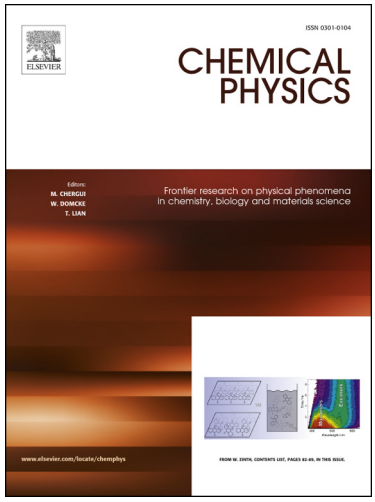

Electronic Structure of PTCDA on Sn/Si(111)- $2\sqrt{3}2\sqrt{3}$

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Electronic Structure of PTCDA on Sn/Si(111)-$2\sqrt{3} \times 2\sqrt{3}$

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Abstract

The electronic structures of PTCDA on the Sn/Si(111)-$2\sqrt{3} \times 2\sqrt{3}$ surface have been thoroughly studied by high-resolution photoelectron spectroscopy and near-edge x-ray absorption fine structure (NEXAFS). Upon deposition of PTCDA, there is an unusual charge transfer from the Sn/Si(111)-$2\sqrt{3} \times 2\sqrt{3}$ surface to the molecules. This is clearly shown by a new component in the Sn $4d$ core-level spectra that shifts towards higher binding energy. In contrast to the literature, the charge provided by Sn is donated to the carbonyl C instead of the O atoms. This is revealed by a new component in the C 1s core-level spectra that shifts towards lower binding energy. The charge transfer causes a splitting of the HOMO level in the valence band spectra. As indicated in the NEXAFS spectra, it also induces a splitting of the LUMO level of the molecules. For thick films the NEXAFS results suggest a layer by layer growth mode.

Keywords: PTCDA; XPS; NEXAFS; electronic structure; molecule-induced reconstruction; metal/semiconductor surface

1. Introduction

In the past years organic semiconducting molecules and their electronic devices have greatly attracted both theoretical and experimental attention [1]. In particular, the interface interaction between molecules and substrates is of special interest, since it affects the electronic structure of deposited

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