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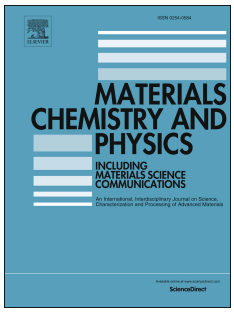


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# *Ab initio* molecular dynamics study of lithium diffusion in tetragonal $Li_7La_3Zr_2O_{12}$

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## Abstract

Using *ab initio* density functional theory the thermally-stimulated migration of lithium ions in the garnet-type material $Li_7La_3Zr_2O_{12}$ is investigated. The methods of *ab initio* equilibrium molecular dynamics have been applied to calculate the lithium ion self-diffusion coefficient and the diffusion barriers as function of lithium ion concentration. The concentration of lithium in the initial $Li_7La_3Zr_2O_{12}$ crystal unit cell is varied from 53 to 59 atoms, where 56 lithium atoms represent the stoichiometric concentration. Almost monotonous dependencies of the main characteristics on the number of lithium atoms $N^{(Li)}$ have been found, except for a non-monotonous peculiarity of the stoichiometric compound ($N^{(Li)} = 56$). Finally, the influence of the unit cell volume change on lithium ion diffusion parameters as well as lithium ion hopping rates has been studied.

*Keywords*: inorganic compounds; ab initio calculations; molecular dynamics; diffusion; transport properties

## Introduction

Over the last 30 years, development and application of solid electrolytes possessing high ionic conductivity at room temperature and high chemical stabilities have been achieved [1]. Currently, there is great interest in the application of solid electrolytes for high-performance lithium batteries because of the high electrical, chemical, and mechanical stability [2]. Therefore, strong efforts are at present directed towards

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