Theoretical study of the structural stability for fcc-CH\textsubscript{x} phases using density functional theory

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(Received 25 July 2010; in final form 11 March 2011)

Abstract
Recently, a new carbon modification, namely n-diamond, have been reported, whose structure is still a matter of debate. It is important to note that the synthesis of n-diamond was carried out in the presence of hydrogen or methan. In this work we evaluate the structural stability of five fcc-CH\textsubscript{x} phases by means of first-principle calculation. The total energy is obtained as a function of the isotropic, tetragonal and rhombohedral deformations for the bulk structures. First, we analyze the C\textsubscript{2}H (cuprite), CH (zincblende), CH (rocksalt) and CH\textsubscript{2} (fluorite) structures. It is found that the four systems show a minimum in the total energy for the isotropic and rhombohedral deformations, but are unstable against tetragonal deformation. In the second part, we explore the structural stability of CH\textsubscript{2} in the pyrite structure. We find that CH\textsubscript{2} (pyrite) with the hydrogen atoms defined by the internal parameter u=0.35 and a lattice parameter of 3.766 Å is elastically stable, providing a possible explanation for the experimental observation of fcc-carbon in materials prepared in the presence of hydrogen or methan. In final, we calculate density of states, band structure and EELS spectrum of CH\textsubscript{2} (pyrite) and compare them with n-diamond

Keywords: DFT, n-diamond, FCC-CHx, EELS, structural properties

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