

Supporting Information

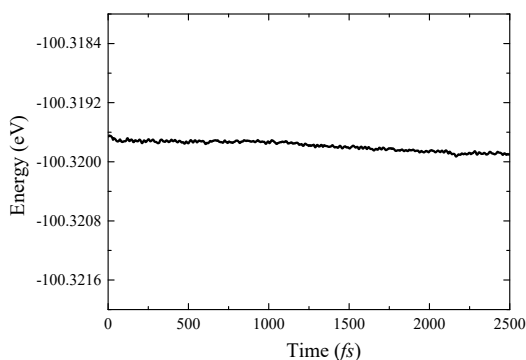


Figure S1 The total energies of $\text{Sc}_2\text{CO}_2\text{-Y}$ as a function of time

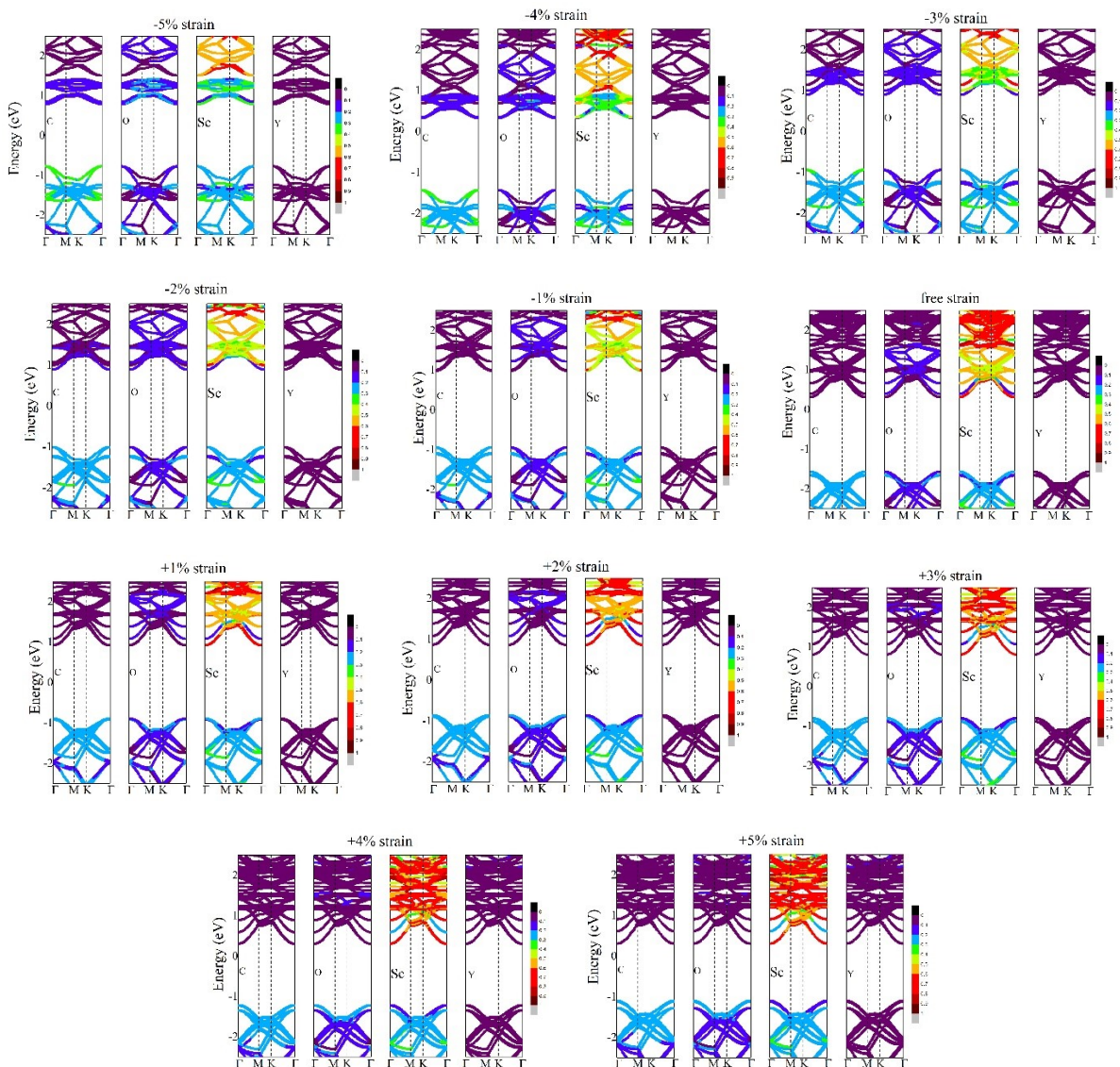


Figure S2 The projected band structures of monolayer $\text{Sc}_2\text{CO}_2\text{-Y}$ under strain from -5% to 5%.

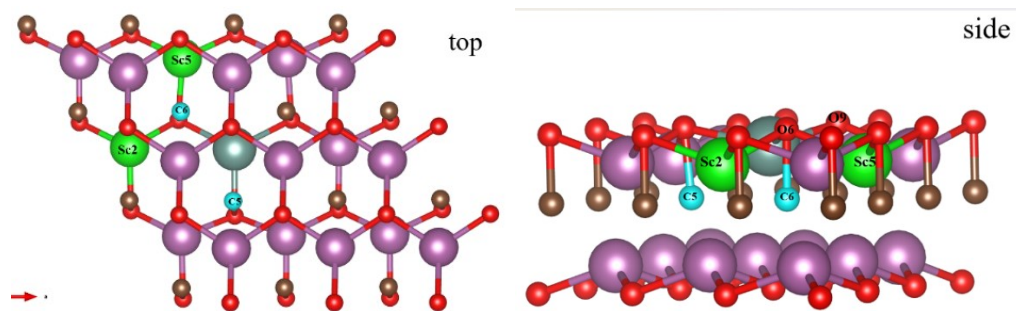


Figure S3 The atomic labels in $\text{Sc}_2\text{CO}_2\text{-Y}$

Table S1 The C_p , C_n , C_p/C_n and electrode type of $\text{Sc}_2\text{CO}_2\text{-Y}$ under strain

system	Aqueous electrolytes				Ionic/organic electrolytes			
	C_p	C_n	C_p/C_n	Electrode type	C_p	C_n	C_p/C_n	Electrode type
-5%	0.02	295.26	6.15×10^{-5}	cathode	0.02	994.74	1.83×10^{-5}	cathode
-4%	0.02	2111.42	8.10×10^{-5}	cathode	0.02	3752.35	4.55×10^{-6}	cathode
-3%	5.19	1387.42	3.73×10^{-3}	cathode	5.19	1917.60	2.29×10^{-3}	cathode
-2%	0.02	1181.15	1.56×10^{-5}	cathode	0.02	1535.16	1.20×10^{-5}	cathode
-1%	4.97	1704.04	2.91×10^{-3}	cathode	4.97	661.02	7.52×10^{-3}	cathode
0	2.55	771	3.31×10^{-3}	cathode	2.55	680.20	3.76×10^{-3}	cathode
1%	0.04	686.03	6.48×10^{-5}	cathode	0.04	846.69	5.25×10^{-5}	cathode
2%	0.04	767.42	5.35×10^{-5}	cathode	0.04	1291.67	3.18×10^{-5}	cathode
3%	7.51	1145.89	6.56×10^{-3}	cathode	7.51	593.31	0.017	cathode
4%	5.63	831.44	6.78×10^{-3}	cathode	5.63	673.03	8.37×10^{-3}	cathode
5%	4.62	987.81	4.67×10^{-3}	cathode	4.62	1037.74	4.45×10^{-3}	cathode