Supplementary Information

One-Dimensional Water Channels in Lanthanum Sulfate:

A First-Principles Study

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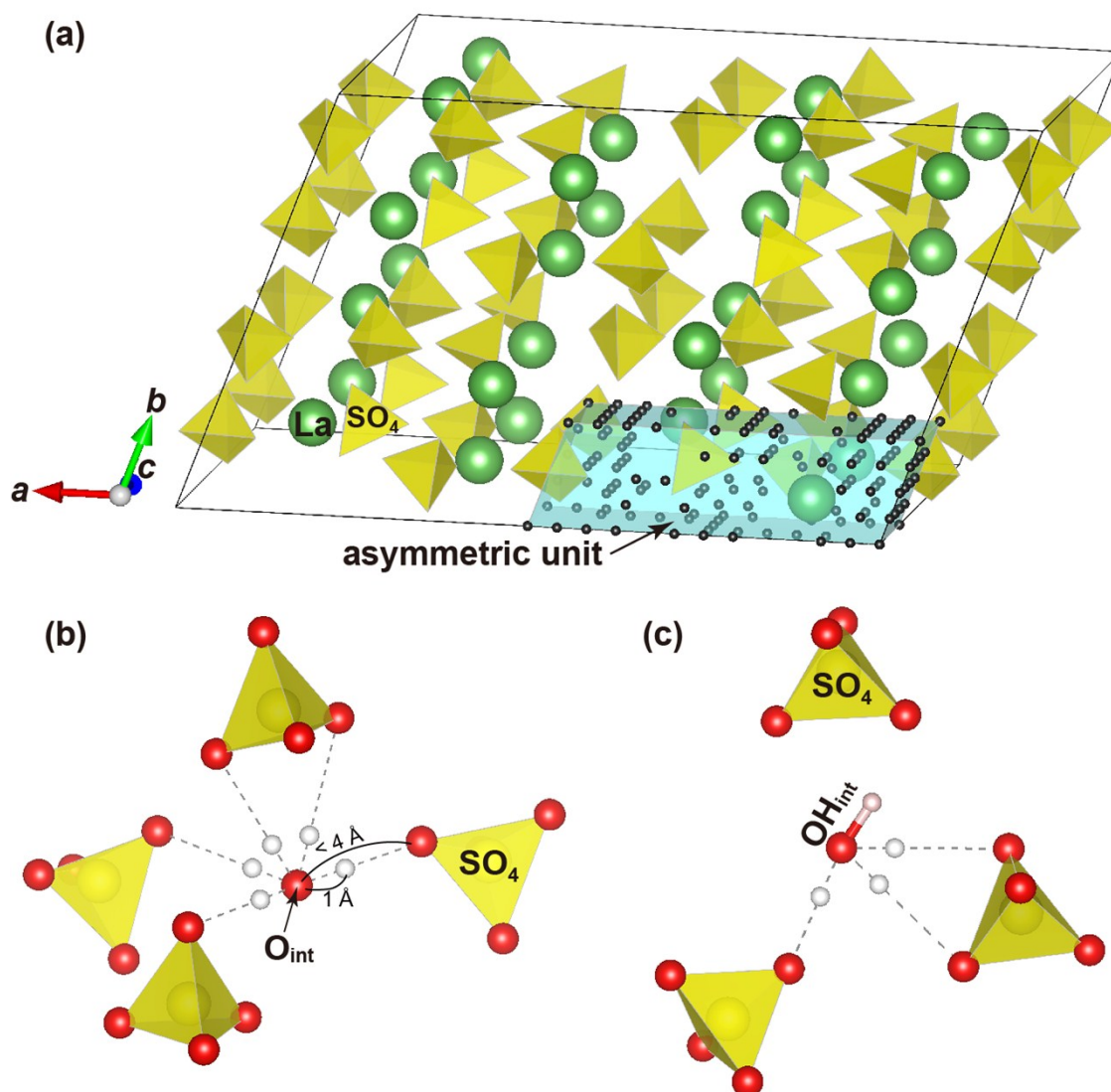
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Figure S1. Three-step procedure (steps 1–3) for determining the H_2O stable structure in $La_2(SO_4)_3$. (a) 144 grid points (black spheres) on the 12×4×4 grid in the asymmetric unit used as the initial positions of an interstitial O ion for structural optimization at step 1. The gird points are shown in the supercell consisting of 1×2×2 unit cells. 48 grid points close to the neighboring host ion are excluded. (b) Initial proton positions (white spheres) around an interstitial O ion (O_{int}) for structural optimization at step 2, to determine the stable structure of an OH ion. These initial positions are on a sphere around the interstitial O ion with a radius of 1 Å and on a line connecting the interstitial and a neighboring O ions. The distance between the two O ions are shorter than 4 Å. (c) Initial proton positions (white spheres) around an interstitial OH ion (OH_{int}) for structural optimization at step 3, to determine the H_2O stable structure. These positions are determined in the same manner at step 2.