Unveiling the effects of A-site substitutions on the oxygen ions migration in

$A_{2-x}A'_{x}NiO_{4+\delta}$ by first principles calculations

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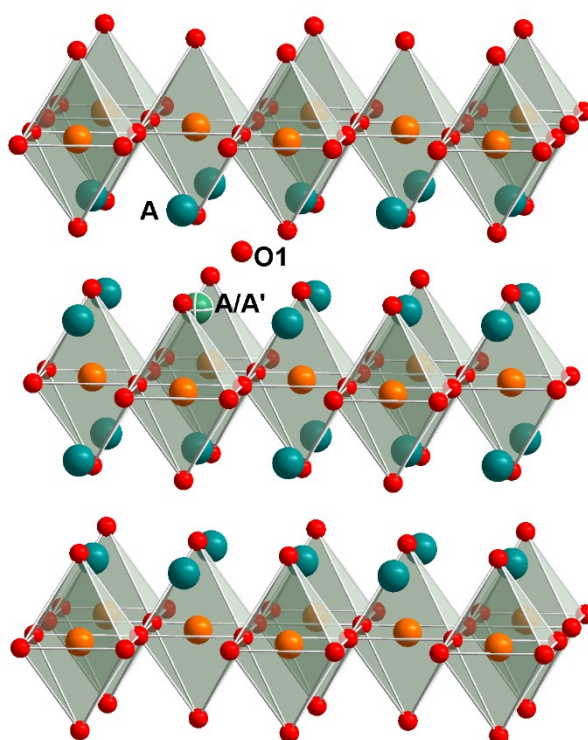
Supporting Information

Figure S1. $2\sqrt{2}\times\sqrt{2}\times1$ supercell with 16(A,A'), 8Ni, 32O atoms for $A_{2-x}A'_{x}NiO_{4+\delta}$ ($\delta = 0.125$)

Table S1. Calculated formation energy of the interstitial oxygen in $A_{2-x}A'_{x}NiO_{4+\delta}$ (A = La, Pr,

Nd, Sm; A' = Ba, Sr, Ca; $x = 0$ and 0.25; $\delta = 0.125$, 0.25 and 0.5). *For this value, experimental parameters ($a = b = \sqrt{2} \times 3.8642$ Å, $c = 12.6869$ Å) were used in the calculations.

composition	formation energy at O1 / eV	formation energy at O5 / eV
$La_2NiO_{4.125}$	-4.43	—
$La_2NiO_{4.25}$	-4.07	—
$La_2NiO_{4.5}$	-1.46	—
$La_2NiO_{4.125}{}^*$	-4.94	—
$La_2NiO_{4.25}{}^*$	-4.41	—
$La_{1.75}Ba_{0.25}NiO_{4.25}$	-3.49	-3.74
$La_{1.75}Sr_{0.25}NiO_{4.25}$	-3.45	-3.82
$La_{1.75}Ca_{0.25}NiO_{4.25}$	-3.57	-3.93
$Pr_2NiO_{4.25}$	-4.81	—
$Nd_2NiO_{4.25}$	-4.61	—
$Sm_2NiO_{4.25}$	-4.24	—