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Lattice Dynamics and Thermal Properties of Materials

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ABSTRACT

In this talk, we present studies on some binaries (SrX (X=S, Se, Te) and ternaries ($LiB^{II}C^{V}$) compounds by using first principles methods. The dynamical and vibrational properties are investigated by the density functional perturbation theory (DFPT). The phonon dispersion curves and their density of states will be presented. Instability and phase transition will be discussed in terms of mode softening. The calculated bond force constants for the ternaries give an indication on the nature of the bonds. The calculated phonon dispersions in conjunction with the quasi- harmonic approximation are used to predict the temperature and pressure dependence of various quantities such as the thermal expansion coefficient, the bulk modulus and the heat capacity.

At the end of this talk the phase transitions and lattice dynamics in perovskite-type hydride $Li_xNa_{1-x}MgH_3$ alloy will be presented.

Keywords: Ab initio methods, VCA, lattice dynamics, thermal expansion.

DOI: 10.21467/abstracts.122 ISBN: 978-81-954993-3-5