

Cation ordering in Bi-based double perovskites: a density functional analysis

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Perovskites with two different types of cations at one of the sublattices, namely the A-site ($AA'B_2O_6$) and the B-site ($A_2BB'O_6$) are called double perovskites. For these compounds, the cation ordering can exist. There are some general rules for such systems [1, 2]. For example, the order at the B-site than at the A-site occurs more frequently. A typical ordering pattern for such compounds is rock-salt. The cation ordering also appears when the difference between the ionic radii and/or oxidation states is significant. Recently, the isovalent cation ordering in the Bi_2FeAlO_6 [3] was observed. In this work, we analyzed the role of ionic radius and magnetic ordering in the formation of the B-site cation ordering in Bi-based perovskite oxides with the general formula Bi_2MFeO_6 and $Bi_2MM'O_6$ where M and M' are Al, Ga, In, and Sc [4]. We found that despite the presence of the lone pairs at the Bi atoms the aforementioned general rules of cations ordering are fulfilled for non-magnetic cations. However, if one of the B-site cations is magnetic the layered ordering has lower energy than the rock-salt one. Finally, for the (pseudo)tetragonal structures the columnar ordering is favored for Bi_2MFeO_6 .

References:

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