Electronic supplementary information

Title

Theoretical investigation of selective CO_2 capture and desorption controlled by the electric field

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Table S1 The formation energy of oxygen vacancy in each doped cation.

Amount of O_{vac} / -	$\Delta E(O_{vac})$ / eV								
	without dopant	Ca^{2+}	Sr^{2+}	Ba^{2+}	Al^{3+}	Ga^{3+}	Sc^{3+}	Y^{3+}	Zr^{4+}
1	2.98	-0.80	-0.66	-0.71	0.59	-0.63	-0.95	-0.72	1.92
2		-1.41	-1.23	-0.61		0.08	0.76	2.36	
3		0.83	1.25	2.49					

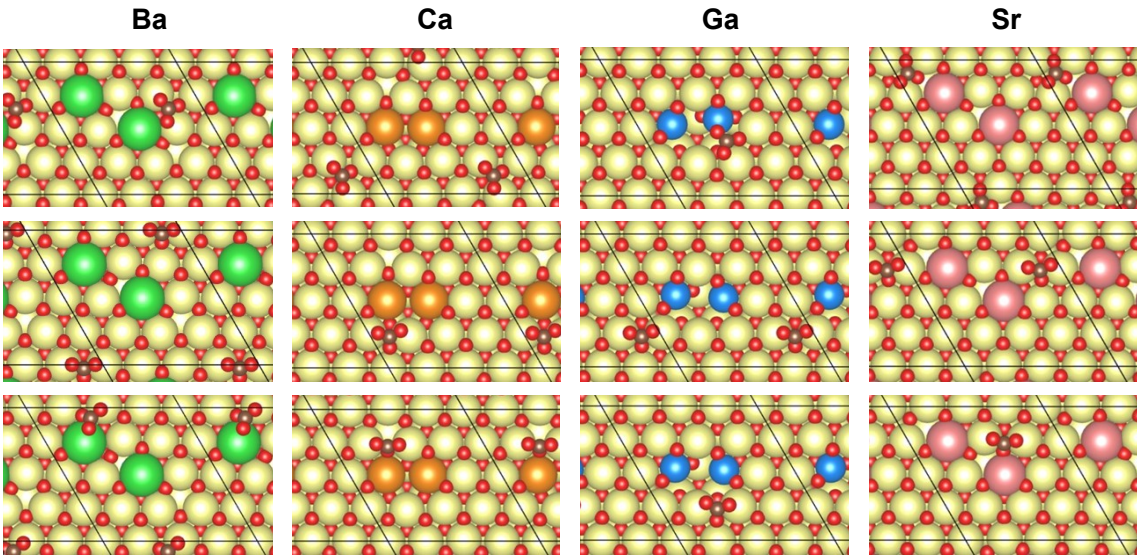

Fig. S1 The surface model for elucidating various factors.

Yellow is Ce, red is O, orange is Ca, pink is Sr, green is Ba, blue is Ga.

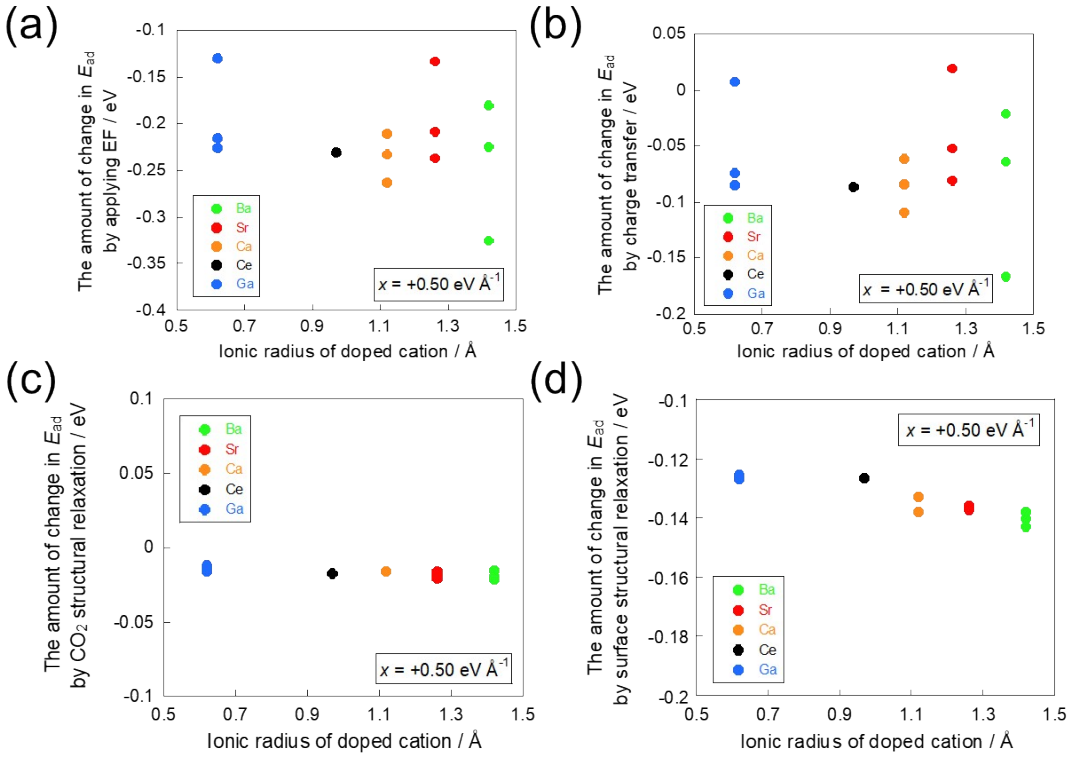

Fig. S2 The effect of each factor on change of CO_2 adsorption energy in +0.50 eV Å^{-1}.

The amount of change in CO_2 adsorption energy (a) by applying EF, (b) by charge transfer,

(c) by changing CO_2 molecule structure, and (d) by relaxation of surface structure.

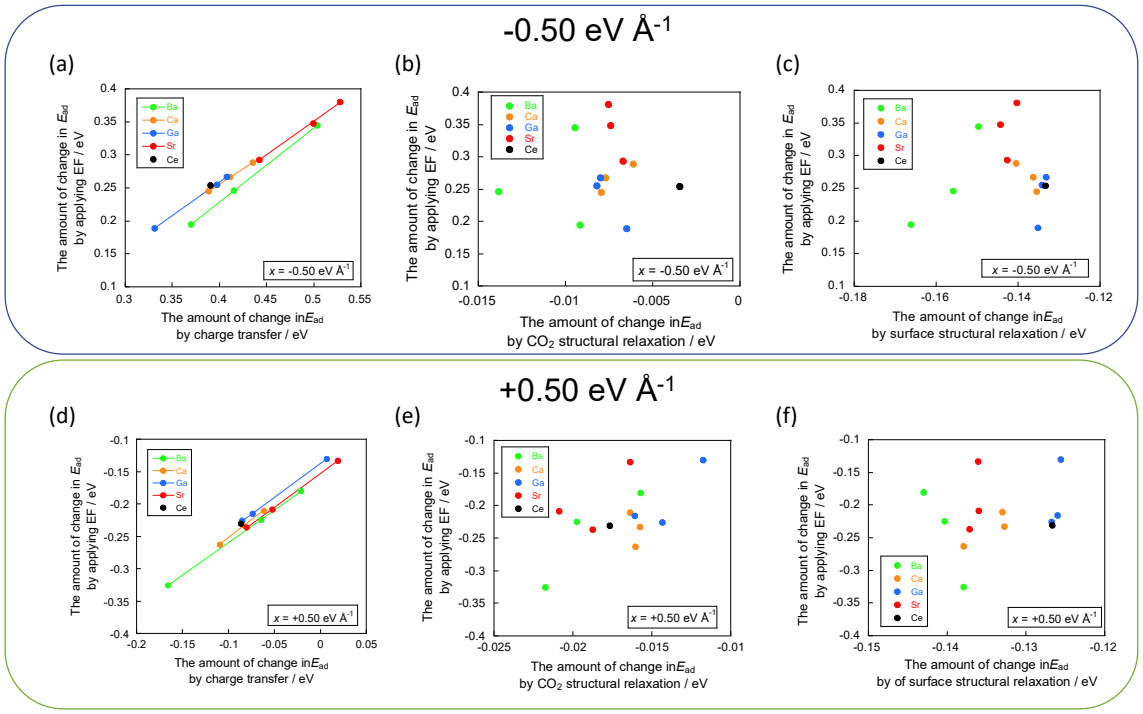

Fig. S3 The relationship between the amount of change in CO_2 adsorption energy by applying EF and the amount of change in CO_2 adsorption energy

(a) by charge transfer in -0.50 eV Å^{-1}, (b) by CO_2 structural relaxation in -0.50 eV Å^{-1}, (c) by surface structural relaxation in -0.50 eV Å^{-1}, (d) by charge transfer in +0.50 eV Å^{-1}, (e) by CO_2 structural relaxation in +0.50 eV Å^{-1}, and (f) by surface structural relaxation in +0.50 eV Å^{-1},