Supporting Information

Oxygen migration performance of $LaFeO_3$ perovskite-type oxygen carrier with Sr doping

Yuan Feng[a], Hanyu Jin [a], Shuai Wang [a*]

a School of Energy Science and Engineering, Harbin Institute of Technology, Harbin, 150001, China

∗ Corresponding author.

E-mail address: shuaiwang@hit.edu.cn

Figure S1 Oxygen vacancy formation energy of a 13-layer $LaFeO_3$ system (ref. bulk value: oxygen vacancy formation energy obtained using the same method from the bulk model)

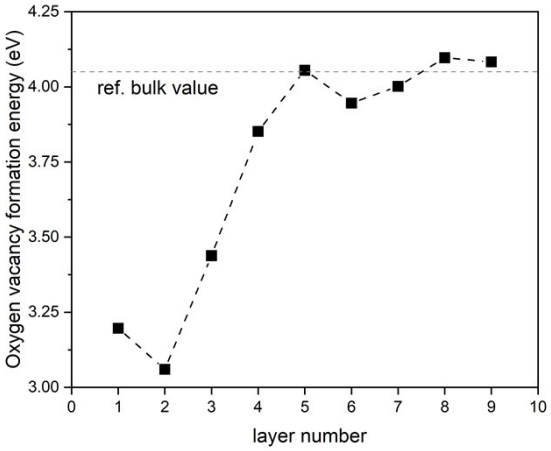

Figure S2 Oxygen migration barrier of a 13-layer $LaFeO_3$ system

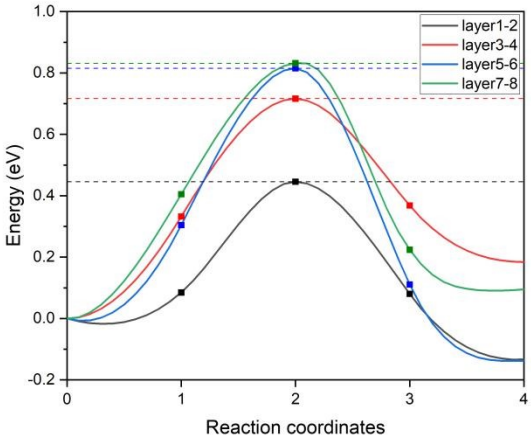

Figure S3 Comparison of oxygen migration barriers from high site and low site at the layer 1-2 process (a), the layer 3-4 process (b) in the undoped $LaFeO_3$ system

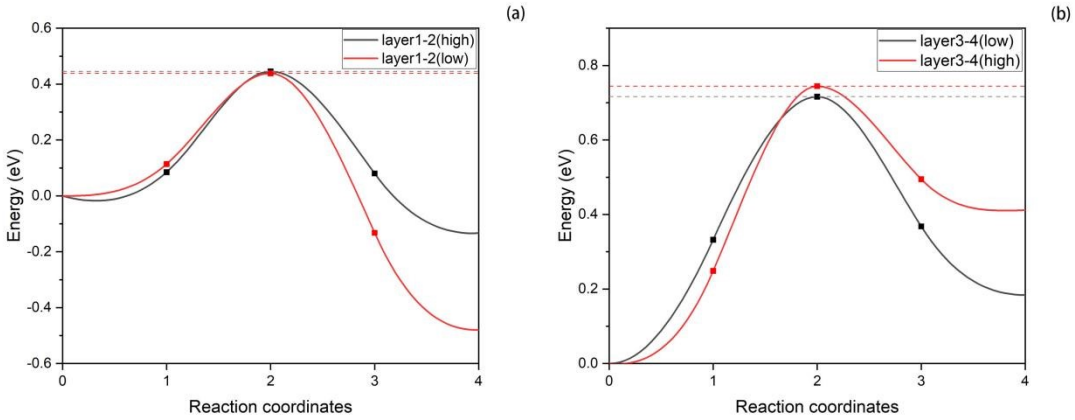

Figure S4 Oxygen migration barrier at the asymmetric location of the 50% Sr doped system from the path away from Sr atom (a) and near Sr atom (b)

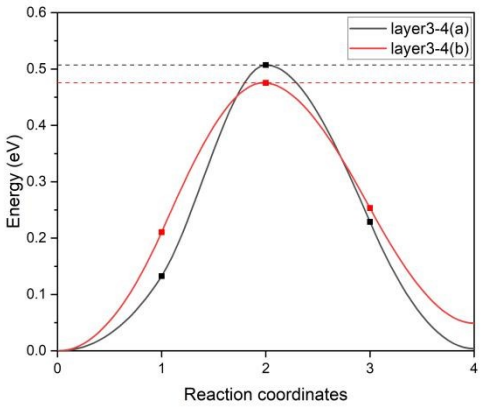

Figure S5 Oxygen migration barrier through A-site atoms in the 50% Sr doped system