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Preparation and passivation of GaAs(001) surfaces for growing organic molecules

N Nicoara¹, I Cerrillo², D Xueming¹, J M García³, B García⁴, C Gómez-Navarro¹, J Méndez^{1,5}

and A M Baró¹

¹ Laboratorio de Nuevas Microscopías, Dept Física de la Materia Condensada, Universidad Autónoma de Madrid, 28049, Spain

² Material Physics Laboratory, University of Wales, Aberystwyth, UK

³ Instituto de Microelectrónica de Madrid CSIC, Spain

⁴ Dept Física Aplicada, Universidad Autónoma de Madrid, 28049, Spain

⁵ Author to whom any correspondence should be addressed.

E-mail: javier.mendez@uam.es

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Abstract. Growth of ordered organic films of 3, 4, 9, 10-perylene-tetracarboxylic-dianhydride (PTCDA), on inorganic substrates of GaAs(001) is investigated by means of low-energy electron diffraction, scanning tunnelling microscopy and atomic force microscopy. The passivation of the sample can be achieved by exposing the substrate to sulphur (the SnS₂ compound) or wet-chemical etching using an S-containing etchant (S₂Cl₂). The sulphur-treated surfaces are less reactive and are suitable as substrates for the growth of epitaxial films. In this work we have compared the growth of organic molecules on substrates prepared by two different methods. The samples prepared by molecular beam epitaxy (MBE) present smoother surfaces compared with chemically treated samples. Therefore, an improvement of the PTCDA molecular order is observed for the MBE samples, which exhibit the formation of crystals.

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Raman spectroscopy: a powerful tool for characterisation of
Ag/3,4,9,10-perylene-tetracarboxylic-dianhydride/GaAs
heterostructures

G. Salvan ^a * salvan@physik.tu-chemnitz.de, D.A. Tenne ^{a,b}, T.U. Kampen ^a, R. Scholz ^a, G.

Jungnickel ^c, Th. Frauenheim ^c and D.R.T. Zahn ^a

^a Institute of Physics, Technical University Chemnitz, 09107 Chemnitz, Germany

b Institute of Semiconductor Physics, 630090 Novosibirsk, Russia

c Institute of Theoretical Physics, University of Paderborn, 33098 Paderborn, Germany

Abstract

The present contribution emphasises the capabilities of Raman spectroscopy for the characterisation of chemical and structural properties of thin organic films. As an example, a perylene derivative is presented, namely 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA). The focus will be directed to the Raman monitoring of dynamic processes. First, the PTCDA film formation on GaAs substrates by organic molecular beam deposition will be followed. The changes in the GaAs bands and PTCDA internal and external vibrational modes will be investigated as indicators for the interface formation. Secondly, the PTCDA internal modes will be monitored upon the deposition of silver onto the PTCDA/GaAs heterostructure.

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Keywords: PTCDA; GaAs; Ag; Raman spectroscopy; SERS

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In-situ monitoring of the growth of copper phthalocyanine
films on InSb by organic molecular beam deposition

D.A. Evans a * a.evans@aber.ac.uk, H.J. Steiner a, R. Middleton b, T.S. Jones b, C.H. Chen

c, K. Horn c, S. Park d, T.U. Kampen d, D. Tenne d, D.R.T. Zahn d, A. Patchett e and

I.T. McGovern e

a Department of Physics, University of Wales, Aberystwyth SY23 3BZ, UK

b Centre for Electronic Materials and Devices, Department of Chemistry, Imperial College,

London SW7 2AY, UK

c Fritz-Haber-Institut der Max-Planck-Gesellschaft, D-14195 Berlin, Germany

d Technische Universität Chemnitz, D-09107 Chemnitz, Germany

e Physics Department, Trinity College, Dublin-2, Ireland

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Abstract

Thin films of the organic semiconductor copper phthalocyanine (CuPc) have been grown on the InSb(111)A 2×2 surface by organic molecular beam deposition (OMBD). Soft X-ray photoelectron spectroscopy (SXPS) using synchrotron radiation, low energy electron diffraction (LEED) and Raman spectroscopy have been applied to monitor the bonding and energy band line-up at the CuPc-InSb interface. LEED shows that the first layer of CuPc is ordered. SXPS data reveal that the chemical interaction between the overlayer and the substrate is limited. The lineshapes of the shallow In and Sb core levels change very little during the growth of the CuPc film. Emission from the valence states of both InSb and CuPc was also monitored and the valence band offset for this hybrid system was determined to be (0.75 ± 0.14) eV. Raman spectroscopy confirms the limited interaction at the junction and further reveals that the structure of the CuPc film changes with increasing thickness.

Keywords: Phthalocyanine; Spectroscopy; Interface

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X-ray standing wave study of wet-etch sulphur-treated
InP(100) surfaces

I.T. McGovern a * iggy.mcgobern@tcd.ie, A. Koebbel a, A. Leslie a, E. Dudzik
a, C.E.J.

Mitchell b, A.B. McLean b, A. Patchett c, D.R.T. Zahn c, D.A. Evans d, D.P.
Woodruff e

and B.C.C. Cowie f

a Physics Department, Trinity College, Dublin 2, Ireland

b Department of Physics, Queen's University, Kingston, Canada

c Halbleiterphysik, Technische Universität Chemnitz-Zwickau, Germany

d Department of Physics, University of Wales, Aberystwyth SY23 3BZ, UK

e Physics Department, University of Warwick, Warwick CV4 7AL, UK

f Daresbury Laboratory, Warrington WA4 4AD, UK

Abstract

Normal incidence X-ray standing wave (NIXSW) measurements are presented for sulphur terminated InP(100) surfaces, prepared by wet-etch in (NH₄)₂S solution followed by UHV anneal. Standing wave profiles for sulphur 1s photoyield in three planes (220, 311 and 31) indicate that sulphur is close to the phosphorus site. Coherent positions and fractions are compared with the predictions of a number of models of the surface, including novel 2×2 structures. The experimental data can be reproduced by a general two-dimer model, but it is more likely that the data are reflecting significant disorder.

Keywords: Semiconductor; Surface; Passivation; Synchrotron radiation

<http://susanna.catchword.com/vl=17992947/cl=55/nw=1/rpsv/catchword/tandf/02678292/v28n7/s18/p1105>

Title: Absorption and luminescence spectra of electroluminescent liquid crystals with triphenylene, pyrene and perylene units

Author(s): Susanne Keuker-Baumann; Harald Bock; Fabio Della Sala; Stephan A. Benning; Thomas Haßheider; Thomas Frauenheim; Heinz-S. Kitzerow

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Abstract: New derivatives of triphenylene, perylene, and pyrene are described, some of which form columnar mesophases. The absorption spectra are investigated both experimentally and

theoretically. The spectra calculated using the density functional tight binding (DFTB) theory are in good agreement with experimental results. The investigated compounds show photoluminescence of violet-blue (triphenylene), yellow-green (pyrene), and orange-red (perylene) colours. In addition, electroluminescence is observed in thin films of these compounds between a positively charged ITO electrode and a negatively charged aluminium electrode. The brightness of the electroluminescence decreases in the order perylene > pyrene > triphenylene. Threshold voltages below 20 V and a luminance up to 100 cd m⁻² were observed.

Reference Links: 29

<http://ojps.aip.org/getabs/servlet/GetabsServlet?prog=normal&id=PRBMD0000063000023233204000001&idtype=cvips&gifs=yes&jsessionid=2751901025688537940>

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Electronic band structure and intermolecular interaction in substituted thiophene polymorphs

J. Widany, G. Daminelli, A. Di Carlo, and P. Lugli
INFM-Department of Electronic Engineering, University of Rome "Tor Vergata,"
Via di Tor Vergata 110, I-00133 Rome, Italy

G. Jungnickel, M. Elstner, and Th. Frauenheim
Universität GH Paderborn, Fachbereich Physik, Theoretische Physik, D-33098
Paderborn, Germany

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Total energy calculations based on a density-functional tight-binding scheme have been performed on polymorphic modifications of various thiophene crystals. The electronic band structures exhibit a quasi-one-dimensional interaction in the triclinic crystals, while the monoclinic modifications show no dispersion over the whole Brillouin zone. The main interaction mechanism can be described as a d-wave function overlap between sulfur and carbon. The strong intermolecular interaction may induce an interchain excitation, responsible for the different optical properties of the polymorphs. ©2001 The American Physical Society

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Coherent External and Internal Phonons in Quasi-One-Dimensional Organic Molecular Crystals

T. Hasche,¹ T. W. Canzler,¹ R. Scholz,² M. Hoffmann,¹ K. Schmidt,¹ Th. Frauenheim,³ and K. Leol

¹Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden, Germany

2Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

3Fachbereich Physik, Theoretische Physik, Universität-Gesamthochschule Paderborn, D-33098 Paderborn, Germany

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We have directly time resolved coherent phonon oscillations in quasi-one-dimensional organic crystals of MePTCDI (N-N-dimethylperylene-3,4,9,10-dicarboximide), using femtosecond pump-probe experiments. We observe both higher-energy oscillations caused by intramolecular vibrations (internal phonons) and, for the first time in a quasi-one-dimensional organic system, lower-energy modulations which are related to coherent lattice phonons (external phonons). For internal Ag vibrations, the coherence decay time of about 2 ps is almost independent of the mode. In contrast, the damping time of the external phonons increases strongly with decreasing energy. ©2001 The American Physical Society

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Tight-binding approach to time-dependent density-functional response theory

T. A. Niehaus and S. Suhai

German Cancer Research Center, Department of Molecular Biophysics, D-60120 Heidelberg, Germany

F. Della Sala and P. Lugli

INFN and Department of Electronic Engineering, University of Rome "Tor Vergata," 00133 Rome, Italy

M. Elstner, G. Seifert, and Th. Frauenheim

Department of Theoretical Physics, University of Paderborn, D-33098 Paderborn, Germany

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In this paper we propose an extension of the self-consistent charge-density-functional tight-binding (SCC-DFTB) method [M. Elstner et al., Phys. Rev. B 58, 7260 (1998)], which allows the calculation of the optical properties of finite systems within time-dependent density-functional response theory (TD-DFRT). For a test set of small organic molecules low-lying singlet excitation energies are computed in good agreement with first-principles and experimental results. The overall computational cost of this parameter-free method is very low and thus it allows us to examine large systems: we report successful applications to C60 and the polyacene series. ©2001 The American Physical Society

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Resonant Raman spectroscopy of
3,4,9,10-perylene-tetracarboxylic-dianhydride epitaxial films

R. Scholz, A.Yu. Kobitski, T. U. Kampen, M. Schreiber, and D. R. T. Zahn
Institut für Physik, Technische Universität, D-09107 Chemnitz, Germany

G. Jungnickel, M. Elstner, M. Sternberg, and Th. Frauenheim
Fachbereich Physik, Theoretische Physik, Universität Gesamthochschule
Paderborn, D-33098 Paderborn, Germany

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We present a comprehensive investigation of Raman-active modes of 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) thin films deposited on H-passivated Si(111) substrates. The experimental data are interpreted with a density-functional tight-binding scheme used for calculating the geometry and vibrational modes of the isolated molecule. These results for the breathing modes are applied to the optical absorption of PTCDA in solution, and the vibrational absorption bands can be related quantitatively to the elongation of the most prominent Raman modes during the highest occupied molecular orbital to lowest unoccupied molecular orbital transition. From a comparison of the calculated deformation of negatively charged PTCDA⁻ with Raman spectra recorded in the region of the charge-transfer exciton, a significant net charge separation during the optical absorption is highly unlikely. ©2000 The American Physical Society

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Resonant Raman Spectroscopy of Organic Semiconductors
R. Scholz 1, A.Yu. Kobitski 1, T.U. Kampen 1, M. Schreiber 1, D.R.T. Zahn 1, G. Jungnickel 2, Th. Frauenheim 2
1Institut für Physik, Technische Universität, D-09107 Chemnitz, Germany
2Fachbereich Physik, Theoretische Physik, Universität Gesamthochschule Paderborn, D-33098 Paderborn, Germany
email: R. Scholz (scholz@physik.tu-chemnitz.de)

Abstract

Epitaxial films of a prototype organic semiconductor, 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) are investigated with resonant Raman spectroscopy and density functional calculations. It is shown that the resonant Raman spectra are mainly determined by the vibrational properties of an isolated molecule, and the pronounced subbands in the absorption spectra of dissolved PTCDA molecules can be related to elongations of the Raman-active breathing modes between the ground state and the relaxed excited state.

