

Electronic Supplementary Information (ESI)

Hydroxide ion incorporation and conduction mechanisms in tin pyrophosphate

– A first-principles study

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Fig. S1 (a) The calculated proton sites (white small balls bonding to an oxide ion) and (b) tin sites (green and purple balls) and their site energies. The site energies in the parentheses are with reference to that at the most stable site in each figure. The atomic positions of the host lattice are shown by their original positions before structural optimizations.

Fig. S2 Hydroxide-ion migration trajectories in SnP_2O_7 evaluated by the NEB calculations. Figures (a)-(c) correspond to the processes of (i)-(ii), (iii), and (iv) in Fig. 6, respectively.

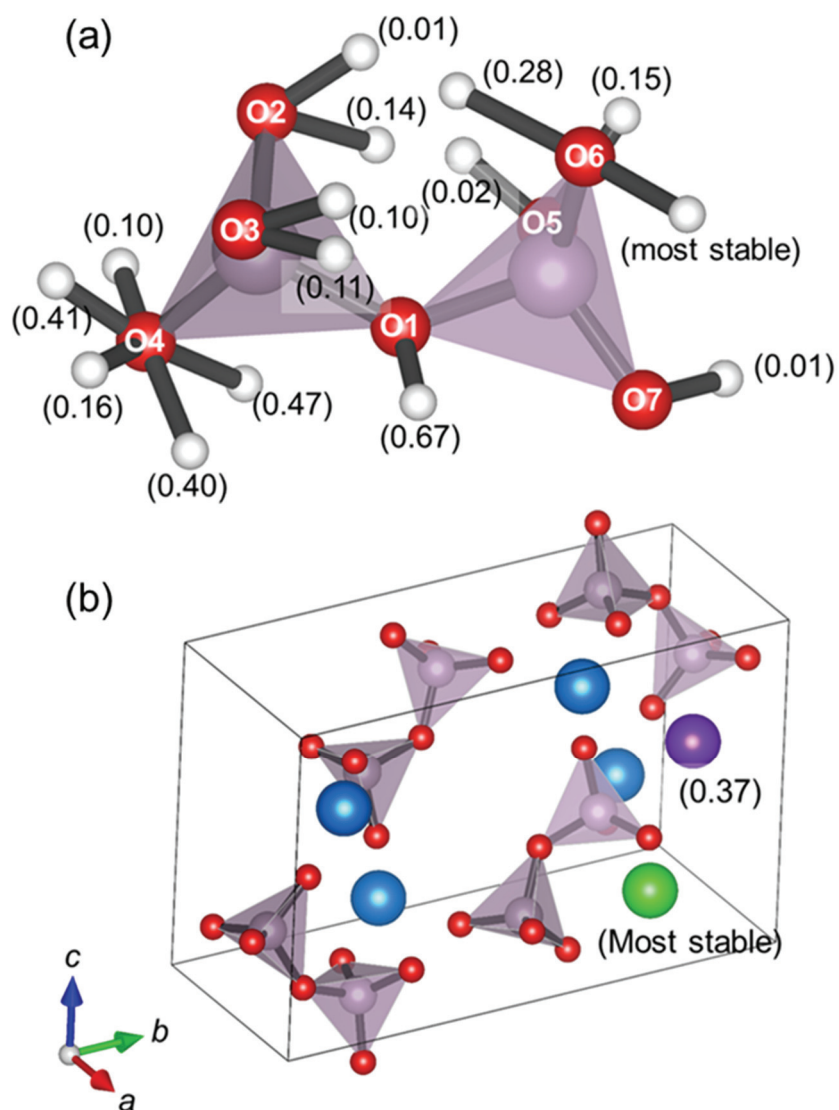


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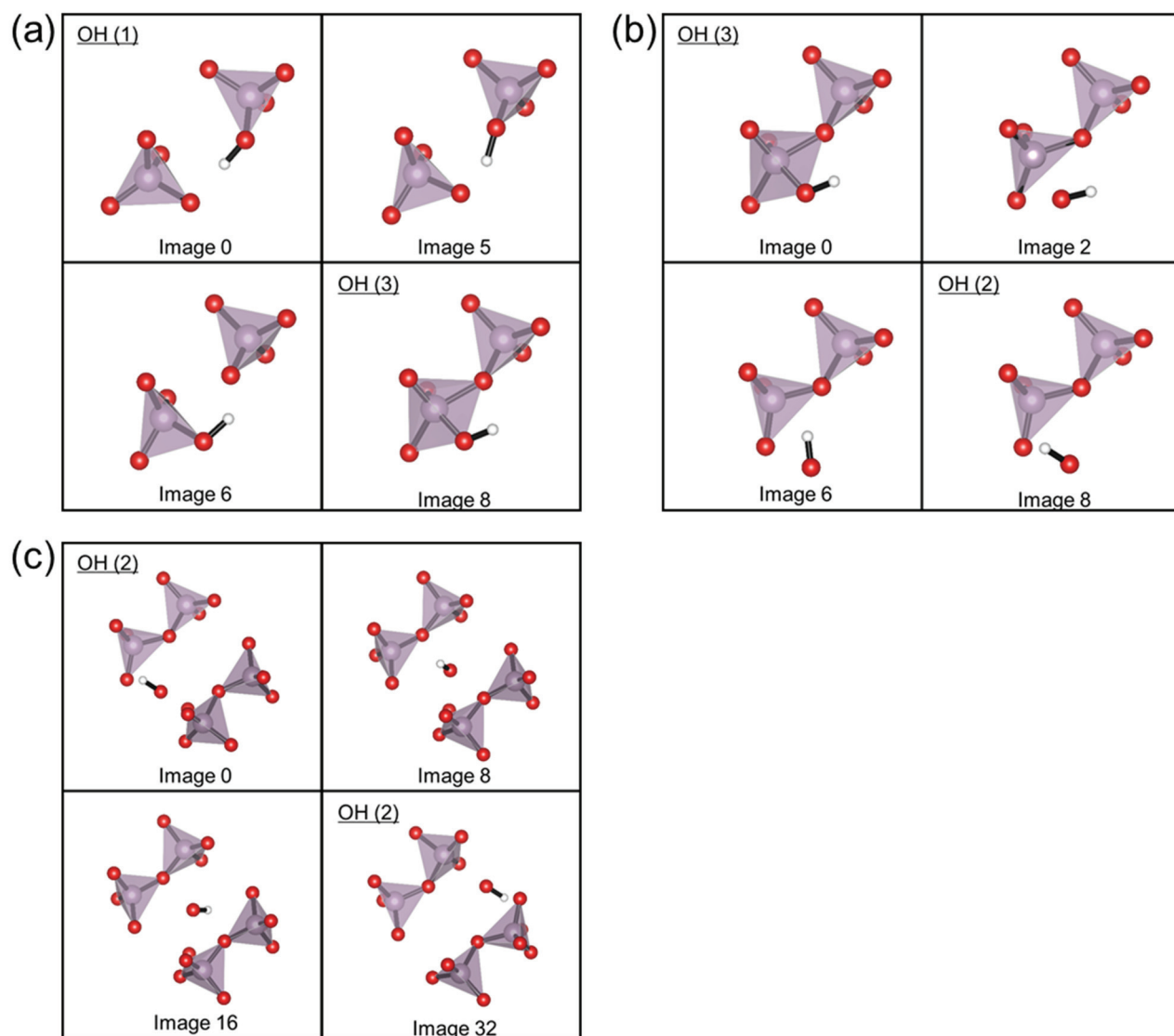


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