Notes

o.m1.o5 Computational simulations of novel a-site substituted perovskites. V.L. Jennings & P.A. Thomas, *Physics Department, University of Warwick, Coventry. U.K.*
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The perovskites (generic formula ABO_3), show many useful properties, such as ferroelectricity, piezoelectricity and high dielectric constant. They are important not only for these properties, but also because their relatively simple basic structure facilitates the study and understanding of the relationship of these properties to the structure.

The structure, minimal energy configurations and possible phases of perovskite and related compounds have been investigated using computational methods. The main interest is the study of novel A-site substituted perovskite compounds, particularly $Na_{0.5}Bi_{0.5}TiO_3$.The methods used were density functional theory (FLAPW method implemented using the WIEN97[1] code) and an empirical potential approach (GULP[2] code). Preliminary results of modeling studies on this class of compounds will be presented.

[1] P.Blaha, K. Schwarz and J. Luitz, WIEN97, Vienna University of Technology, Vienna 1997, Updated version of P. Blaha, K. Schwarz, P. Sorantin and S. B. Trickey, Comp. Phys. Commun. 59, 399, 1990.
[2] General Utility Lattice Program, Julian Gale, Imperial College, London, U.K. (1993).