

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Ab-initio study of the electronic structure and optical properties for carbon in the glitter phase JUAN ANDRES DIAZ-CELAYA, EDUARDO CIFUENTES-QUINTAL, JOSE LUIS CABELLOS, ROMEO DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico — Experimental evidence has showed the existence of a new crystalline phase of carbon. Electron diffraction studies show that this new phase of carbon has the same reflections that diamond but showing additional reflections that are forbidden for diamond. This new carbon has been called n-diamond. Although the results suggest that n-diamond correspond to a cubic phase, the crystal structure remains unclear. Thus, based on theoretical computational studies have been proposed different cubic structures to explain the observed diffraction patterns in n-diamond. However, recently has been proposed that the n-diamond could be explained by a tetragonal structure, which is called glitter. More recently, based on ab-initio calculations has been shown that the glitter structure is vibrationally stable. In this work, we study the electronic structure and optical properties of carbon in the glitter structure by means of first principles calculations. The electronic density of states of that carbon in glitter structure corresponds to a metallic material which is corroborating by the optical conductivity.

Romeo de Coss
Department of Applied Physics, Cinvestav-Merida, Mexico

Date submitted: 14 Nov 2013

Electronic form version 1.4