Molecular orientation and weak-charge transfer dynamics of PTCDI-C4 molecules on MoS₂ interfaces

Arramel1, Xinmao Yin1,2,3, Qixing Wang1, Yu Jie Zheng1, Song Zhibo1, Mohammad Heider bin Hassan1, Dianyu Qi1, Andrivo Rusydi1,2,4, and Andrew Thye Shen Wee1

1Department of Physics, National University of Singapore, 2 Science Drive 3, 117542, Singapore.
2Singapore Synchrotron Light Source. National University of Singapore, 5 Research Link, Singapore 1176033
3SZU-NUS Collaborative Innovation Center for Optoelectronic Science and Technology, Key Laboratory of Optoelectronic Devices and Systems of Ministry of Education and Guangdong Province, Shenzhen University, Shenzhen 518060, China
4NUS/NIN-NanoCore, National University of Singapore, Singapore 117411.

Abstract

Two-dimensional layered semiconductors have proven to be versatile examples in the exploration of their unique layer-number dependent electronic and optical properties. Recent progress on altering the physical properties of transition metal dichalcogenides (TMDs) using surface molecular doping effect has much interest.[1-2] In this study, we investigate the molecular alignment and the ultrafast charge transfer dynamics of N,N'-Dibutyl-3,4,9,10-perylenedicarboximide (PTCDI-C4) molecules at different molecular thicknesses on molybdenum disulphide (MoS₂) substrates using near edge X-ray absorption fine structure spectroscopy (NEXAFS) and Resonant Photoemission Spectroscopy (RPES), respectively. The average tilt angle analysis revealed a strong anisotropy in the π* symmetry transition (284-288 eV range) across the absorption threshold. The non-planar molecular configuration was extracted from the carbon K-edge of the perylene spectrum.[3] Core hole clock spectroscopies at the few monolayer sample displayed a resonant enhancement of the occupied state level which indicates the existence of a moderate interfacial electronic coupling between the adsorbed molecules and substrate. These findings provide a deeper understanding of the interfacial interaction of organic semiconductors on transition metal dichalcogenide surfaces, which is essential for the development of non-planar geometry-based organic devices.

Background

The perylene derivative family is one of the most extensively studied organic semiconductor in the field of organic electronics

Goal

To investigate the molecular orientation and the charge transfer dynamics of the hybrid organic/inorganic heterostructures.

Synchrotron radiation technique

SINS : Surface, Interface and Nanostructure Science

RPES results

NEXAFS results

Carbon K-edge NEXAFS spectra of PTCDI-C4 film as a function of deposition time.

Average tilt angle

$$J_{\text{avg}} A \cdot \left( \frac{2}{\sin^2 \alpha} \right)$$

For 1 min sample, we can deduce that the molecule has a stronger tendency to stand upright with respect to the MoS₂ surface. The extracted tilt angles for the other two thicker samples are close to the magic angle (54.7˚), implying that a random PTCDI-C4 molecular orientation exists in the multilayer samples.

Summaries

1. A polarization dependence is clearly resolved in the case of submonolayer coverage (1 min). In contrast, the degree of polarization of the other two cases (3 min and 5 min) showed negligible changes in both π* and σ* electronic transition as a function of incident photon angle.
2. Thickness-dependent of RPES profile suggested that a weak electronic coupling was established at the PTCDI-C4/MoS₂ interface.

References


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