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P.S.A.44.

CHANGES IN THE ELECTRONIC STRUCTURE DURING THE HYDROGEN-INDUCED LITHIUM AMIDE/IMIDE TRANSFORMATION

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The reversible transformation of lithium amide ($LiNH_2$) into lithium imide (Li_2NH) during the absorption/desorption of hydrogen (H) is a potentially important process for H storage applications. However, its investigation is difficult due to the competition of many complicated Li_2NH structures with ground state energies very close to one another. In order to establish the most probable pathways of the transformation, we have examined the changes in electronic structure of all the relevant molecular species and clusters involved in the processes, using *ab-initio* calculations based either on the linear combination of atomic orbitals (LCAO), or a real-space Green's function formalism. The influence of the replacement of Li with some other elements of interest on the system behaviour has been also investigated in this sense. The cluster calculations were conducted so to link the results obtained for molecules and the density functional theory (DFT) calculations of various crystal structures appearing as the end-points of the process. In this way, an atomic-level insight into the changes of the electronic structure during the H-induced $LiNH_2/Li_2NH$ transformation has been obtained. Calculations have revealed that the changes of particular molecular and cluster structures have a determining role during the transformation, and that the appearance of several Li_2NH structures is the long-range ordering response to particular local ordering possibilities during the process.

P.S.A.45.

STRUCTURAL CHARACTERIZATION OF MECHANICALLY ACTIVATED MgO-TiO_2 SYSTEM

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Mixtures of MgO-TiO_2 powders were mechanically activated in a planetary ball mill for time interval from 0 to 120 minutes. On thus obtained powders, structural investigations have been performed. N_2 adsorption method was used to determine the BET specific surface area and pore size distribution. Unusual results are obtained: specific surface area continuosly decreases up to 40 minutes of activation and after that increases, reaching its minimun value of 4.4 m^2/g. The influence of mechanical activation on lattice vibrational spectra was examined by Raman spectroscopy at room temperatures. The differential thermal analysis has been performed in order to investigate thermal behavior of the mixtures, indicating at several endothermal peaks in range of RT to 1100^{o}C. SEM gave information about changes in microstructures, showing the clear decrease in particle size.