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Bonding Structure of Phenylacetylene on Hydrogen-Terminated Si(111) and Si(100): Surface Photoelectron Spectroscopy Analysis and Ab-Initio Calculation MASAKAZU KONDO, Chisso Corporation and Materials Research Laboratory, UCSB, EDWARD KRAMER, Materials Research Laboratory and Materials Department, UCSB — Organic monolayers formed by reaction on hydrogen-terminated silicon have potential in future device applications. Although previous studies showed that monolayers may be fabricated via a surface hydrosilylation reaction scheme, controversy exists regarding the bonding structure at the interface. In the present study, we shed light on the interfaces between phenylacetylene (PA) and two different H-terminated silicon surfaces, H:Si(111) and H:Si(100). We utilize X-ray photoelectron spectroscopy, ultraviolet photoelectron spectroscopy, and near-edge X-ray absorption fine structure spectroscopy for the purpose. Features arising from the valence/unoccupied bands in photoelectron spectra suggest that a large number of the PA molecules retain their π-electronic character for both of the systems. We further discuss these experimental findings and their interpretation based on ab-initio quantum chemical calculations.

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