Atomistic simulations of Li-ion diffusion in $LiZr_2(PO_4)_3$ solid electrolyte for Li-air batteries

Bhargav Akkinepally[1], Minsik Yang[1], Jaehun Chung[1], Migyung Cho[2$], Jaesool Shim[1*]

[1]School of Mechanical Engineering, Yeungnam University, Republic of Korea

[2]Dept. of Game Engineering, Tongmyong University, Republic of Korea

*Corresponding author: Email address: jshim@ynu.ac.kr (J. Shim)
[$]Co-corresponding author: Email address: mgcho@tu.ac.kr (M. Cho)

Abstract:

In the last few decades, crystalline group of NASICON due to its high ionic conductivity have experienced a sharp development and became a promising candidate for the future lithium batteries. In this research, we focused on the Al doping effects on the pure LZP (Lithium Zirconium Phosphate) and also the diffusion phenomenon of Li-ion due to temperature variations using molecular dynamics simulations. LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) tool had been used for the purpose mentioned. These simulations were based on the reactive force-field (Reaxff) potentials. The framework of $Li_{1+x}Al_xZr_{2-x}(PO_4)_3$ solid electrolyte for Li-air batteries have been analyzed at different temperatures. The computational results for pure LZP matches with the previous literatures and hence validating the computation code. The Li diffusion path and the activation energy are in well agreement with the literatures. The Al doping significantly improves both the Li-ion conductivity and the diffusivity.

Keywords: NASICON, MD simulations, Li air batteries, solid electrolyte

Acknowledgement

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2018 R1A2B6002849).

References

[1] Xu, H. H.; Wang, S. F.; Wilson, H.; Zhao, F.; Manthiram, A. Y-Doped NASICON-Type $LiZr_2(PO_4)_3$ Solid Electrolytes for Lithium Metal Batteries. *Chemistry of Materials, 29 (17) (*2017) 7206-7212, DOI: 10.1021/acs.chemmater.7b01463

[2] Noda, Y.; Nakano, K.; Takeda, H.; Kotobuki, M.; Lu, L.; Nakayama, M. Computational and Experimental Investigation of the Electrochemical Stability and Li-Ion Conduction Mechanism of $LiZr_2(PO_4)_3$. *Chemistry of Materials, 29 (17) (*2017) 8983-8991, DOI: 10.1021/acs.chemmater.7b01703