Iranian Journal of Physics Research, Vol. 23, No. 2, 2023
DOI: 10.47176/ijpr.23.2.51681

Investigating and comparing the penetration mechanism and diffusion path of sodium and lithium in the structure of NaSICONs

M R Valizadeh and F Marsusi

Department of Physics, Amirkabir University of Technology (Tehran Polytechnic), Tehran, Iran.

E-mail: marsusi@aut.ac.ir

(Received 07 May 2023 ; in final form 20 May 2023)

Abstract

The design and identification of solid electrolytes can lead to finding safer and more efficient solid state batteries in a wider temperature range for fuel cells. There are more than 200,000 crystal structures in the ICSD database for finding solid electrolytes, and among them, more than 44,000 experimental structures have been considered in the search for solutions for advances in energy storage. Therefore, before making solid electrolytes, we need new calculation methods so that we can choose the appropriate structure among all these existing structures with the help of it, more quickly and accurately than in the past. Super ionic conductor solids are one of the main components in energy storage and conversion, and the development of these new conductors is impossible without a comprehensive understanding of ion migration mechanisms in these structures. NaSICON is an oxide-based solid electrolyte with a three-dimensional framework. NZP (NaZr2P3O12) and rhombohedral LiZr2P3O12 (LZP) are the two prototypes of all NaSICONs. In this research, with a new computational approach, we showed that by changing the sodium ion with lithium in the structure of NaSICONs, the amount of activation energy, which plays a decisive role in the design and production of all-solid-state batteries, changes and we have answered the question whether with this change, the path of movement of sodium and lithium ions inside the crystal structure remains constant or not.

Keywords: solid electrolyte, molecular dynamics, super ionic conductor, sodium ion, bond valence

For full article, refer to the Persian section