**Supplementary Information**

The Effect of Lanthanum Doping and Oxygen Vacancy on Perovskite, Pyrochlore Oxide and Lanthanide Titanates: A First Principle Study

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Figure S1: Effect of mix oxidation state of Ti on the Bader charge of cations in La2/3TiO3 system. Multiple Bader charges at a fixed # additional electron represent all La/Ti atoms. The large sphere represents their average.

Figure S2: Effect of mix oxidation state of Ti on the Bader charge of anions in La2/3TiO3 system. Multiple Bader charges at a fixed # additional electron represent all O atoms. The large sphere represents their average.



Figure S3: Contour plots of charge-density difference the La2/3TiO3 0 and 4 additional electrons system. Yellow and blue colors indicate positive (charge accumulation) and negative (charge depletion) regions, respectively.