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Structural, Electronic and Optical Properties of Li_xNa1-_xH for Hydrogen Storage

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Abstract : This study investigates the structural, electronic, and optical properties of LiH and NaH compounds, as well as their ternary mixed crystals Li_xNa1-_xH, adopting a face-centered cubic structure with space group Fm-3m (number 225). The structural and electronic characteristics are examined using density functional theory (DFT), while empirical methods, specifically the modified Moss relation, are employed for analyzing optical properties. The exchange-correlation potential is determined through the generalized gradient approximation (PBEsol-GGA) within the density functional theory (DFT) framework, utilizing the projected augmented wave pseudopotentials (PAW) approach. The Quantum Espresso code is employed for conducting these calculations. The calculated lattice parameters at equilibrium volume and the bulk modulus for x=0 and x=1 exhibit good agreement with existing literature data. Additionally, the Li_xNa1-_xH alloys are identified as having a direct band gap.

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