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Electronic properties of carbon in the fcc phase. CESAR CAB, ALEJANDRO TAPIA, ROMEO DE COSS, GERKO OSKAM, Department of Applied Physics, Cinvestav-Merida, Mexico., GABRIEL CANTO, Centro de Ciencias de la Materia Condensada, UNAM, Mexico. — The observation of a new carbon phase in nanoparticles obtained from Mexican crude oil having the face-centered-cubic structure (fcc) has been reported. However, more recently has been suggested that hydrogen is present in the samples forming CH with the zincblende structure. The structural and electronic properties of C(fcc) and CH(zincblende) are unknown. In the present work we have studied the electronic structure of C(fcc) and CH(zincblende) 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 analyzed the band structure, the local density of states (LDOS), and orbital population. We find that in contrast to graphite and diamond, both fcc carbon and CH with the zincblende structure exhibit metallic behavior. This research was supported by Consejo Nacional de Ciencia y Tecnología (Conacyt-México) under Grants No. 43830-F, No. 44831-F, and No. 43828-Y.

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