

ADSORPTION OF ACETYLENE MOLECULES AT Si(111) AND Si(100) SURFACES.

C. A. Pignedoli¹, R. Di Felice¹, C. M. Bertoni¹, A. Catellani²,
C. Sbraccia³, P. L. Silvestrelli³, F. Ancilotto³.

¹*INFN and Dipartimento di Fisica, Università di Modena e Reggio E., via Campi 213/A, I-41100, Modena, Italy*

²*CNR-IMEM, Parco Area delle Scienze, 37a, I-43010, Parma, Italy*

³*INFN and Dipartimento di Fisica "G. Galilei", Università di Padova, via Marzolo 8, I-35131, Padova, Italy*

We performed DFT ab-initio calculations to characterize the early stages of SiC growth on Si substrates. We considered the adsorption of C₂H₂ and other C-containing molecules on Si(100) and Si(111) surfaces. We modeled a portion of the 7x7 reconstructed Si(111) surface through a 2x2 unit cell containing an ad-atom and a rest-atom: this portion of the 7x7 reconstruction plays a relevant role in the adsorption of the acetylene molecule. We found that, for both the surfaces, the preferred adsorption geometry for the acetylene molecule is a “bridge” configuration between two surface Si atoms. Other metastable adsorption configurations are discussed. The results obtained shed light on controversial experimental findings regarding the stability of acetylene on both Si Surfaces.

Our results point at the formation of a highly stable C-C dimer at the surface, irrespectively of the substrate orientation.

We propose a possible mechanism for the dissociation of the C dimer and for the early stage formation of a carbonized layer on the Si(111) surface.