

Dr. Johannes Gierschner



Address:

Madrid Institute for Advanced Studies, IMDEA in Nanoscience

Facultad de Ciencias Módulo C-IX, 3^a planta

Avda. Fco. Tomás y Valiente, 7

Ciudad Universitaria de Cantoblanco

28049, Madrid, SPAIN

Tel.: + 34 91 497 6836

Fax: + 34 91 497 6855

Institute website: www.nanoscience.imdea.org

Group website: www.nanochannel.de/gierschner/index.html

e-mail: johannes.gierschner@imdea.org

OUTLINE

Since the discovery of conducting polymers in the 1960's (Aust. J. Chem. 1963, 16, 1056), conjugated polymers have made their way from basic research to real applications in optoelectronic devices. To improve the performance of these devices several processes have to be optimized, e.g. in solar cells optical absorption, exciton diffusion, charge generation, recombination and transport. These processes are governed by the electronic nature of the film-constituting molecules as well as by their mutual arrangement, which in turn is controlled by the intramolecular geometrical and electronic properties. The versatility of organic materials through the synthetic route thus demands a thorough understanding of structure-property relationships in a multi-disciplinary approach for the rational design of tailor-made materials prior to synthesis.

The expertise of my research brings together a strong background in materials, in common & advanced techniques of optical spectroscopy and in quantum-chemical & (semi-)classical theoretical methods. This crossroad approach allows for a thorough and systematic insight into the electronic, optical and photophysical properties of novel conjugated oligomeric & polymeric materials from diluted systems, via nanostructured supramolecular host-guest compounds, to condensed phases, such as nanoparticles, thin films and liquid & single crystalline systems.

The multi-disciplinary character of the field calls for intense collaboration with synthesists, material scientists, quantum chemists, laser physicists, and device engineers, which I have established in the past years through international research projects, inter alia funded through my coordinated EC projects RTN NANOCHANNEL and NANOMATCH

BASIS DATA

peer-reviewed publications > 60
citations > 1500
h-index (m-index) 21 (1.3)

EDUCATION & PROFESSION

2008 Senior Researcher (*Ramón y Cajal* Fellow) at the IMDEA Nanoscience Institute, Madrid, Spain

2004 - 2007 Research fellow at the Laboratory for Chemistry for Novel Materials, University Mons-Hainaut, Belgium (group of David Beljonne & Jérôme Cornil)

2003 - 2004 Research fellow at the Institute of Physical and Theoretical Chemistry (IPTC), University of Tübingen, Germany

2000 - 2003 Researcher, lecturer and administration manager of the IPTC

2000 PhD, University of Tübingen, Germany (D. Oelkrug)

1987 - 1995 Studies in chemistry at the University of Tübingen, Germany

1992 Participation in a research project '*Transport phenomena in polymer-substrate interfaces*' funded by the German Ministry of Science, at the IPTC

Studies-related activities: seminars in *Ethics and Responsibility in Science, History of Science, Ecology, Philosophy, Psychology, History*

VISITING RESEARCH POSITIONS

since 2009 regular visiting researcher at Seoul National University, with S. Y. Park

2008 - 2010 ICMol, University of Valencia, Spain

2005 with Jean-Luc Brédas, Georgia Institute of Technology, Atlanta, USA

since 2005 regular visiting researcher at the IPTC, Univ. Tübingen, Germany

SCIENTIFIC STAYS

2008 with Soo Young Park, Seoul National University, South Korea

2007 with Carlos Silva, Department of Physics, University of Montreal, Canada

2006 with Francesco Minardi & Riccardo Tubino, Milano Bicocca, Italy

2006 with Larry Lüer & Guglielmo Lanzani, Politecnico di Milano, Milano, Italy

2005 with Frank Spano, Temple University, Philadelphia (PA), USA

2004 LSF, Rutherford-Appleton Laboratories, Chilton, Didcot, UK

1999 Institute for Fluorescence Spectroscopy, J. Lakowicz, Baltimore, USA

1998 with Michele Muccini & Carlos Taliani, C.N.R. Bologna, Italy

MANAGEMENT

- 2011 - 2014 Principle Investigator of a MICINN project CONMOL [CTQ2011-27317]
2006 - 2010 Coordination of a European Marie Curie Research Training Network RTN NANOMATCH [MRTN-CT-2006-035884]: 15 groups
2002 - 2006 Coordination of a European Marie Curie Research Training Network RTN NANOCHANNEL [HPRN-CT-2002-00323]: 8 groups
2000 - 2003 Head of the institute administration at the Institute of Physical and Theoretical Chemistry, University of Tübingen, Germany

PROJECTS

Current collaborations inter alia with D. Beljonne & J. Cornil (Mons, B), L. De Cola (Münster, D), A. Meixner (Tübingen, D), H.-J. Egelhaaf (Nürnberg, D), J. Hulliger (Bern, CH), S. Y. Park (Seoul, SK), E. Ortí (Valencia, E), G. Farinola (Bari, I), M. Heeney & I. McCulloch (London, UK), M. Watson (Lexington, KY), R. Martinez Alvarez & N. Martín (Madrid, E).

TALKS

More than 30 talks at international conferences, symposia & workshops (9 invited), and more than 30 poster presentations. 48 invited seminars at institute departments and 20 lectures at research meetings.

SERVICE TO THE COMMUNITY

- 2010 Guest Editor for 'Materials' (Special Issue on 'Organic Electronic Materials')
since 2010 Board member of the CPIC conference series
since 2002 Board member of the European School 'Nanostructured Supramolecular Materials'
since 2002 Organization of 1 Internat. Conference, 4 Summer Schools, 11 Research Meetings
since 2002 Peer reviewer for ACS, Wiley VCH, AIP, RSC, Springer & Elsevier journals
2000 - 2003 Academic advisor in physical chemistry at the IPTC, University of Tübingen
Organization of undergraduate student & school visits, student excursion
Training courses for high-school teachers in physical chemistry
Contributions to Industrial Training Courses in Spectroscopy

TEACHING

- since 1995 Lecturer, director and assistant supervisor / advisor of experimental courses in all field of physical chemistry, but particularly in optical spectroscopy.
since 1995 Supervision of Postdocs, PhD students, and Undergraduates
1987 - 1995 Tutoring of students (high school & university): mathematics, chemistry, physics

BIBLIOGRAPHIC RECORDS

Who's Who in Science and Engineering

PUBLICATIONS

- 1) *π -Conjugation*
B. Milián-Medina, J. Gierschner, WIREs Comput. Mol. Sci., accepted
- 2) *π -Conjugated Cyanostilbene Derivatives: A Unique Self-Assembly Motif for Molecular Nanostructures with Enhanced Emission and Transport*
B.-K. An, J. Gierschner, S. Y. Park, Acc. Chem. Res. in press
- 3) *UV/Vis Spectra of Natural Polyphenols: a Time-dependent Density Functional Theory Study*
E. H. Anouar, J. Gierschner, J.-L. Duroux, P. Trouillas, Food. Chem. 131 (2012) 79-89.
- 4) *Tuning Interchain and Intrachain Interactions in Polyfluorene Copolymers*
Y.-S. Huang, J. Gierschner, J. P. Schmidtke, R. H. Friend, D. Beljonne, Phys. Rev. B. 84 (2011) 205311
- 5) *Excited State Switching by Per-Fluorination of para-Oligophenylenes*
B. Milián-Medina, S. Varghese, R. Ragni, H. Boerner, E. Ortí, G. M. Farinola, J. Gierschner, J. Chem. Phys. 135 (2011) 124509.
- 6) *Polarized Fluorescence from Single Stopcock Molecules at Channel Entrances of an All-Organic Host-Guest Compound*
A. M. Chizhik, R. Berger, A. I. Chizhik, A. Lyubimtsev, L. Viani, J. Cornil, S. Bär, M. Hanack, J. Hulliger, A. J. Meixner, H.-J. Egelhaaf, J. Gierschner, Chem. Mater. 23 (2011) 1088-1090.
- 7) *Oligothienoacenes versus oligothiophenes: Impact of ring fusion on the optical properties*
J. Aragón, P. M. Viruela, J. Gierschner, E. Ortí, B. Milián Medina, Phys. Chem. Chem. Phys. 13 (2011) 1457-1465.
- 8) *Electronic properties and supramolecular organization of terminal bis-alkylethynyl-substituted benzodithiophenes*
M. A. M. Leenen, F. Cucinotta, L. Viani, A. Mavrinskiy, W. Pisula, J. Gierschner, J. Cornil, A. Prodi-Schwab, H. Thiem, K. Müllen, L. De Cola, J. Phys. Chem. B. 114 (2010) 14614–14620.
- 9) *Multi-Stimuli Two-Color Luminescence Switching via Different Slip-Stacking of Highly Fluorescent Molecular Sheets*
S.-J. Yoon, J. W. Chung, J. Gierschner, K. S. Kim, M.-G. Choi, D. Kim, S. Y. Park, J. Am. Chem. Soc. 132 (2010) 13675–13683.
- 10) *Alignment and Relaxation Dynamics of Dye Molecules in Host-Guest Inclusion Compounds as Probed by Dielectric Spectroscopy*
J. Tsuwi, R. Berger, G. Labat, G. Couderc, N.-R. Behrnd, P. Ottiger, F. Cucinotta, K. Schürmann, M. Bertoni, L. Viani, J. Gierschner, J. Cornil, A. Prodi-Schwab, L. De Cola, M. Wübbenhorst, J. Hulliger, J. Phys. Chem. A 114 (2010) 6956-6963.
- 11) *Theoretical Characterization of Charge Transport in One-dimensional Collinear Arrays of Organic Conjugated Molecules*
L. Viani, Y. Olivier, S. Athanasopoulos, D. A. de Silva Filho, J. Hulliger, J.-L. Brédas, J. Gierschner, J. Cornil, ChemPhysChem 11 (2010) 1062-1068.
- 12) *Weak Forces at Work in Dye-Loaded Zeolite Materials: Spectroscopic Investigation on Cation-Sulfur Interactions*
G. Macchi, C. Botta, G. Calzaferri, M. Catti, J. Cornil, J. Gierschner, F. Meinardi, R. Tubino, Phys. Chem. Chem. Phys. 12 (2010) 2599-2605.

- 13) *Conjugated Polymers with Large Effective Stokes Shift: Benzobisdioxole-based Poly(phenylene-ethynylene)s*
T. Dutta, K. B. Woody, S. R. Parkin, M. D. Watson, J. Gierschner, *J. Am. Chem. Soc.* 131 (2009) 17321–17327.
- 14) *A Deep Red-Emitting Perylenediimide-Iridium-Complex Dyad: Following the Photophysical Deactivation Pathways*
R. D. Costa, F. J. Céspedes-Guirao, H. J. Bolink, F. Fernández-Lázaro, A. Sastre-Santos, E. Ortí, J. Gierschner, *J. Phys. Chem C* 113 (2009) 19292–19297.
- 15) *A White-Light-Emitting Molecule: Frustrated Energy Transfer Between Constituent Emitting Centers*
S. Park, J. E. Kwon, S. H. Kim, J. Seo, K. W. Chung, S.-Y. Park, D.-J. Jang, B. Milián Medina, J. Gierschner, S. Y. Park, *J. Am. Chem. Soc.* 131 (2009) 14043–14049.
- 16) *On the origin of small band gaps in alternating thiophene – thienopyrazine oligomers*
B. P. Karsten, L. Viani, J. Gierschner, J. Cornil, R. A. J. Janssen, *J. Phys. Chem. A* 113 (2009) 10343–10350.
- 17) *Spatial Control of Energy Transfer in Supramolecular Host-Guest Architectures*
L. Viani, L. Poulsen Tolbod, M. Jazdyk, G. Patrinoiu, F. Cordella, A. Mura, G. Bongiovanni, C. Botta, D. Beljonne, J. Cornil, M. Hanack, H.-J. Egelhaaf, J. Gierschner, *J. Phys. Chem. B.* 113 (2009) 10566–10570.
- 18) *Efficient Deep-Red Light-Emitting Electrochemical Cells based on a Perylenediimide-Iridium-Complex Dyad*
R. D. Costa, F. J. Céspedes-Guirao, E. Ortí, H. J. Bolink, J. Gierschner, F. Fernández-Lázaro, A. Sastre-Santos, *Chem. Comm.* (2009) 3886-3888.
- 19) *Electronic Structure of Small Bandgap Polymers Based on Cyclopentadithiophenes and Acceptor Units*
B. P. Karsten, J. C. Bijleveld, L. Viani, J. Cornil, J. Gierschner, R. A. J. Janssen, *J. Mater. Chem.* 19 (2009), 5343-5350.
- 20) *Dynamics of Guest Molecules in PHTP Inclusion Compounds as Probed by Solid-State NMR and Fluorescence Spectroscopy*
G. Srinivasan, J. A. Villanueva-Garibay, K. Müller, D. Oelkrug, B. Milián Medina, D. Beljonne, J. Cornil, M. Wykes, L. Viani, J. Gierschner, R. Martinez Alvarez, M. Jazdyk, M. Hanack, H.-J. Egelhaaf, *Phys. Chem. Chem. Phys.* 11 (2009) 4996-5009.
- 21) *Exciton versus Electronic Couplings in Molecular Assemblies: The Importance of Non-Nearest Neighbour Interactions*
J. Gierschner, Y.-S. Huang, B. Van Averbeke, J. Cornil, R. H. Friend, D. Beljonne, *J. Chem. Phys* 130 (2009) 044105.
- 22) *Spectroscopic Signatures for Planar Equilibrium Geometries in Methyl-Substituted Oligothiophenes*
G. Macchi, B. Milián Medina, M. Zambianchi, R. Tubino, J. Cornil, G. Barbarella, J. Gierschner, F. Meinardi, *Phys. Chem. Chem. Phys.* 11 (2009) 984-990.
- 23) *Conformational Disorder and Ultrafast Exciton Relaxation in PPV-family Conjugated Polymers*
T. E. Dykstra, E. Hennebicq, D. Beljonne, J. Gierschner, G. Claudio, E. R. Bittner, J. Knoester, G. D. Scholes, *J. Phys. Chem. B* 113 (2009) in press.
- 24) *EDOT-type Materials: Planar but not Rigid*
B. Milián Medina, D. Wasserberg, S. C. J. Meskers, E. Mena-Osteritz, P. Bäuerle, J. Gierschner, *J. Phys. Chem. A* 112 (2008) 13282–13286.

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- 25) *An Oligomer Study on Small Bandgap Polymers*
B. P. Karsten, L. Viani, J. Gierschner, J. Cornil, R. A. J. Janssen, *J. Phys. Chem. A* 112 (2008) 10764–10773.
- 26) *Molecular Packing Effects on the Optical Spectra and Triplet Dynamics in Oligofluorene Films*
J. Cabanillas-Gonzalez, C. Sciascia, G. Lanzani, S. Toffanin, R. Capelli, M. C. Ramon, M. Muccini, J. Gierschner, T.-Y. Hwu, K.-T. Wong, *J. Phys. Chem. B* 112 (2008) 11605-11609.
- 27) *Highly fluorinated Benzobisbenzothiophenes*
Y. Wang, S. R. Parkin, J. Gierschner, M. D. Watson, *Org. Lett.* 10 (2008) 3307-3310.
- 28) *Independent Tuning of Electronic Levels in Pentacene by Site-Specific Substitution*
B. Milián Medina, J. E. Anthony, J. Gierschner, *ChemPhysChem.* 9 (2008) 1519-1523.
- 29) *Oligophenylenevinylenes in Spatially Confined Nanochannels: Monitoring Intermolecular Interactions by UV/Vis and Raman Spectroscopy*
M. Alosyna, B. Milián Medina, L. Poulsen, J. Moreau, D. Beljonne, J. Cornil, G. Di Silvestro, M. Cerminara, F. Meinardi, R. Tubino, H. Detert, S. Schrader, H.-J. Egelhaaf, C. Botta, J. Gierschner, *Adv. Funct. Mater.* 18 (2008) 915-921.
- 30) *A New Functionalization Strategy for Pentacene*
J. E. Anthony, J. Gierschner, C. A. Landis, S. R. Parkin, J. B. Sherman, R. C. Bakus II, *Chem. Comm.* (2007) 4746-4748.
- 31) *Optical spectroscopy of a polyfluorene copolymer at high pressure: intra- and inter-molecular interactions*
J. P. Schmidtke, J.-S. Kim, J. Gierschner, C. Silva, R. H. Friend, *Phys. Rev. Lett.* 99 (2007) 167401.
- 32) *Electronic Structure and Charge Transport Properties of Polythiophene Chains Containing Thienothiophene Units: A Joint Experimental and Theoretical Study*
B. Milián Medina, A. Van Vooren, P. Brocorens, J. Gierschner, M. Shkunov, M. Heeney, I. McCulloch, R. Lazzaroni, J. Cornil, *Chem. Mater.* 19 (2007) 4949-4956.
- 33) *Three-Dimensional Energy Transport in Highly Luminescent Host-Guest Crystals: A Quantitative Experimental and Theoretical Study*
L. Poulsen, M. Jazdyk, J.-E. Communal, J. C. Sancho-García, A. Mura, G. Bongiovanni, D. Beljonne, J. Cornil, M. Hanack, H.-J. Egelhaaf, J. Gierschner, *J. Am. Chem. Soc.* 129 (2007) 8585-8593.
- 34) *Migration-Assisted Nonlinear Quenching in Random Media*
D. Khoptyar, J. Gierschner, H.-J. Egelhaaf, *J. Opt. Soc. Am. B* 24 (2007) 1527-1534.
- 35) *Liquid Crystalline Octaalkoxycarbonyl Phthalocyanines: Design, Synthesis, Electronic Structure, Self-aggregation and Mesomorphism*
S. Sergeev, E. Pouzet, O. Debever, J. Levin, J. Gierschner, J. Cornil, R. Gómez Aspe, Y. H. Geerts, *J. Mater. Chem* 17 (2007) 1777-1784.
- 36) *Hole-Vibronic Coupling in Oligothiophenes: Impact of Backbone Torsional Flexibility on Relaxation Energies*
D. A. da Silva Filho, V. Coropceanu, D. Fichou, N. E. Gruhn, T. Bill, J. Gierschner, J. Cornil, J.-L. Brédas, *Phil. Trans. R. Soc. A* 365 (2007) 1435-1452.
- 37) *Effect of Fluorination on the Electronic Levels and Optical Excitations of π -Conjugated Oligomers*
B. Milián Medina, D. Beljonne, H.-J. Egelhaaf, J. Gierschner, *J. Chem. Phys.* 126 (2007) 111101.

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- 38) *Optical Bandgaps of π -Conjugated Organic Materials at the Polymer Limit: Experiment and Theory*
J. Gierschner, J. Cornil, H.-J. Egelhaaf, Adv. Mater. 19 (2007) 173-191.
- 39) *Tuning of Molecular and Solid State Properties by Fluorination: A Theoretical Study*
J. Gierschner, B. Milián Medina, H.-J. Egelhaaf, D. Beljonne, J.-L. Brédas, Polym. Mater. Sci. Eng. 96 (2007) 753-754.
- 40) *Highly Fluorescent Crystalline and Liquid Crystalline Columnar Phases of Pyrene-Based Structures*
A. Hayer, V. de Halleux, A. Köhler, A. El-Garouhy, E.W. Meijer, J. Barberá, J. Tant, J. Levin, M. Lehmann, J. Gierschner, J. Cornil, Y. H. Geerts, J. Phys. Chem. B (2006), 7653-7659.
- 41) *Solid State Optical Properties of Polyconjugated Molecules: π -Stack contra Herringbone*
J. Gierschner, M. Ehni, H.-J. Egelhaaf, B. Milián Medina, D. Beljonne, H. Benmansour, G. C. Bazan, J. Chem. Phys. 123 (2005) 144914.
- 42) *Comment on 'Structure-Property Relationships for Electron-Vibrational Coupling in Conjugated Organic Oligomeric Systems'*
J. Gierschner, J. Phys. Chem. B 109 (2005) 22081.
- 43) *Nanometric scale investigation of the nonlinear efficiency of perhydrotriphenylene inclusion compounds*
K. Komorowska, S. Brasselet, G. Dutier, I. Ledoux, J. Zyss, L. Poulsen, M. Jazdyk, H.-J. Egelhaaf, J. Gierschner, M. Hanack, Chem. Phys. 318 (2005) 12-20.
- 44) *Design of π -Conjugated Organic Materials for One-Dimensional Energy Transport in Nanochannels*
J. C. Sancho Garcia, J. L. Brédas, D. Beljonne, J. Cornil, R. Martinez Alvarez, M. Hanack, L. Poulsen, J. Gierschner, H.-G. Mack, H.-J. Egelhaaf, D. Oelkrug, J. Phys. Chem. B. 109 (2005) 4872-4880.
- 45) *Breakdown of the Mirror Image Symmetry in the Optical Absorption/Emission Spectra of Oligo(paraphenylenes)*
G. Heimel, M. Daghofer, J. Gierschner, E. J. W. List, A. C. Grimsdale, K. Müllen, D. Beljonne, J. L. Brédas, E. Zojer, J. Chem. Phys. 122 (2005) 054501.
- 46) *Theoretical Characterization and Design of End-substituted Distyrylbenzenes as Excitation Shuttles in One-dimensional Channels*
J. C. Sancho Garcia, L. Poulsen, J. Gierschner, R. Martinez Alvarez, E. Hennebicq, M. Hanack, H.-J. Egelhaaf, D. Oelkrug, D. Beljonne, J. L. Brédas, J. Cornil, Adv. Mater. 16 (2004) 1193-1197.
- 47) *Optical Properties of Oligophenylenevinylenes*
J. Gierschner, D. Oelkrug, in H. Nalwa (Ed.): Encyclopedia of Nanoscience and Nanotechnology, Vol. 8, American Scientific Publishers (2004) 219-238.
- 48) *Modeling of the Optical Properties of Cofacial Chromophore Pairs: Stilbenophane*
J. Gierschner, H.-G. Mack, D. Oelkrug, I. Waldner, H. Rau, J. Phys. Chem. A. 108 (2004) 257-263.
- 49) *Time-resolved Fluorescence Spectroscopy on Single Oligophenylenevinylene Nanoparticles*
J. Gierschner, H.-J. Egelhaaf, D. Oelkrug, S. Botchway, A. W. Parker, Tech. Rep. - Counc. Cent. Lab. Res. Counc. 2003-2004, 131-133.
- 50) *Luminescence of Molecules Confined in Nanochannels*
J. Gierschner, H.-J. Egelhaaf, H.-G. Mack, D. Oelkrug, R. Martinez Alvarez, M. Hanack, Synth. Met. 137 (2003) 1449-1450.
- 51) *Optical Spectra of Oligothiophenes: Vibronic States, Torsional Motions, and Solvent Shifts*
J. Gierschner, H.-G. Mack, H.-J. Egelhaaf, S. Schweizer, B. Doser, D. Oelkrug, Synth. Met. 138 (2003) 311-315.

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- 52) *Fluorescence and Absorption Spectra of Oligophenylenevinylenes: Vibronic Coupling, Band Shapes and Solvatochromism*
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- 56) *One Dimensional Coupling of Oligophenylenevinylenes in Perhydrotriphenylene Matrices*
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- 57) *Preparation and Optical Properties of Oligophenylenevinylene/Perhydrotriphenylene Inclusion Compounds*
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