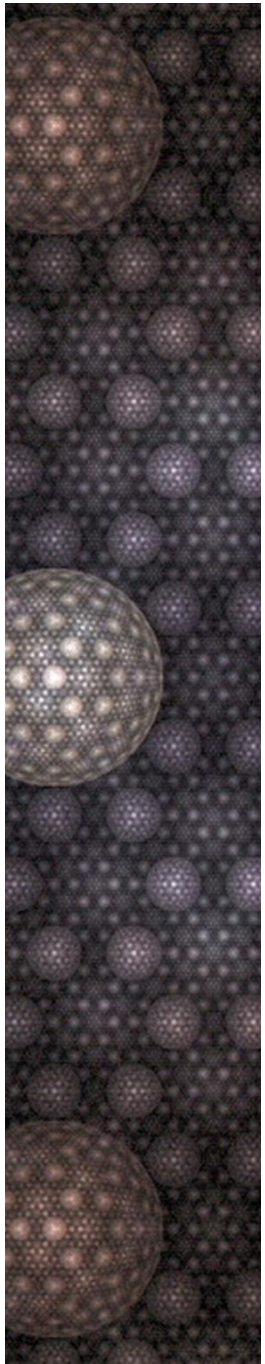

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Photophysics of Conjugated Organic Materials

Part A: Chromophores in Solution

Part B: Chromophores in the Solid State

Part C: Techniques

Johannes Gierschner

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Tübingen, 03/2021 - online

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- **questions, comments, understanding, too fast**: just interrupt! ...microphone, chat
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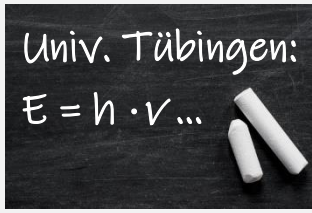
- **length**... ...let's see



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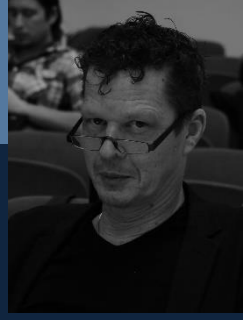
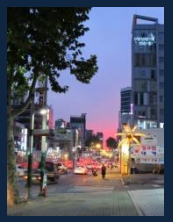
short CV



2000	Ph.D. in Physical Chemistry, IPTC, University of Tübingen, Germany
2000 - 2004	Researcher, Lecturer and Head of the Institute Administration, IPTC
2004 -2007	Research Fellow at University of Mons, Belgium and GiorgiaTech, Atlanta, USA
since 2008	Research Professor IMDEA Nanoscience, Madrid, Spain (2008-2017 Ramón y Cajal, I3 & IED Fellow of the Spanish Ministry)
2014	Habilitation Tübingen, Adjunt Prof. (Priv. Doz.) : Annual Lectures in Photophysics

Visiting Prof. Positions

since 2009	Regular Visiting Researcher, Seoul Nat. University (SNU)
since 2014	Visiting Researcher Univ. Valencia
	2014/2015 Visiting Prof. Univ. Mons & SNU
	2008-2010 Visiting Res. ICMol, Valencia



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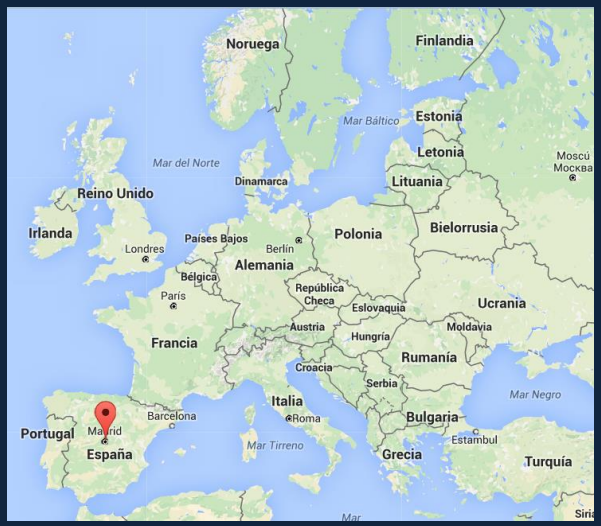

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- 70% external funds
- Severo Ochoa International Center of Excellence 2017

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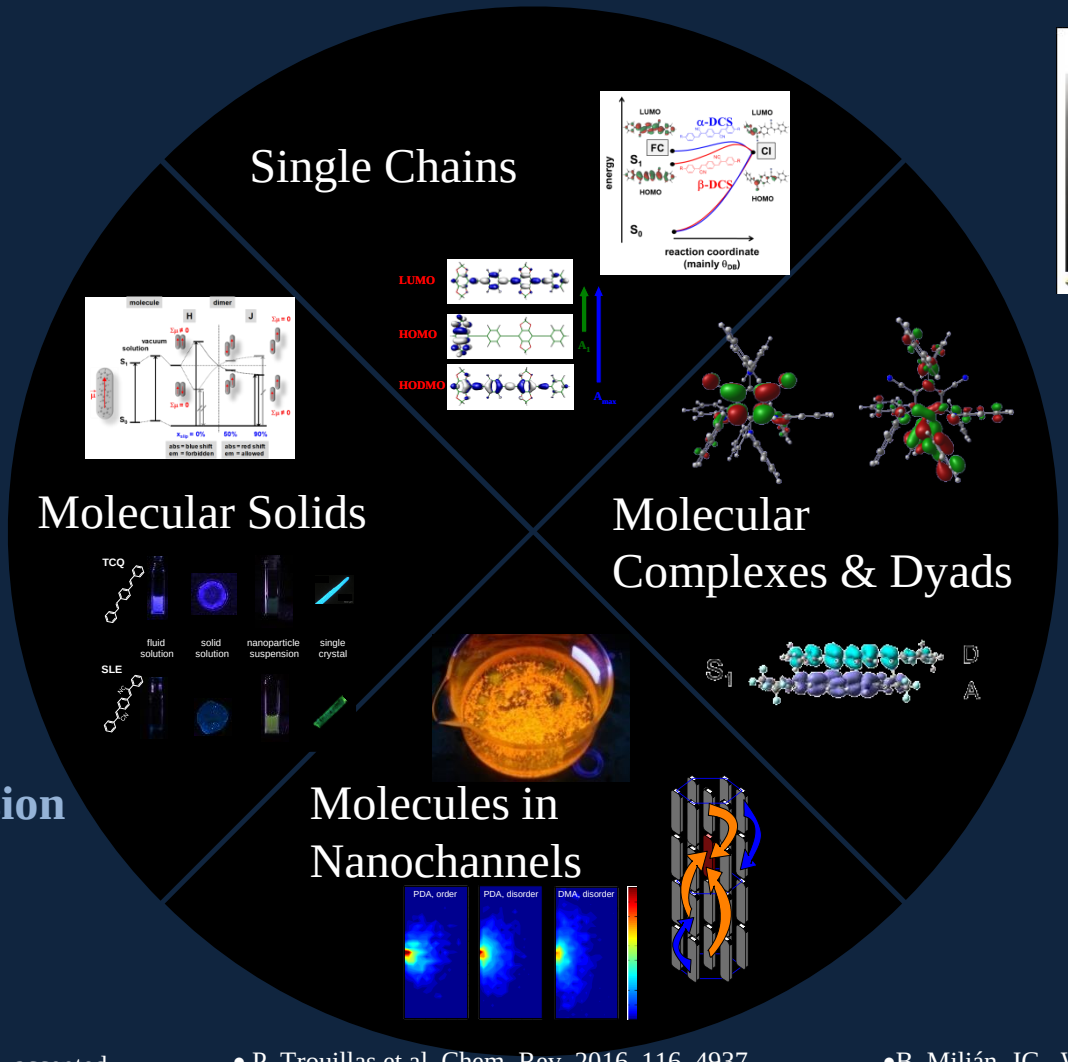
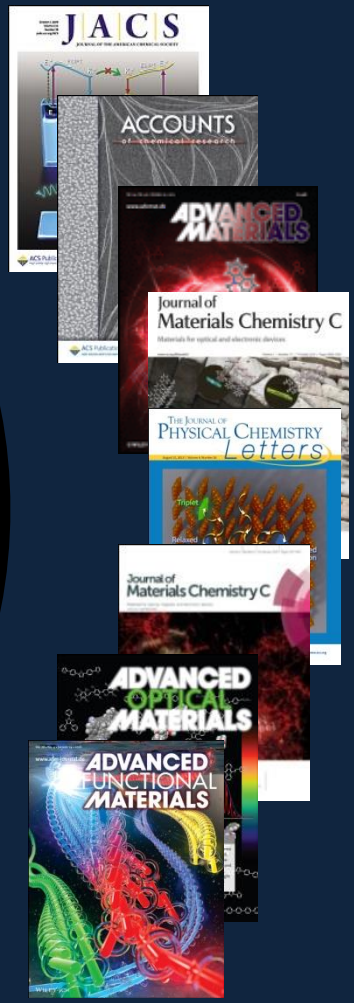
OFETs, Lasers...

Bioprobes
labels, sensors

Colorants
dyes, pigments
in food, pharma,
analytics

Energy Conversion
photocatalysts
photosensitizer





overviews JG:
- JG et al, Adv. Opt. Mater. 2021, accepted
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Targeted Materials Design: Integrating Materials, Spectroscopy & Computations

Quantum Chemistry in Materials Science

- **Understanding** of Properties & Processes

  i.e. geometry & arrangement,

  electronic & spectroscopic prop.

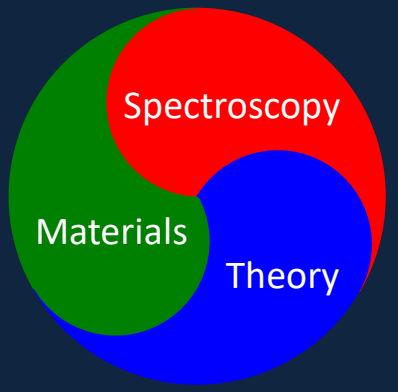
  charge, exciton, heat transfer/transport

  reactivity

- **Prediction** of Properties & Processes:

  qualitative (trends!)

  quantitative (numbers!)



...requires:

- detailed insight in *all* factors, which possibly contribute to the targeted properties & processes
- knowledge of definitions etc. (often originating from experiment)

...communication of theory with experiment!

Part A: Chromophores in Solution

1. Introduction
   - 1.1. Light and Color
   - 1.2. Dyes and Pigments
   - 1.3. Classic Light-Matter Interaction
   - 1.4. Quantum Mechanics
2. Electronic Transitions
   - 2.1. Molecular Symmetry
   - 2.2. QM Treatment of Light-Matter Interaction
   - 2.3. The Hückel Method for Butadiene
   - 2.4. Electronic States & Spectra
   - 2.5. Selection Rules
3. Chemical Constitution & Absorption
   - 3.1. Conjugated Oligomers & Polymers
   - 3.2. The Polymer Limit
   - 3.3. Substituent Effects
   - 3.4. Solvent Shifts
   - 3.5. Bandgap Engineering
   - 3.6. Polymer Frontier MO Localization
   - 3.7. Spectral Modelling
4. Molecular Spectra
   - 4.1. Terms and Principles
   - 4.2. Vibronic Coupling in Diatomic Molecules
   - 4.3. Polyatomic Molecules
   - 4.4. Reorganization and Molecular Structure
   - 4.5. Line Broadening Processes
5. Excited State Deactivation
   - 5.1. Basic processes
   - 5.2. Internal Conversion and Vibrational Relaxation
   - 5.3. The Fluorescence Process
   - 5.4. The Efficiency of Fluorescence
   - 5.5. Dual Emission
   - 5.6. Intersystem Crossing & Phosphorescence
   - 5.7. Quenching
   - 5.8. Photochemistry

Part B: Chromophores in the Solid State

6. Interacting Chromophores
   - 6.1. Molecular Excitons
   - 6.2. Photoinduced Bimolecular Processes
   - 6.3. Dimers in the PDA Regime and beyond
7. Weakly Interacting 3D Assemblies
   - 7.1. HGC Structures and Properties
   - 7.2. Excitons in HGCs
   - 7.3. Applied HGC Systems
8. Molecular Solids & Aggregates
   - 8.1. Introduction
   - 8.2. Formation of Molecular Solids & Aggregates
   - 8.3. Excitons in Molecular Solids & Aggregates
   - 8.4. Symmetry Breaking and Spectral Bandshapes
   - 8.5. Intermolecular Vibronic Coupling
   - 8.6. Exciton Transport and Fate
9. Organic Solid State Systems
   - 9.1. Fluorescent Single Crystals
   - 9.2. Fluorescent Poly- and Nanocrystals
   - 9.3. Chromism in Molecular Solids
   - 9.4. Phosphorescent Single Crystals
   - 9.5. Fluorescent Co-Crystals
   - 9.6. Molecular Liquids & Liquid Crystals
   - 9.7. Polymers

Part C: Techniques

10. UV/Vis Absorption
    - 10.1. Spectrometer Parameters
    - 10.2. Stray Light & Photometric Accuracy
    - 10.3. Light Scattering
    - 10.4. Special Techniques
11. Fluorescence Spectrosocpy
    - 11.1. Steady-State Fluorescence Spectrometer
    - 11.2. Instrument Parameters
    - 11.3. The Sample
    - 11.4. Spectral Analysis
    - 11.5. Time-Resolved Fluorescence
    - 11.6. Polarized Fluorescence Spectroscopy
12. Light-Scattering
    - 12.1. Basics
    - 12.2. Rayleigh Scattering
    - 12.3. Mie Theory
    - 12.4. Particle Sizing

Part A

Dual Emission: Classes, Mechanisms and Conditions
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Part B

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Highly Emissive H-Aggregates or Aggregation-Induced Emission Quenching? The Photophysics of All-Trans Para-Distyrylbenzene
J. Gierschner et al, J. Phys. Chem. Lett. 2013, 4, 2686

π-Conjugated Cyanostilbene Derivatives: A Unique Self-Assembly Motif for Molecular Nanostructures with Enhanced Emission and Transport
B.-K. An et al, Acc. Chem. Res. 2012, 45, 544

Directional Exciton Transport in Supramolecular Nanostructured Assemblies
J. Gierschner, Phys. Chem. Chem. Phys. 2012, 14, 13146

Conclusions

...after a 32h journey through the photophysics of conjugated organic materials

...strong advance in the field due to interdisciplinary character of collaborative schemes:

- imaginative materials science & chemistry
- novel cheaper & faster synthesis protocols
- widely available computational techniques
- elaborated photophysical characterization and understanding

impressive twist of the field
must be properly contextualized with
the **long tradition in the understanding** of the principal photophysical pathways, established in the last 100 years.
...evidently often not sufficiently recognized and acknowledged in our fast moving and economy-driven times.

awareness for the achievements of the past:

- crucial step for rapid & straight, targeted progress

(...avoiding misinterpretations, pitfalls, blind alleys & false claims)

- essential part of good scientific practice:

antidote against the increasing dispraise of science as an opinion among others