FIRST-PRINCIPLES CALCULATIONS OF THE STRUCTURAL, ELECTRONIC AND ELASTIC PROPERTIES OF $SrGeO_3$ AND $SrZrO_3$ CUBIC PEROVSKITES

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Abstract. *The structural, electronic, elastic and thermodynamic properties of two cubic perovskites – $SrGeO_3$ and $SrZrO_3$ – were calculated using the first-principles methods for the pressure range from 0 to 25 GPa. Comparison of the calculated results with other literature data (whether available) yielded good agreement. Dependencies of all calculated properties – such as lattice constants, relative change of the unit cell volume, elastic constants and Debye temperature – on pressure were obtained, which enables reliable estimations of all these parameters for any value of hydrostatic pressure in the studied range.*

Keywords: Perovskite; First-principles calculations; Electronic properties; Elastic properties

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1. Introduction

Perovskites is a common name for a large group of compounds with the general chemical formulas ABX_3 (if A and B are the di- and tetravalent metals, then X is oxygen; if A and B are the mono- and divalent metals, then X is a halogen). The possible combinations of these chemical elements should satisfy the stability criterion: the so called Goldschmidt tolerance factor $t = \frac{r_A + r_X}{\sqrt{2}\,(r_B + r_X)}$ (r_i is the ionic radius, the subscript i denotes an element in the chemical formula) should be confined in the range between 0.75 and 1 [1,2,3]. It is also possible to make the doubled perovskites $A_2BB'X_6$ by doubling a unit cell of an ABX_3 perovskite along the c crystallographic direction [4]. Versatile chemical composition of perovskites and their ability to accommodate organic complexes instead of some cations may also lead to a variety of stable crystallographic structures, such as cubic, rhombohedral, tetragonal, orthorhombic, and monoclinic.

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