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First-principles prediction of a new metallic carbon hydride: bcc-CH_2[1] CESAR CAB, ROMEO DE COSS, GERKO OSKAM, Department of Applied Physics, CINVESTAV-Merida, Mexico, GABRIEL MURRIETA, Facultad de Matematicas, UADY, Yucatan, Mexico, GABRIEL CANTO, CCMC-UNAM, Ensenada, Mexico. — The observation of a new carbon phase in nanoparticles having the body-centered-cubic structure (bcc) has been reported very recently. However, has been suggested that hydrogen is present in the samples forming solid CH_2 with the anti-cuprite structure. The structural and electronic properties of bcc-C and bcc-CH_2 are unknown. In the present work we have studied the elastic stability and the electronic structure of these systems by means of first-principles total-energy calculations. The results were obtained with the pseudopotentials LCAO method (SIESTA code) and the Generalized Gradient Approximation (GGA) for the exchange-correlation potential. We have evaluated the structural stability via the elastic properties, we find that bcc-CH_2 is stable with a lattice parameter very close to the experimental value. In addition, we find that the electronic structure of bcc-CH_2 exhibits metallic behavior with a relatively high density of states at the Fermi level. The relevance of this new hydride to the problem of hydrogen storage is discussed.

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Romeo de Coss
CINVESTAV-Merida

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