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The molecular orientation of DNA bases on H-passivated Si(1 1 1) surfaces investigated by means of near edge X-ray absorption fine structure spectroscopy

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Abstract

Layers of the DNA bases adenine, cytosine, and guanine were deposited onto hydrogen passivated Si(1 1 1) surfaces. The average tilt angles of these molecules with respect to the substrate surface were determined by the angular dependence of the Near Edge X-ray Absorption Fine Structure (NEXAFS) of the carbon K-edge. The interpretation of the NEXAFS spectra was assisted by a semi-empirical approach to the calculation of the π^*-transition region which employs density functional theory calculations and core level photoemission data.

Keywords: DNA base; Adenine; Cytosine; Guanine; Molecular orientation; Near edge X-ray absorption fine structure spectroscopy; NEXAFS; Core level; Photoemission spectroscopy