Role of divalent cation (Ba) substitution in Li$^+$ ion conductor LiTi$_2$(PO$_4$)$_3$: Molecular dynamics study

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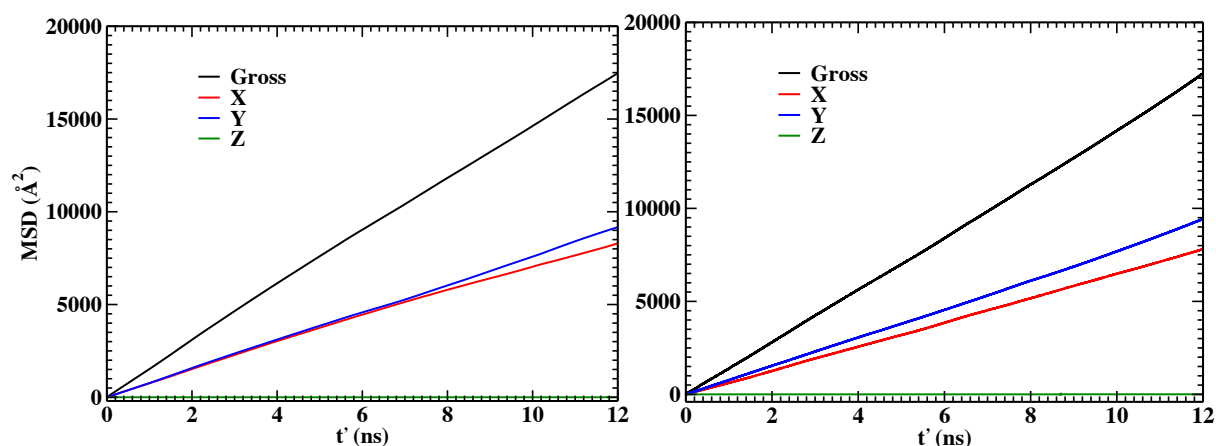[b]Institute of Physics, Academia Sinica, Taiwan

Fig. S1 Mean Square Displacement of Li$^+$ ion for x, y, z component and total for $x = 0.67$ (left) and $x = 0.83$ (right) composition.
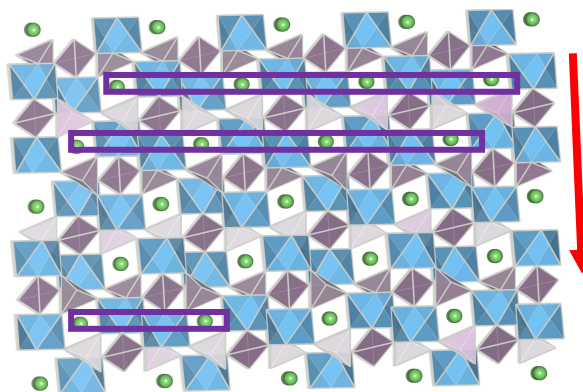

Fig. S2 Polyhedral model of LiTi$_2$(PO$_4$)$_3$ for super-cell consists of $4 \times 4 \times 1$-unit cells. The TiO$_6$ octahedra is represented by cyan and PO$_4$ tetrahedra is represented by blue. The Li1-site is indicated by green ball. The purple box indicates the plane where Ba^{2+} is located for ordered cases in Li1-sites. The purple box will be filled one by one from top to bottom (indicated by red arrow) depending on the compositions. This order arrangement is different than Fig. 1 in term of Ba^{2+} filling order.