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DYNAMICAL AND THERMODYNAMIC PROPERTIES OF $NaMgH_3$: IMPLICATIONS FOR HYDROGEN STORAGE

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RÉSUMÉ

The ability to store hydrogen gas makes this particularly attractive compared to electricity which is difficult to store. The storage of hydrogen-based metal hydride, also known as storage in solid form, is very safe. It also offers significant improvements in terms of weight and costs for applications related to transport. These new materials have a significant impact on the marketing of cars with fuel-cells to achieve the goals set by the automotive sector. Indeed, several manufacturers, including General Motors, Toyota, Nissan, Renault, Volkswagen, Peugeot and Hyundai are testing prototypes using fuel-cells. General Motors and the american Sandia Laboratories have invested millions of dollars to develop the storage of hydrogen using sodium and aluminium hydrides.

In this work, we present a study of the structural, electronic, optical and thermodynamic properties of $NaMgH_3$, a compound utilized for hydrogen storage. This study was made by the density functional theory using pseudo-potential methods in both the local density approximation (LDA) and the generalized gradient approximation (GGA). Good agreement between the calculated structural parameters and the experimental ones was found. The gap between valence and conduction bands was estimated to be 3.5 eV and indicates that $NaMgH_3$ is an insulator. The enthalpy of hydrogenation of the compound was calculated and compared to experiment. Using the density functional perturbation theory, we calculate the phonon dispersion curves and the phonon density of states. The thermodynamic functions are calculated by using this phonon density of states.

MOTS-CLÉS : hydride, density functional theory, DFT, lattice dynamics, thermodynamic functions, $NaMgH_3$, storage