Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Absence of B1-B2 structural transition in lithium halides under hydrostatic pressure ROMEO DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico, GABRIEL MURRIETA, Facultad de Matematicas, Universidad Autonoma de Yucatan, Mexico. — We have investigated the B1-B2 structural transition in LiF, LiCl, LiBr, and LiI under hydrostatic pressure by means of first-principles total-energy calculations using the Full- Potential LAPW method. In order to analyze the gradient effects, we have performed calculations using the local density approximation (LDA) and the generalized gradient approximation (GGA), for the exchange and correlation potential. In agreement with the experimental observations, we find that even for pressures higher than 100 GPa, the Li halides do not present the B1-B2 structural transition. In order to understand this behavior, we have calculated the distribution of the electron densities. From the analysis of the distribution of electron densities for the Li halides in the B1 and B2 phases, we find that for this group of ionic compounds the B1 phase have a distribution of electron densities more homogeneous than in the B2 phase, preventing the B1-B2 structural transition. This work was partially supported by Consejo Nacional de Ciencia y Tecnología (CONACYT, México) under Grant No. 43830-F.

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Date submitted: 01 Dec 2004 Electronic form version 1.4