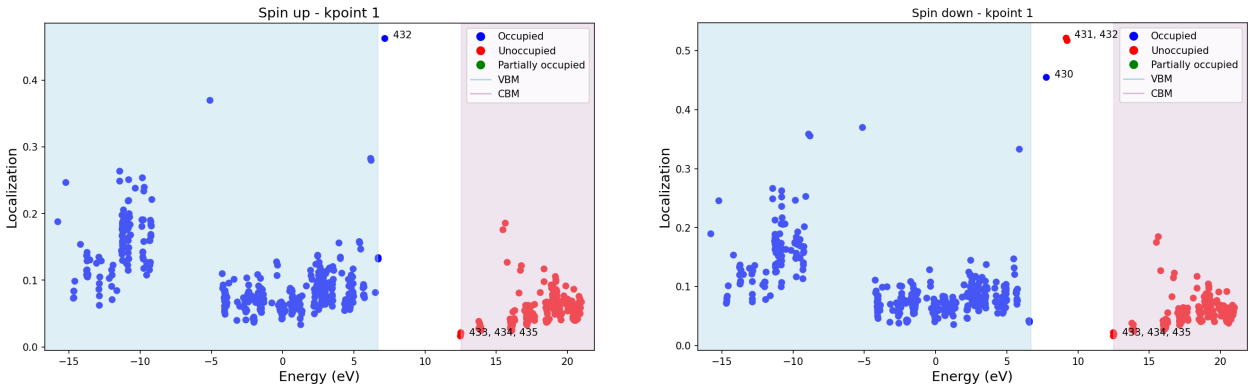


Figure 7: Kohn-Sham states.



(a) Spin up - Kpoint 1

(b) Spin down - Kpoint 1

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

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

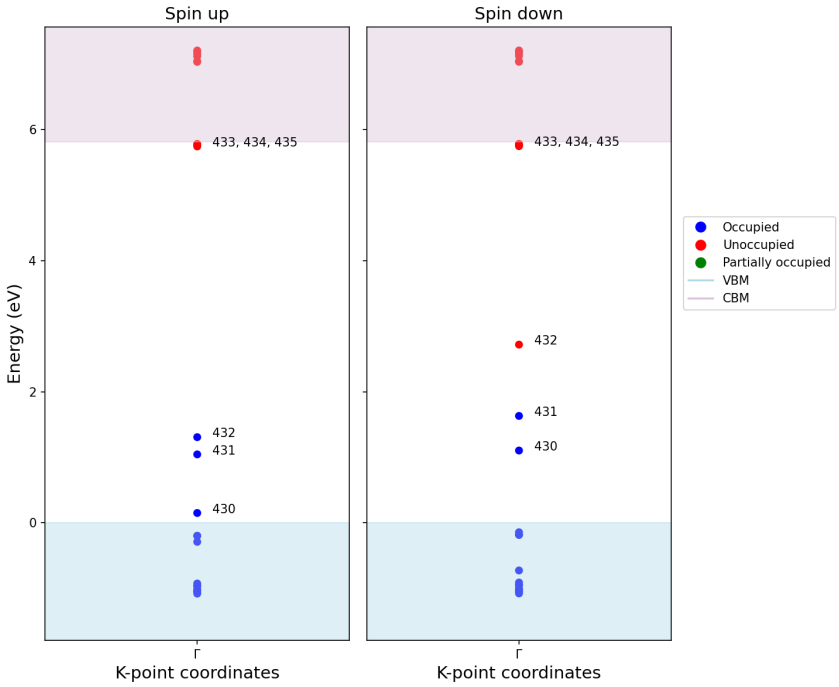
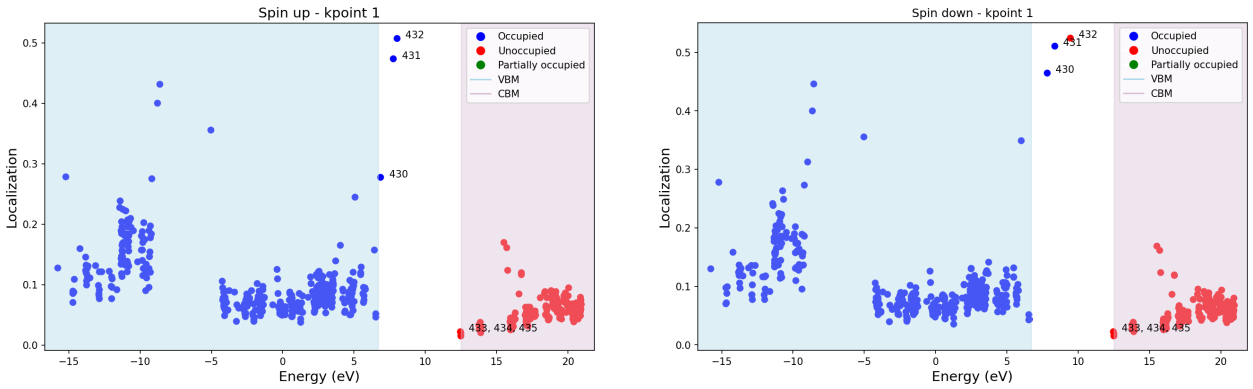


Figure 9: Kohn-Sham states.



(a) Spin up - Kpoint 1

(b) Spin down - Kpoint 1

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

2.6 Divacancy: $(V_B - V_N)^0$

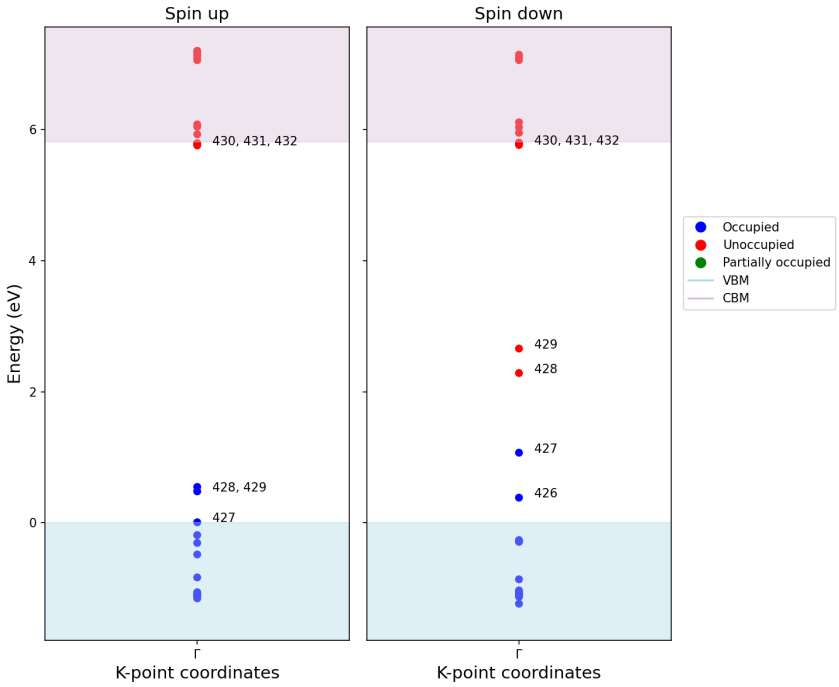
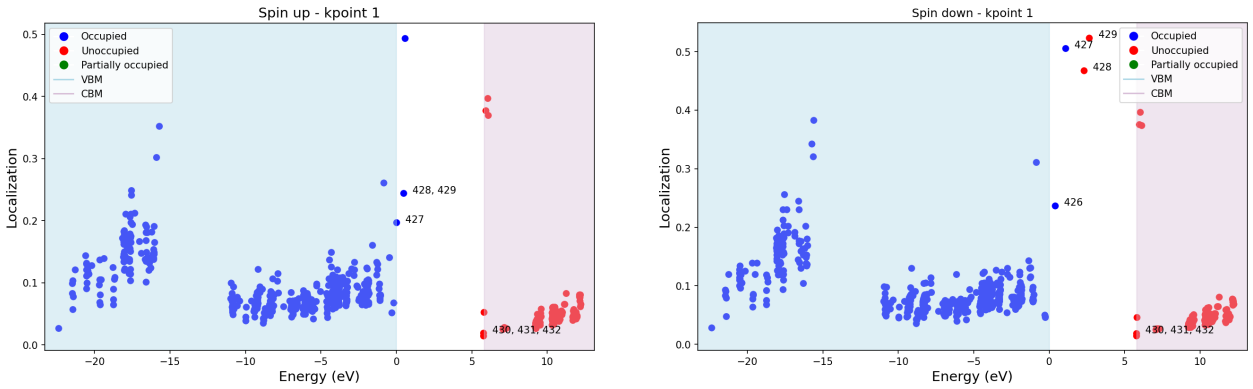


Figure 11: Kohn-Sham states.



(a) Spin up - Kpoint 1

(b) Spin down - Kpoint 1

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

2.7 Divacancy: $(V_B - V_N)^{-1}$

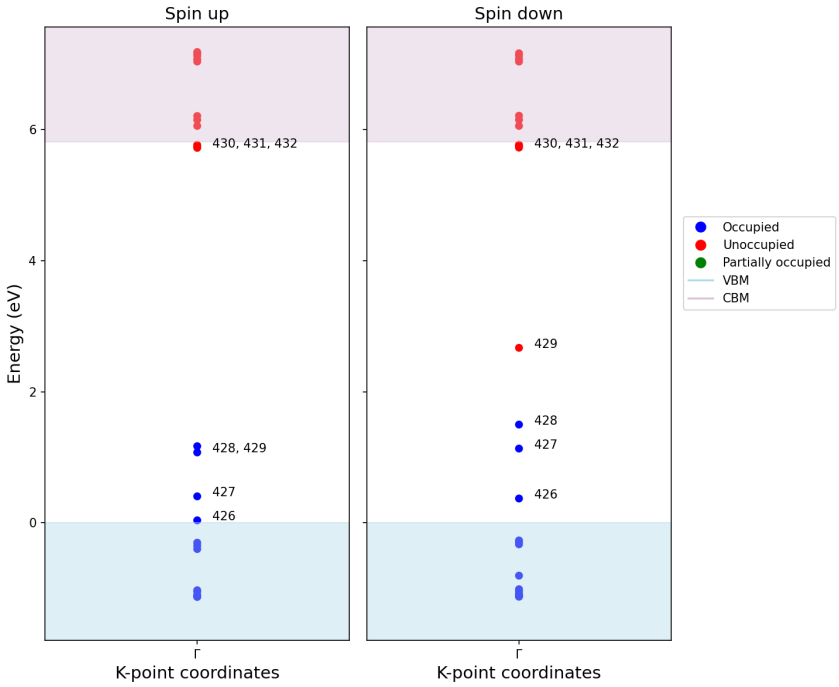
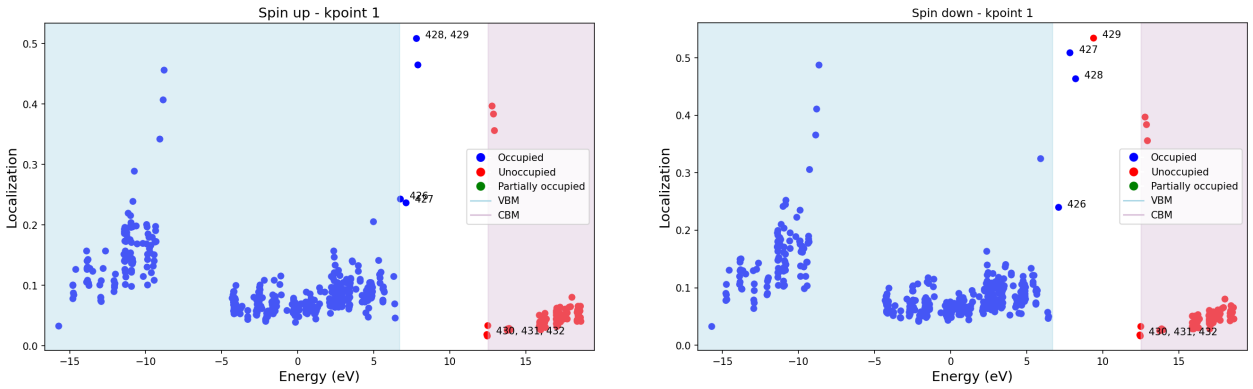


Figure 13: Kohn-Sham states.



(a) Spin up - Kpoint 1

(b) Spin down - Kpoint 1

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