Electronic supplementary information

Title
Theoretical investigation of selective CO\textsubscript{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.

<table>
<thead>
<tr>
<th>Amount of O\textsubscript{vac} / -</th>
<th>\Delta\textit{E}(O\textsubscript{vac}) / eV</th>
</tr>
</thead>
<tbody>
<tr>
<td>without dopant</td>
<td>Ca\textsuperscript{2+}</td>
</tr>
<tr>
<td>1</td>
<td>2.98</td>
</tr>
<tr>
<td>2</td>
<td>-1.41</td>
</tr>
<tr>
<td>3</td>
<td>0.83</td>
</tr>
</tbody>
</table>
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 CO₂ molecule structure, and (d) by relaxation of surface structure.

Fig. S3 The relationship between the amount of change in CO₂ adsorption energy by applying EF and the amount of change in CO₂ adsorption energy (a) by charge transfer in -0.50 eV Å⁻¹, (b) by CO₂ 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 CO₂ structural relaxation in +0.50 eV Å⁻¹, and (f) by surface structural relaxation in +0.50 eV Å⁻¹,