Supporting information for:

Improved conductivity of $NdFeO_3$ through partial substitution of Nd by Ca: a theoretical study

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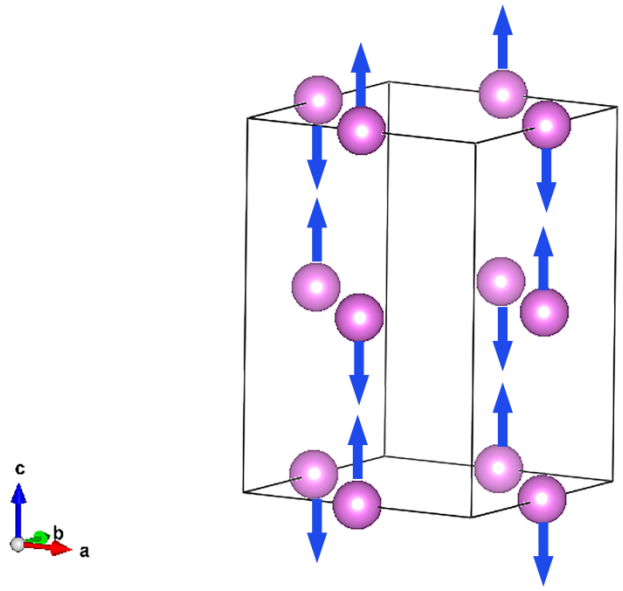


Fig. S1 The G-type antiferromagnetic structure of $NdFeO_3$.

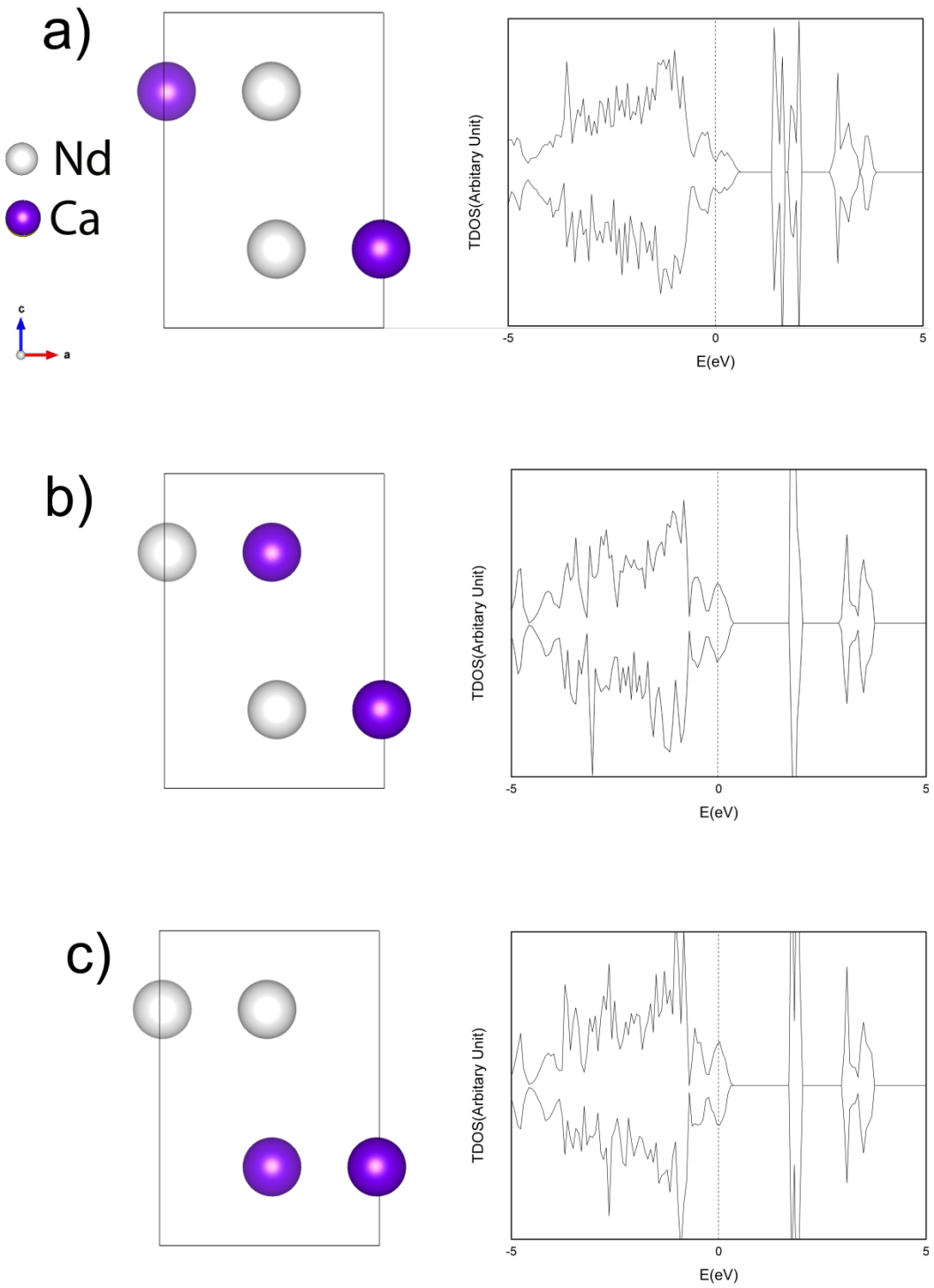


Fig. S2 Three types of Nd/Ca arrangements and their total density of states of $Nd_{0.5}Ca_{0.5}FeO_3$. For clarity, we only show the arrangements of Nd and Ca from the supercell structures.

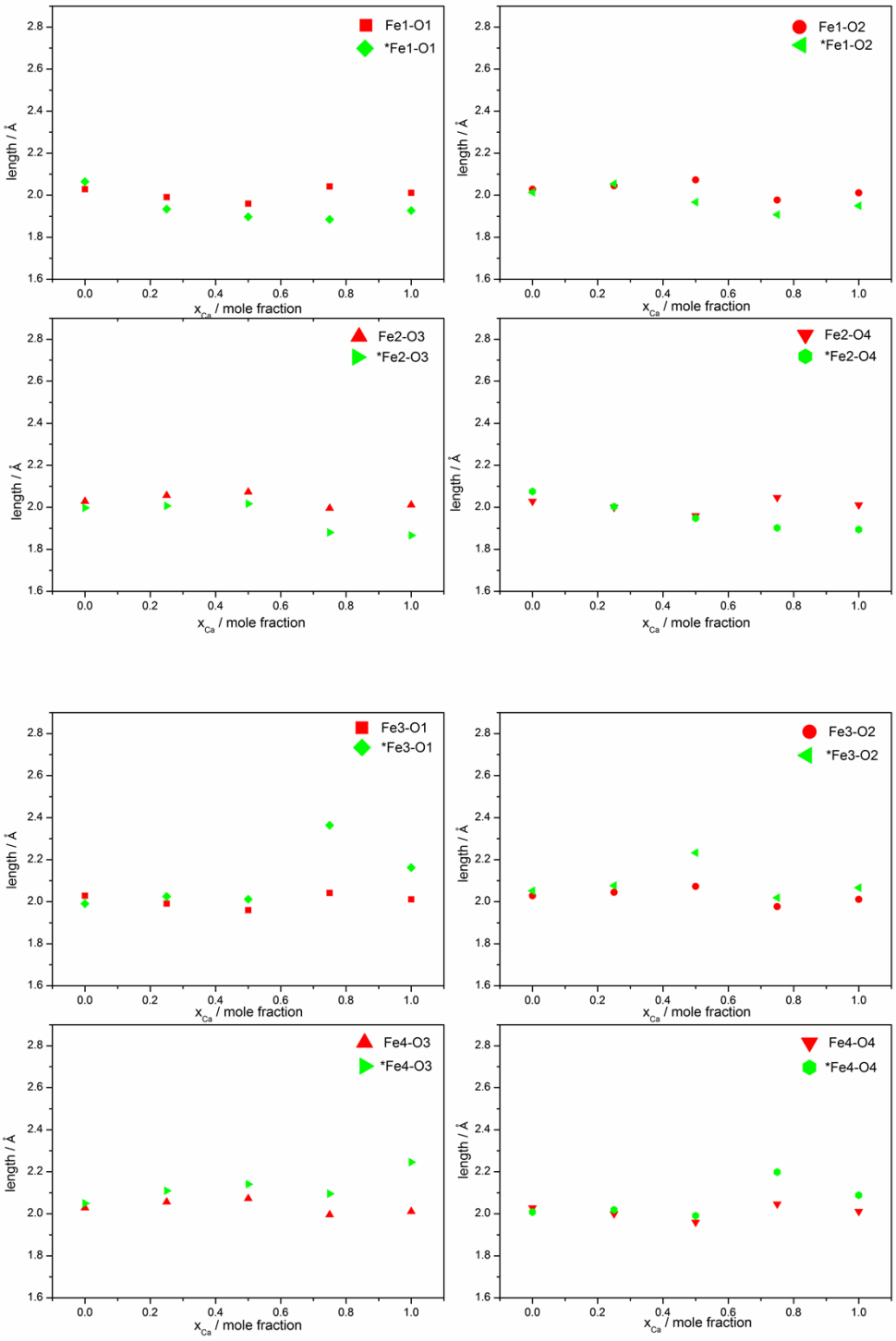
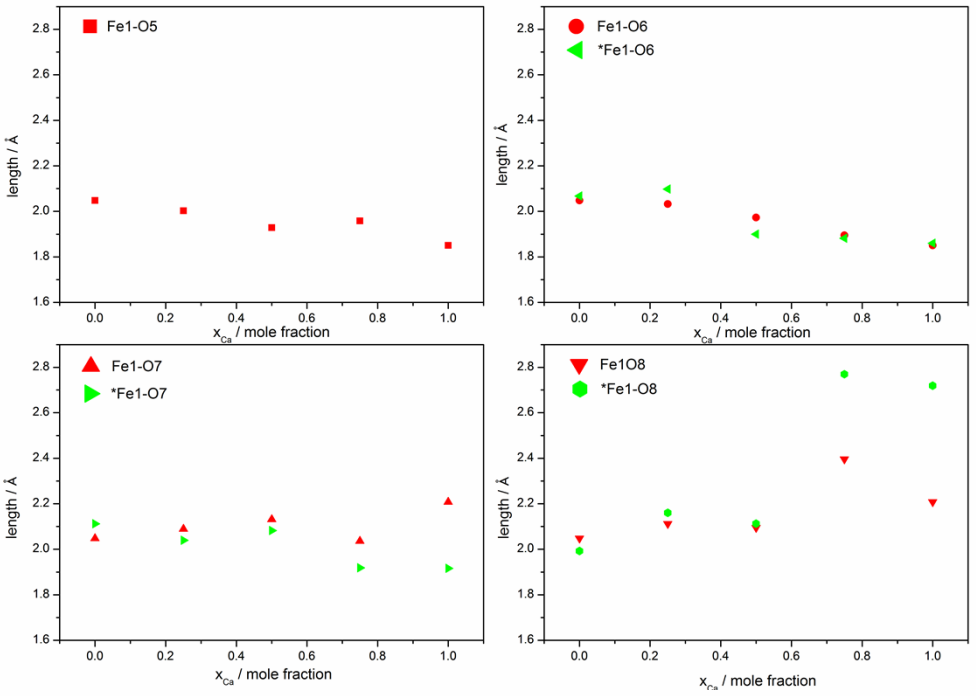
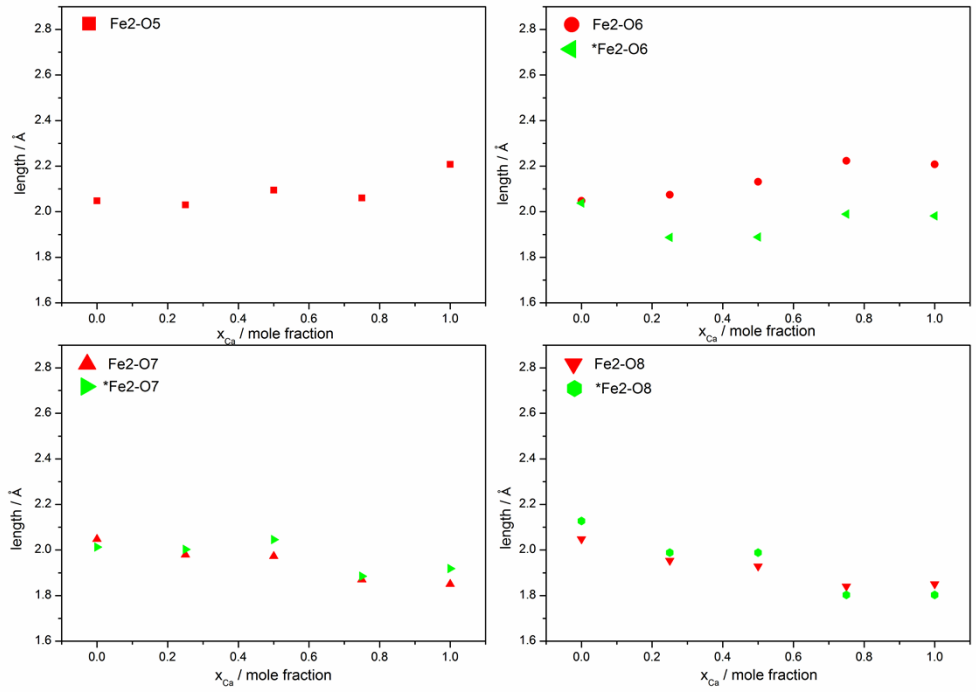


Fig. S3 The axial Fe-O bond length (Å) for $Nd_{1-x}Ca_xFeO_3$ (red) and $Nd_{1-x}Ca_xFeO_{2.75}$ (green) (x=0.00, 0.25, 0.50, 0.75, 1.00). See Fig. S7 for the numbering of Fe and O ions.


Fe1-O5
Fe1-O6
*Fe1-O6
Fe1-O7
*Fe1-O7
Fe1O8
*Fe1-O8
length / Å
x_Ca / mole fraction


Fe2-O5
Fe2-O6
*Fe2-O6
Fe2-O7
*Fe2-O7
Fe2-O8
*Fe2-O8
length / Å
x_Ca / mole fraction

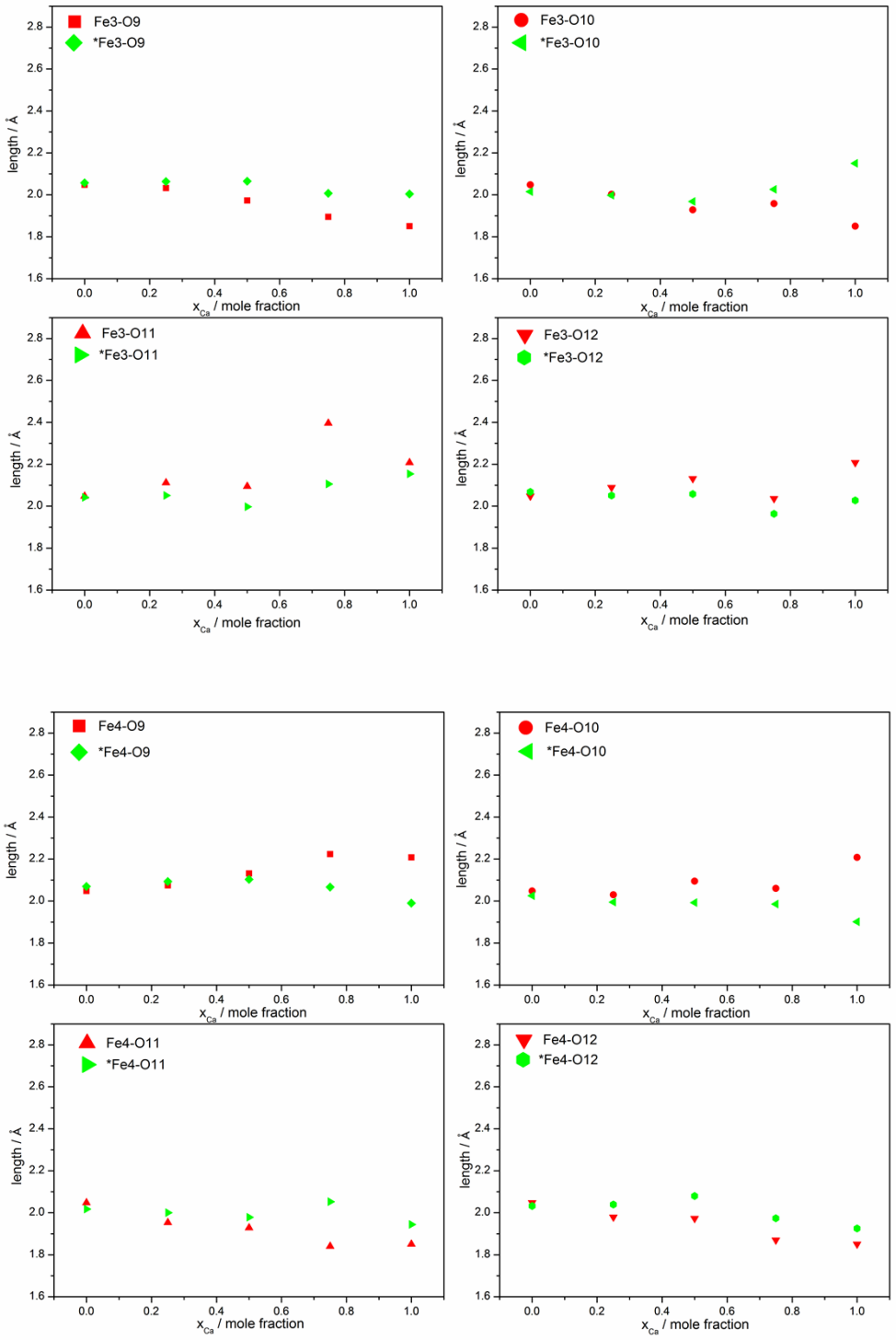


Fig. S4 The equatorial Fe-O bond length (Å) for $Nd_{1-x}Ca_xFeO_3$ (red) and $Nd_{1-x}Ca_xFeO_{2.75}$ (green) (x=0.00, 0.25, 0.50, 0.75, 1.00).

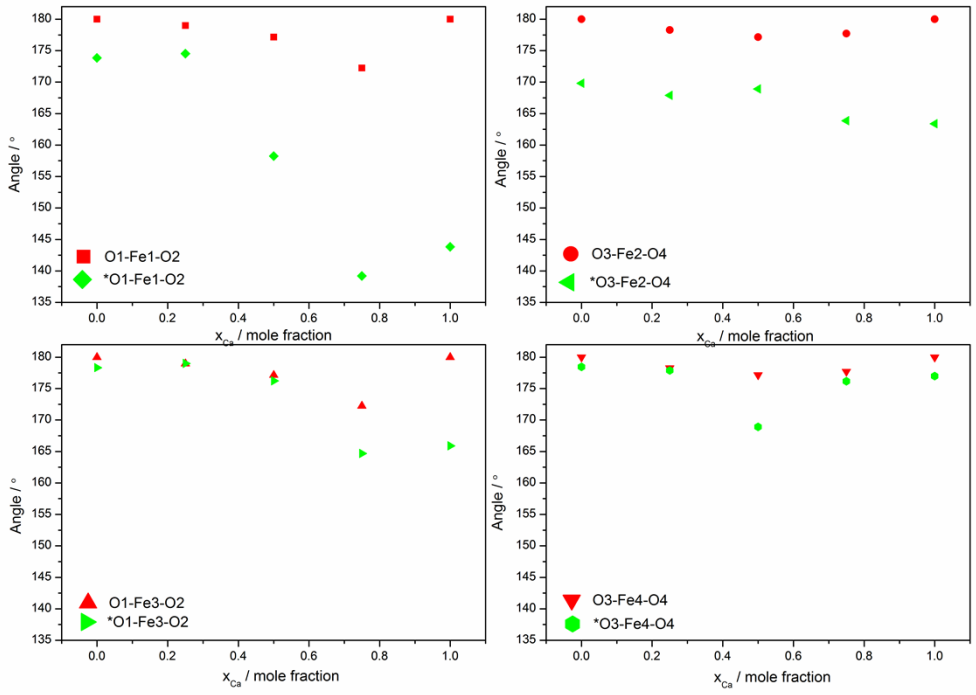


Fig. S5 The axial O-Fe-O bond angle (º) for $Nd_{1-x}Ca_xFeO_3$ (red) and $Nd_{1-x}Ca_xFeO_{2.75}$ (green) (x=0.00, 0.25, 0.50, 0.75, 1.00).

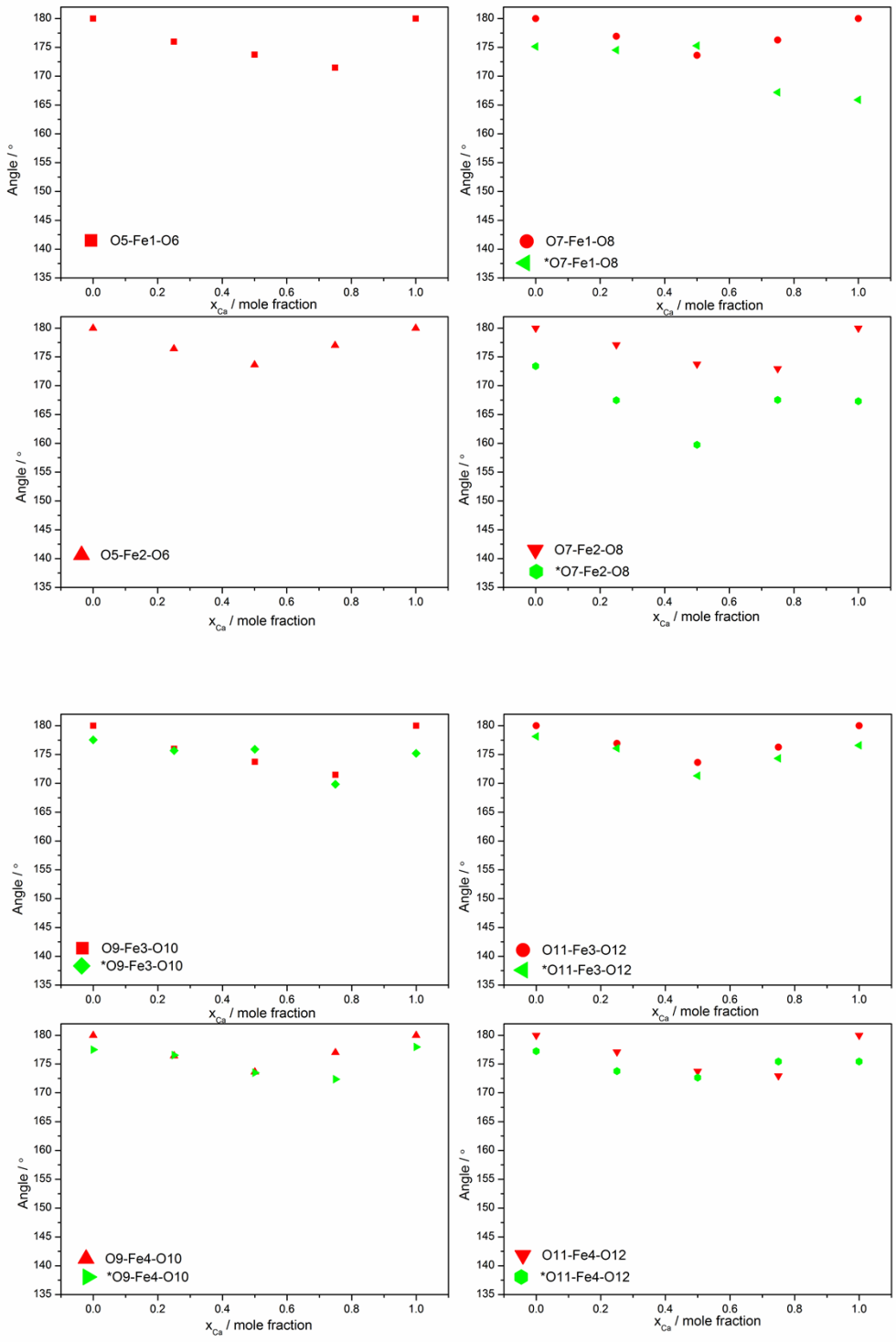


Fig. S6 The equatorial O-Fe-O bond angle (º) for $Nd_{1-x}Ca_xFeO_3$ (red) and $Nd_{1-x}Ca_xFeO_{2.75}$ (green) (x=0.00, 0.25, 0.50, 0.75, 1.00).

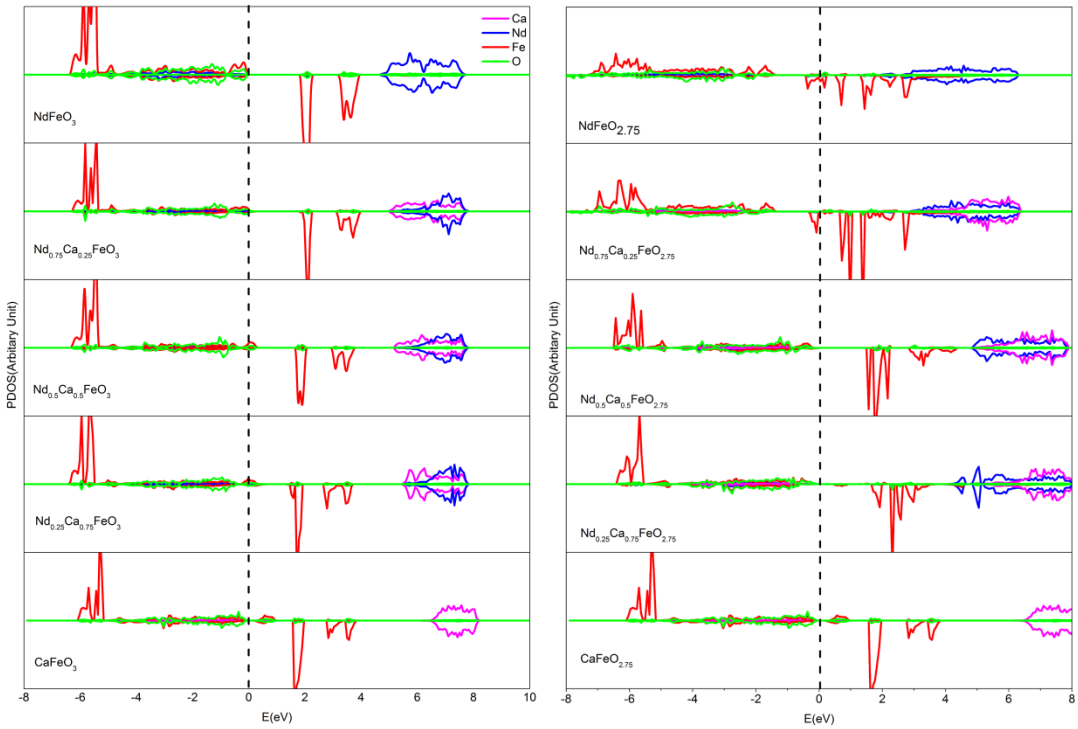


Fig. S7 Partial density of states (PDOS) of $Nd_{1-x}Ca_xFeO_3$ (x=0.00, 0.25, 0.50, 0.75 or 1.00, δ=0.00 or 0.25).

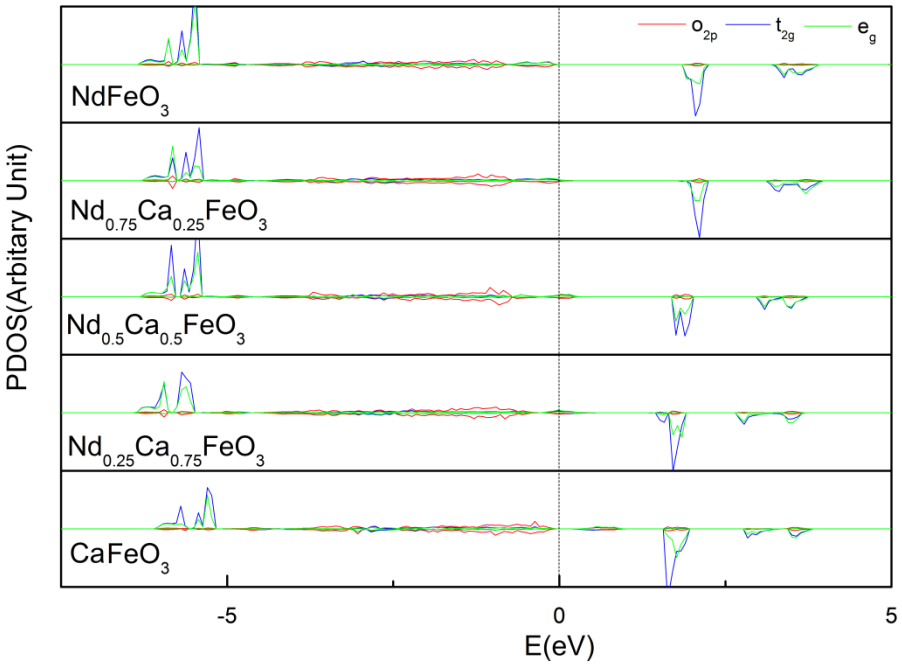


Fig. S8 The PDOS images of O 2p, Fe t_{2g} and Fe e_g are shown for the structures of $Nd_{1-x}Ca_xFeO_3$ (x=0.00, 0.25, 0.50, 0.75 and 1.00).

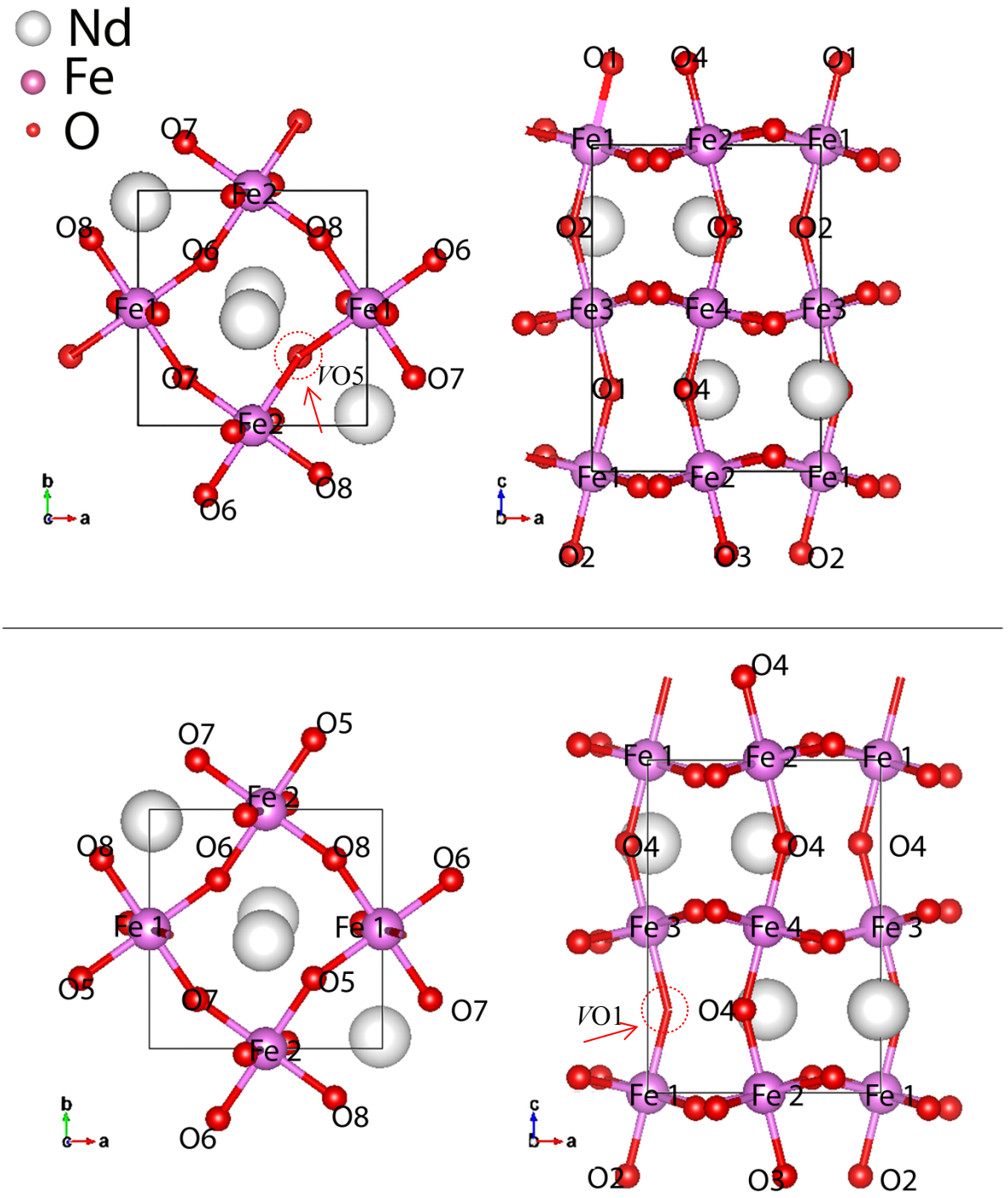


Fig. S9 Top views and side views of $NdFeO_{2.75}$. Oxygen vacancies formed along axial Fe-O-Fe bond (lower) and equatorial (upper). Structures are visualized with VESTA.