Supporting Information

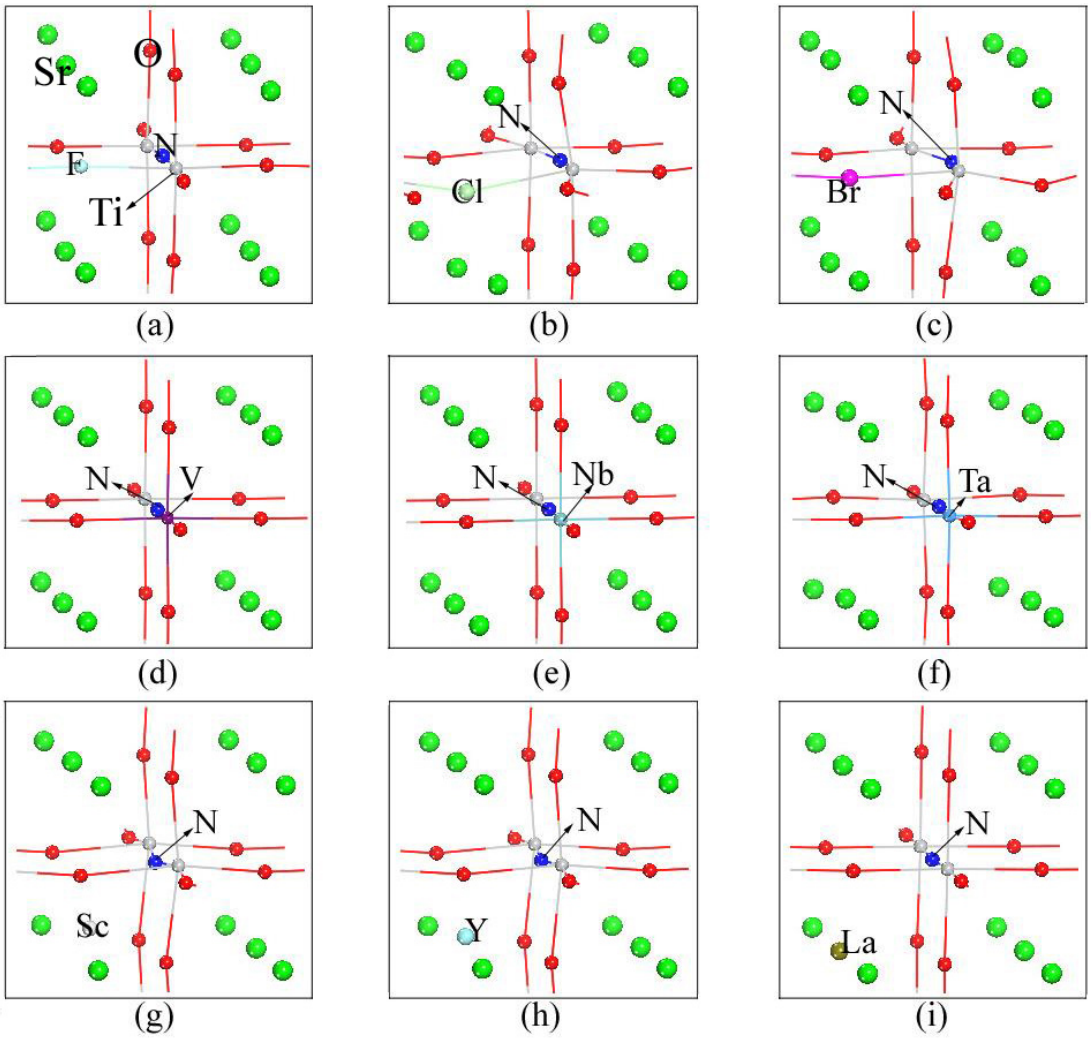

Figure S1: An octahedron taken from (a) N/F-, (b) N/Cl-, (c) N/Br-, (d) N/V-, (e) N/Nb-, (f) N/Ta-, (g) N/Sc-, (h) N/Y- and (i) N/La-codoped $SrTiO_3$. All the elements are labeled.

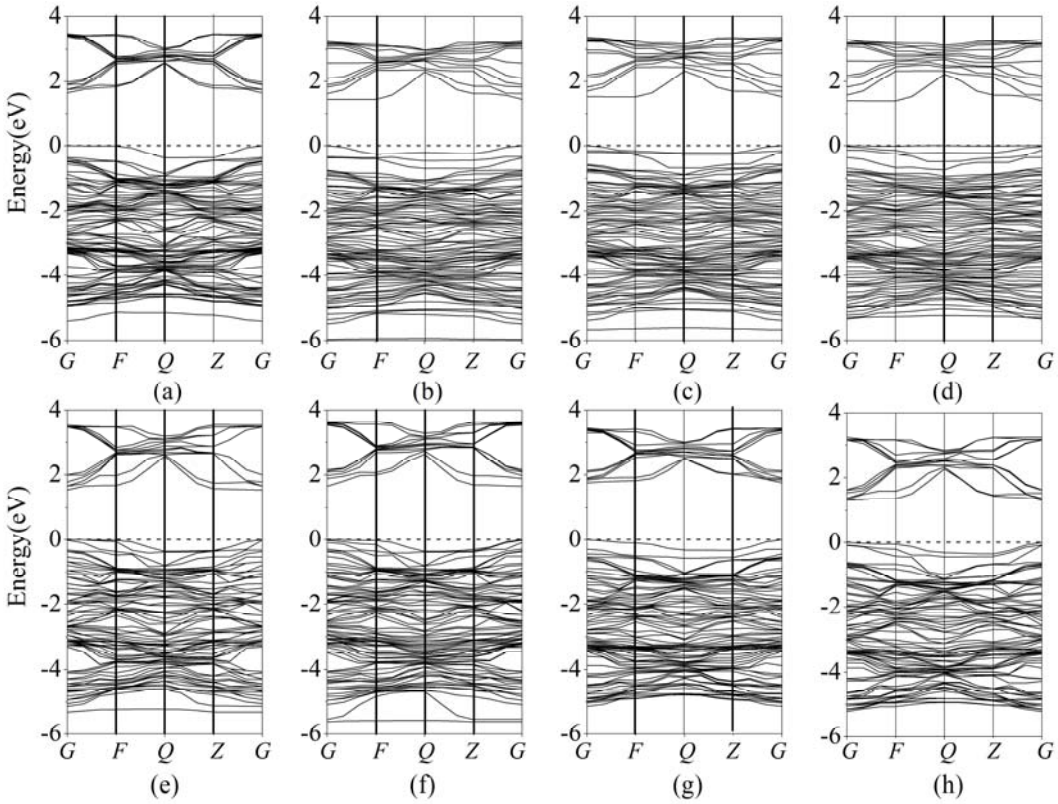

Figure S2: Band structure of (a) N/H-, (b) N/Cl-, (c) N/Br-, (d) N/I-, (e) N/Nb-, (f) N/Ta-, (g) N/Y- and (h) N/La-codoped $SrTiO_3$. The highest occupied level is set at zero.

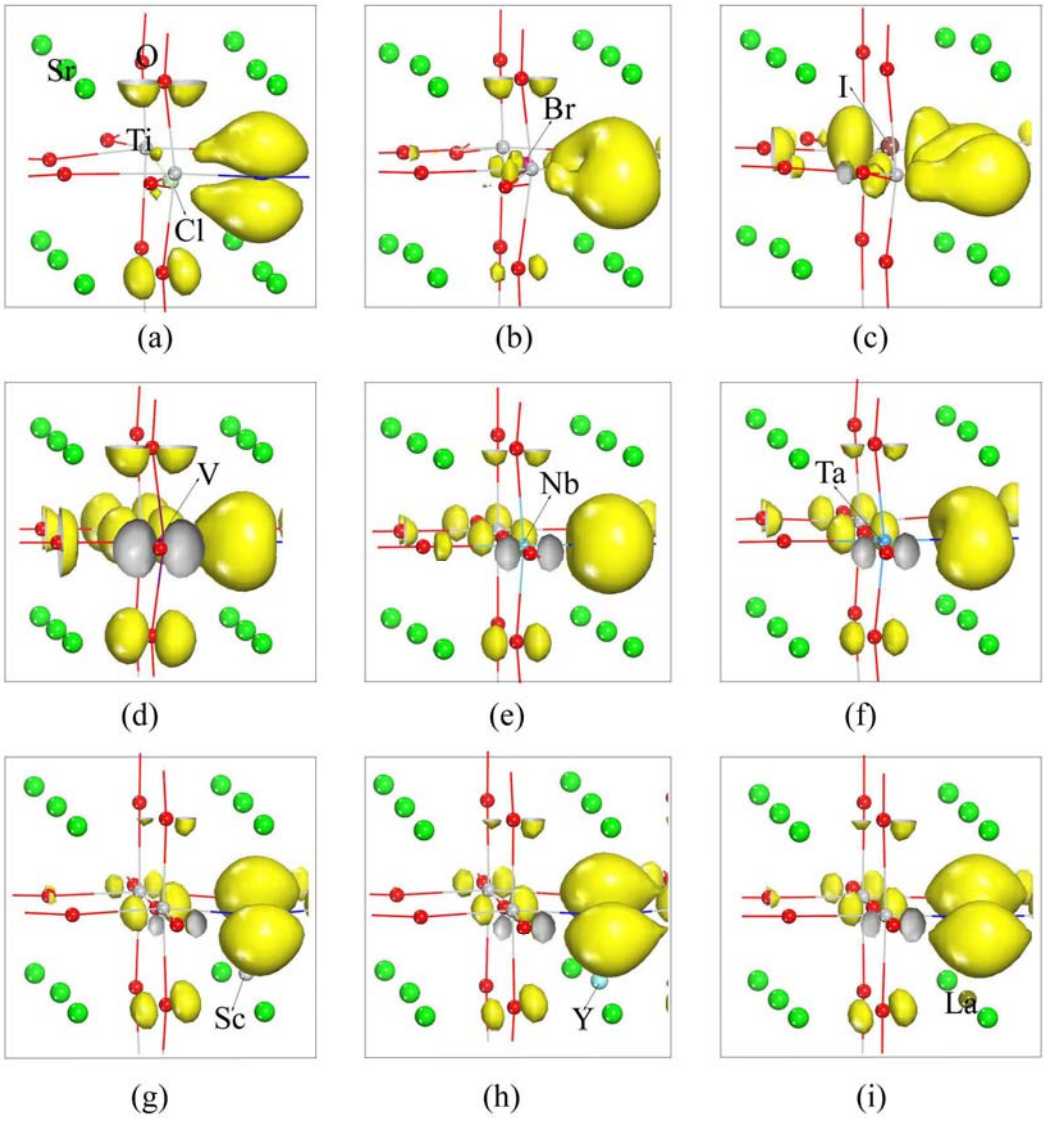

Figure S3: The highest occupied molecular orbital (HOMO) in (a) N/Cl-, (b) N/Br-, (c) N/I-, (d) N/V-, (e) N/Nb-, (f) N/Ta-, (g) N/Sc-, (h) N/Y- and (i) N/La-codoped $SrTiO_3$. The isovalue for orbital contour plots is 0.02 electron/ $Å^3$. All the elements are labeled.

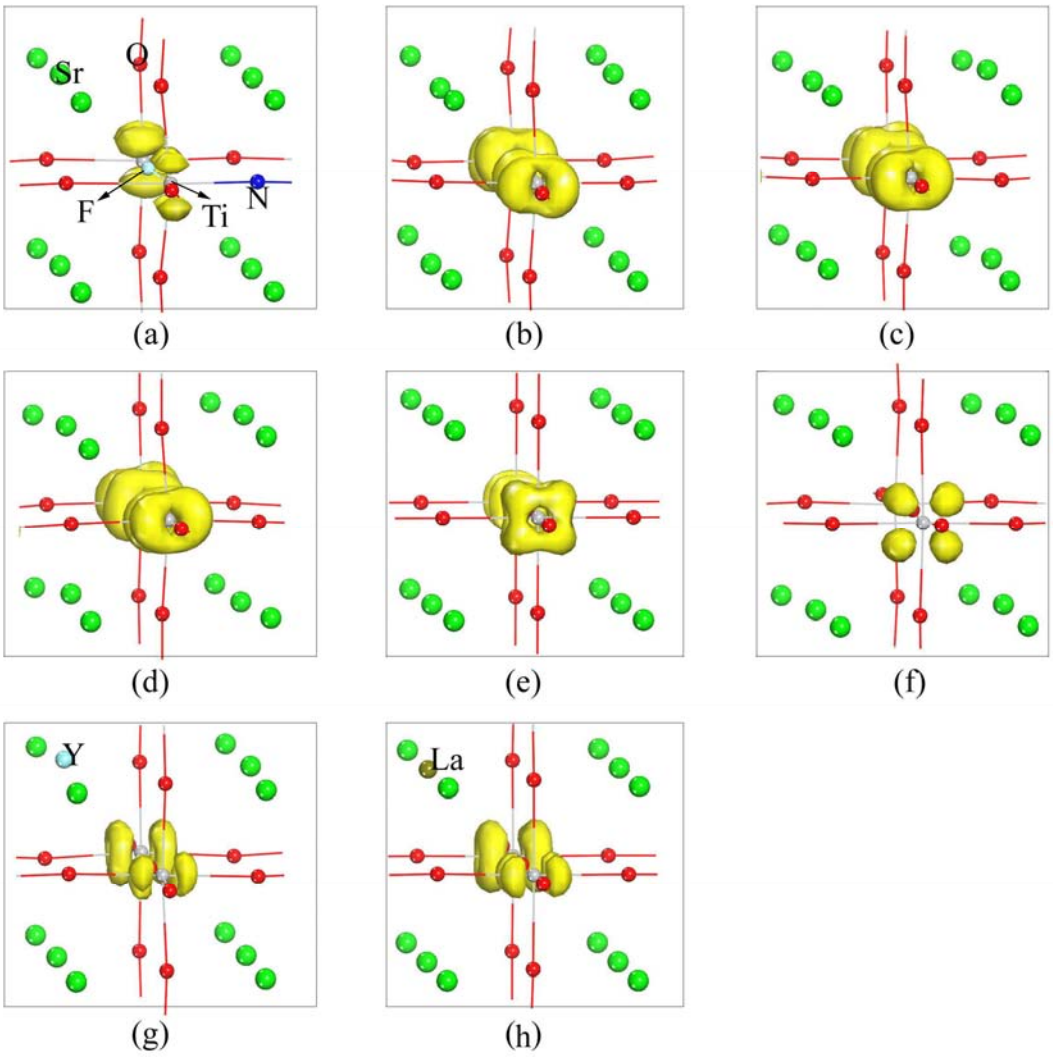

Figure S4: The lowest unoccupied molecular orbital (LUMO) in (a) N/F-, (b) N/Cl-, (c) N/Br-, (d) N/I-, (e) N/Nb-, (f) N/Ta-, (g) N/Y-, (h) N/La-codoped $SrTiO_3$. The isovalue for orbital contour plots is 0.02 electron/ $Å^3$. All the elements are labeled.