The theoretical study on the new perovskite-type transition metal fluorides with lithium ion conductivity

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Abstract

Previously, hybrid-DFT calculations were performed for the perovskite-type manganese fluorides of $RMnF_3$ (R=K, Rb, Li).[1] The calculated activation energies for the lithium ion conduction were enough small, in comparison with that of $La_{2/3-x}Li_{3x}TiO_3$.[2] It was concluded that the lithium ion conduction in $RMnF_3$ is possible, if the vacancy at R site is doped. In this study, the effects of the oxygen doping on $RMnF_3$ were investigated in order to realize the high lithium ion conductivity.

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References

[1]T. Onishi, Polyhedron., in press

[2]T. Onishi, Solid. State. Ionics., in press