**Functional -Systems – Organic Materials Design by Molecular and Supramolecular Engineering [20 hours lectures; in total 40 hours workload]**

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|  | Monday, 19.7.2021 | Tuesday, 20.7.2021 | Wednesday, 21.7.2021 | Thursday, 22.7.2021 | Friday, 23.7.2021 |
| 8:00 - 9:00 Germany  14:00-15:00 China | Opening Remarks;  Dyes: Absorption Properties 1 (**Würthner**) | Molecular Redox Systems 1 (**Lambert**) | Organic Semiconductors 1: Fundamentals (**Lambert**) | Organic Semiconductors 2: Fundamentals (**Lambert**) | Scientific Talk 1: From Squaraine Dye Monomers to Polymers (**Lambert**) |
| 9:00 - 10:00 Germany  15:00-16:00 China | Dyes: Absorption Properties 2 (**Würthner**) | Molecular Redox Systems 2 (**Lambert**) | Dye Aggregates 3: Thermodynamics and Mechanisms of Self-assembly (**Würthner**) | Organic Semiconductors 3: Applications  (**Lambert**) | Scientific Talk 2: CT States in Organic Optoelectronics and Energy Conversion (**Gierschner**) |
| 30 min break |  |  |  |  |  |
| 10:30-11:30 Germany  16:30-17:30 China | Molecular Luminescence 1  (**Gierschner**) | Dye Aggregates 1: Structural Aspects by Theory and Experiment  (**Würthner**) | Luminescent Molecular Solids 1  (**Gierschner**) | Dye Aggregates 4: Photophysical Properties (**Würthner**) | Scientific Talk 3: Supramolecularly Engineered Organic Electronic Devices (**Würthner**) |
| 11:30-12:30 Germany  17:30-18:30 China | Molecular Luminescence 2  (**Gierschner**) | Dye Aggregates 2: Understanding Absorption Spectra: Kasha Exciton Theory  (**Würthner**) | Luminescent Molecular Solids 2  (**Gierschner**) | Luminescent Molecular Solids 3  (**Gierschner**) | Closing Remarks (**Würthner**) |
|  |  |  |  |  | **Examination Friday, 30.7.2021** |

**Contents**

**Dyes: Fundamentals** (2h; Würthner): Structure of important dyes and pigments; Light-Matter Interaction; UV/Vis spectrum, selection rules, transition dipole moment, vibronic coupling, solvent effects; Types of chromophores, Hückel MO

**Molecular Luminescence** (2h; Gierschner): Excited state deactivation (Jablonski term scheme), internal conversion (energy gap law, Kasha's rule, conical intersections, environmental effects), fluorescence (Einstein equations, Strickler-Berg, spontaneous vs. induced processes, non-Kasha, thermal activation, dual emission), inter-system processes (ISC, phosphorescence, triplet recycling), quenching, photochemistry

**Molecular Redox Systems** (2h, Lambert): experimental techniques (cyclic voltammetry, square wave voltammetry,…), determination of redox potentials, multiredox systems, radical cations/anions, polarons, mixed valence compounds

**Dye Aggregates** (4h; Würthner): pi-pi-stacking (theoretical methods, energy decomposition analysis); structural methods, X-ray diffraction, packing arrangements, polymorphism, microscopic methods, MS and NMR, optical spectroscopy (UV/Vis, CD), molecular exciton model (Kasha), [Exciton-vibrational coupling, CT coupling, heteroaggregates, etc], self-assembly models (isodesmic, cooperative, anticooperative), solvent-dependent binding strength, Kinetic control, living supramolecular polymerizations, supramolecular block copolymers, [functional dye aggregates: examples for applications]

**Organic Semiconductors** (3h, Lambert): band vs hopping transport; Fermi level; small molecules and polymers; polarons; excitons; band gap; cyclic voltammetry; UPS; conductivity measurements, charge carrier mobility determination; organic semiconductor materials, polyacetylene, MEH-PPV, P3HT, PEDOT, PANI, acenes, copper phthalocyanine; PTCDA and perylene bisimides; triarylamines; oligothiophenes; organic photoconductors, OFETs, OLEDs, organic solar cells.

**Luminescent Molecular Solids** (3h; Gierschner): bimolecular deactivation processes (annihilation, fission, energy transfer, photoinduced electron transfer), weakly interacting 3D systems (exciton migration, fluorescence polarization), solid state arrangements (classification, polymorphism), spectral shifts, radiative decay in molecular excitons, excitons vs. excimers, solid state luminescence enhancement, non-radiative deactivation, exciton trapping & sensitization, luminescent solid state systems (luminescent single crystals and polycrystals, co-crystals, stimuli-responsive materials, luminescent molecular liquids and liquid crystals)