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ATOMISTIC LATTICE SIMULATION STUDIES OF BINARY AND TERNARY FLUORIDES

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Solid inorganic fluorides are playing an increasingly important role in such areas as novel glasses for optical fibres, solid state lubricants, lasers and thin-film solid electrolytes in addition to their established use as fluorination catalysts. However, apart from the binary alkaline-earth fluorides, the amount of experimental and theoretical information available on, for example, the defect structure, which determines many physical and chemical properties, is very limited.

This paper presents preliminary results for a range of binary and ternary fluorides. The theoretical methods are similar to those used previously for a variety of oxides [1]. The calculations are formulated within the framework of an ionic model and are based on two-body, electron-gas potentials [2] which incorporate the Dick-Overhauser shell approach to ionic polarization [3]. A consistent set of potentials have been generated for the binary fluorides, AF (A=Li, Na, K) and BF_2 (B=Mg, Ca, Ba), using a single F^{-}- F^{-} potential for the entire range. These are then used unchanged to predict the structures and properties of the full range of ternary fluorides ABF_3. Among the properties considered are the lattice structure, phonon densities of states and the fundamental defect structure. Only $LiBaF_3$, $KCaF_3$, $KMgF_3$ and $NaMgF_3$ are known experimentally and this is consistent with our calculated heats of formation [4]. In each case our calculations predict correctly the observed low temperature crystal structure and lattice parameters to within 1% of the measured value.

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