Supplementary Data

Electronic Structure of the Oxygen Interstitials in $La_{10}(SiO_4)_4(AlO_4)_2O_2$

The local densities of states (LDOS) at atoms surrounding $V_O^{\cdot\cdot}$ and O_i'' are presented in Fig. S1. The figure also includes the total DOS for the model host crystal, which exhibits an energy gap of 4.6 eV. The middle and lower panels in Fig. S1 show the LDOS for La at 4f, Si at 6h, and O at the 2a sites (see Fig. 1 in the main text) adjacent to $V_O^{\cdot\cdot}$ and O_i'''. The formation of $V_O^{\cdot\cdot}$ induces a gap state with the La 5d character in the proximity of CBM, as shown in Fig. 1. For $V_O^{\cdot}$ and $V_O^{\times}$, a similar state is obtained with partial and full occupation, respectively.

The gap state of O_i'' appears above the top of the valence band, which consists mainly of O_i p orbitals, while these states are shown as a tail of the valence band in the figure, due to the supercell approximation and Gaussian broadening to obtain the LDOS.

The LDOS for O_i displayed in the bottom panel of Fig. S1(b) shows a similar distribution to that for the adjacent oxygen in the cluster. Thus, the electronic structure around O_i appears to be almost the same as that for other oxygen ions in the Al-O cluster. The LDOS for the Al-site adjacent to O_i (middle panel in Fig. S1(b)) has a small but visible amplitude for those states that are dominated by the oxygen orbitals, which indicates that O_i forms a bond to the aluminum atom with some covalent character.

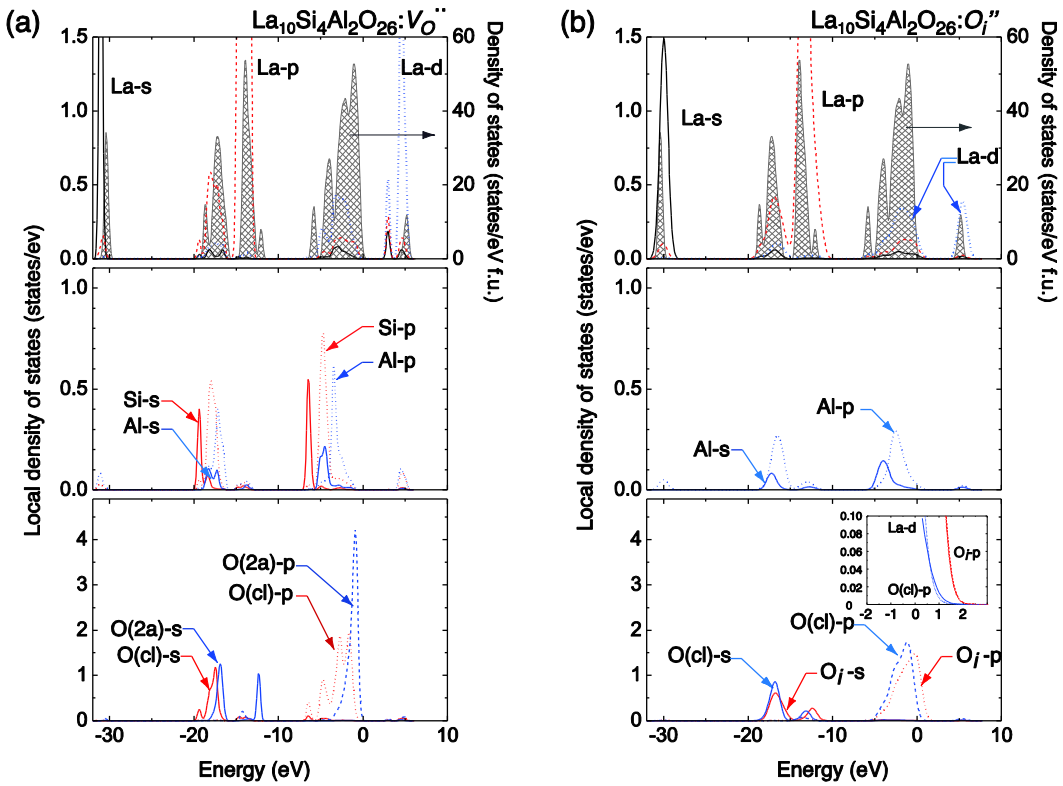

FIGURE S1. Calculated LDOS for (a) $V_O^{\cdot\cdot}$ and (b) O_i'' in $La_{10}(SiO_4)_4(AlO_4)_2O_2$. The total DOS of the model host crystal is also plotted as a hatched area in both panels. O(cl) denotes the nearest oxygen atom in the AlO_4 or SiO_4 cluster. The top of the valence band is set to zero. The inset in the bottom panel of (b) is an enlargement around zero with the La-d component.

Potential Energy Surfaces and Atomic Configurations for the Vacancy Mediated Model

The results of the potential energy surface calculations for the vacancy mechanism are shown in Fig. S2. The atomic configuration changes are also indicated in the figure.

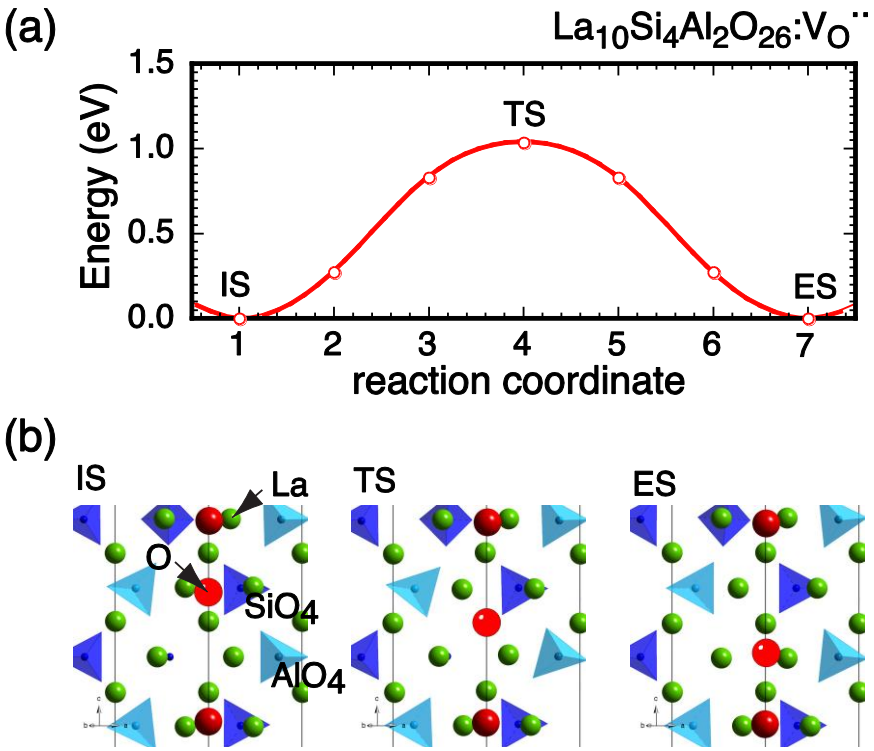

FIGURE S2. Calculated potential energy surfaces and the atomic configurations of the oxygen migration via the vacancy mechanism and (b) the interstitial and interstitialcy mechanism. The oxygen ions exhibiting large displacement are denoted by arrows.