Electronic Supplementary Information

Computational investigation of the Mg-ion conductivity and phase stability of $MgZr_4(PO_4)_6$

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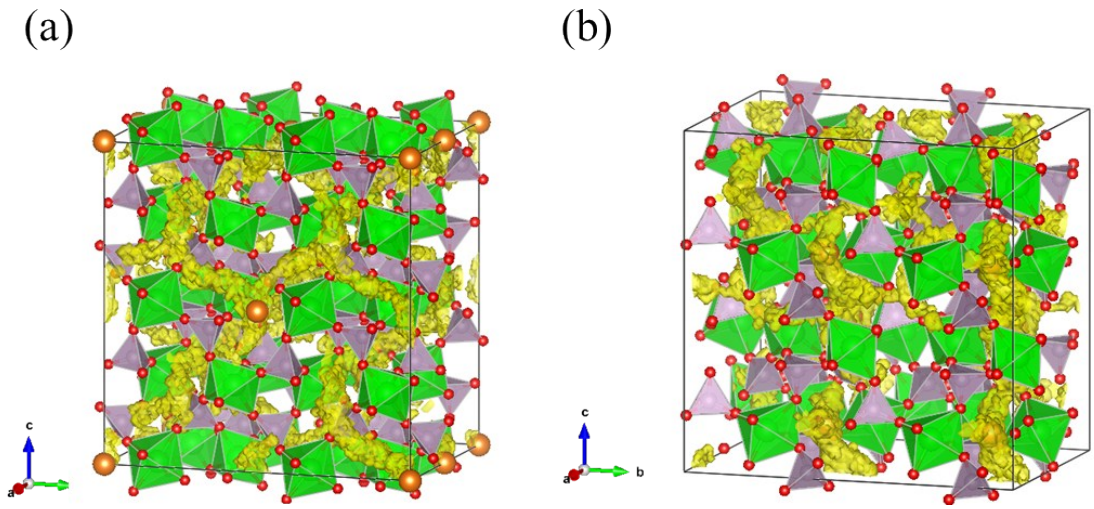

Supporting Figure S1. Trace of Mg atom in FPMD simulation at 1573 K. (a) and (b) show the NASICON-type and β–iron sulfate-type structures, respectively.

Supporting Table S1. Mg-Ion Conductivity (σ_{Mg}) and Activation Energy (E_{act}) of Mg-Ion Conductors

Study	σ_{Mg} [S cm^{-1}]	E_{act} [eV]
Theoretical (β-iron sulfate-type, this paper)	3.9×10^{-3} (bulk, 873 K)	0.71
Theoretical (NASICON-type, this paper)	7.1×10^{-3} (bulk, 873 K)	0.63
Experimental[21] (β-iron sulfate-type)	1×10^{-5} (873 K)	1.6
Experimental[21] $Mg_{0.7}(Zr_{0.85}Nb_{0.15})_4P_6O_{24}$ (β-iron sulfate-type)	1.1×10^{-7} (573 K)	0.92
Experimental[22] $Mg_{0.7}(Zr_{0.85}Nb_{0.15})_4P_6O_{24}$ (β-iron sulfate-type)	1.1×10^{-6} (total, 623 K)	1.18
Experimental[18] $(Mg_{0.1}Hf_{0.9})_{4/3.8}Nb(PO_4)_3$ (NASICON-type)	2.1×10^{-6} (bulk, 573 K)	0.68