

Optical properties and molecular orientation in organic thin films

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[M Friedrich](#)¹, [G Gavrilă](#)¹, [C Himcinschi](#)¹, [T U Kampen](#)¹, [A Yu Kobitski](#)¹, [H Méndez](#)¹, [G Salvan](#)¹, [I Cerrillo](#)², [J Méndez](#)³, [N Nicoara](#)², [A M Baró](#)² and [D R T Zahn](#)¹

¹ Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

² Laboratorio de Nuevas Microscopías, Departamento Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049, Spain

³ Instituto de Ciencia de Materiales de Madrid, CSIC, E-28049, Spain

Author to whom any correspondence should be addressed

E-mail: friedrich@physik.tu-chemnitz.de

Abstract. The optical properties and the molecular orientation in thin films of 3,4,9,10-perylenetetracarboxylic dianhydride (PTCDA) and *N,N*-dimethyl-3,4,9,10-perylenetetracarboxylic diimide (DiMePTCDI) were studied by means of variable angle spectroscopic ellipsometry (VASE), atomic force microscopy (AFM), near edge x-ray absorption fine structure (NEXAFS) spectroscopy, and infrared (IR) and Raman spectroscopy. VASE reveals that both kinds of film exhibit a strong optical anisotropy. For PTCDA, the optical constants are found to have much higher values in the substrate plane than perpendicular to it. While the anisotropy measured in the substrate plane on passivated GaAs(100) is very small for PTCDA a giant anisotropy is observed for DiMePTCDI. This difference in the optical properties is attributed to the different orientation of molecules in the thin organic films. While the PTCDA molecules lie flat on the substrate with their molecular plane parallel to the substrate surface, the DiMePTCDI molecules are tilted with respect to the substrate surface and are predominantly oriented with their long axis parallel to the [011] direction of the substrate as confirmed by VASE, NEXAFS, and Raman and IR results.

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