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Electronic structure and bonding in NaLi, LiMg and LiAl alloys: a MS X_α SCF approach

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Abstract. A MS X_α SCF method has been initiated to calculate the charge distribution, bonding properties and the density of states in NaLi, LiMg and LiAl alloys. No ionicity is seen in NaLi but a high covalency of different degree is detected in all the three alloys. The ionizations potentials calculated are 5·05, 5·5 and 5·58 eV respectively. Comparison with other calculations and experiments is found to be in fair agreement.

Keywords. Multiple scattering X_α self consistent field; bonding; alloys; electronic structure.

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1. Introduction

The electronic structure calculations by different cluster methods are widely used to study the localized properties in solids. The main points of interest have been bonding properties, transition between different energy states, magnetic properties, gap levels in semiconductors (Adachi *et al* 1979; Khowash *et al* 1985; DeLeo *et al* 1984) etc. Of the many calculation procedure the multiple scattering X_α self-consistent field (MS X_α SCF) method (Johnson 1967, 1968, 1971; Slater 1972, 1974) stands out. In this paper, we report the electronic structure, bonding properties and the density of states for NaLi, LiMg and LiAl alloys. Alkali metal dimers (NaLi) can be efficiently used as high power lasers near the infrared region. LiAl being light in weight and at the same time not easily breakable has attracted attention due to its potential usefulness in high energy density batteries as an anodic material and relatively high electrochemical activity. The equilibrium geometries and the bond length of small clusters of different sizes of LiNa, LiMg and LiAl have recently been given considerable importance (Rao *et al* 1986, 1987).

2. Methods

The MS X_α SCF method (Johnson 1967, 1968, 1971; Slater 1974) considers a cluster scooped out of the solid. The rest of the solid manifests its presence by providing a static electrostatic field through the Watson sphere truncation technique. The cluster is divided into: (i) atomic region with a spherical potential; (ii) interatomic region with a volume averaged potential, and (iii) extramolecular region where the potential