

## MO 21 Molecular Electronics and Energy Transfer

Zeit: Dienstag 10:40–12:40

Raum: H12

**Hauptvortrag**

MO 21.1 Di 10:40 H12

**Molecules in Electronic Circuits: from integrated single molecules to SAMs in CMOS technology** — ●MARCEL MAYOR — University of Basel, Department of Chemistry and Forschungszentrum Karlsruhe GmbH, Institute for Nanotechnology

The integration of molecular structures in electronic circuits is a concept that has already been proposed in the sixties, when Hans Kuhn presented his vision of molecular engineering. Limited by the available techniques, Kuhn and coworkers mainly investigated molecular monolayers deposited on electrodes. In the last few years, the tools to investigate nanoscale objects have improved tremendously, mainly driven by the invention of the scanning probe methods. Furthermore, feature sizes in semiconductor technology have been reduced very fast and continuously. However, this feature size reduction seems to hit soon both, physical and economical limits. With that background, the revival of the idea to integrate molecules in electronic circuits is not surprising.

Molecules are well defined nanoscale objects consisting of a definite structure leading to particular electronic properties. As these structures can be tailored by chemical synthesis, the visionary concept of molecular electronics is geared by the hope that electronic functions can be realized by carefully designed molecular structures.[1] Apart from the huge variety given by the immenseness of possible molecular structures, the incredible smallness of a functional unit based on a molecule is a main driving force. However, integration of molecular structures in electronic circuits is still an experimental challenge and the field is still at the level of exploring the potential as well as the limitations.

In close cooperation with physicists and engineers from academics and industry, single molecules and assemblies of molecules have been integrated in electronic circuits. Correlations between the molecular structure and the observed I/V characteristics have been investigated. The findings allow to further optimize the molecules for particular electronic functions. Several molecular systems have been synthesized and studied to collect the required comprehension to design particular electronic functions. Recently, a molecular rod acting as a single molecule rectifier has been designed, synthesized and integrated.[2] Indeed rectification was observed, however, it does not yet match the rectification ratios known from its silicon opponents.

[1] a) R. L. Carroll, C. B. Gormann, *Angew. Chem. Int. Ed.* (2002) 41, 4378. b) M. Mayor, H. H. Weber, *Chimia* (2002), 56, 494. c) M. Mayor, H. B. Weber, R. Waser in *Nanoelectronics and Information Technology. Advanced Electronic Materials and Novel Devices* (Ed.: R. Waser), Wiley-VCH, Weinheim (2003) 501. d) M. A. Reed, J. M. Tour, *Scientific American* (2000) 282, 86. e) C. Joachim, J. K. Gimzewski, A. Aviram, *Nature* (2000) 408, 541.

[2] M. Elbing, R. Ochs, M. Koentopp, M. Fischer, C. von Hänisch, F. Weigend, F. Evers, H. B. Weber, M. Mayor, *Proc. Natl. Acad. Sci. U.S.A.* (2005) 102, 8815.

**Hauptvortrag**

MO 21.2 Di 11:10 H12

**Single-molecule electronics: Conductance mechanisms** — ●GIANAURELIO CUNIBERTI — Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

Since few years, several quantum transport experiments employing unimolecular systems have been proven. Some of related emerging phenomena, however, are still missing sound theoretical explanations. One principal limitation is the “static” description of molecular bridges typically assumed for transport processes. Molecules, indeed, are flexible objects and their nuclear “dynamics” plays in general a fundamental role in charge transfer as well as transport mechanisms. In this talk, I will give an overview on the role of vibrations and inelastic transport in molecular systems, and show how such phenomena do dramatically affect the overall conduction properties of molecular junctions.

MO 21.3 Di 11:40 H12

**Schwingungsenergie- und Informationstransfer über molekulare Brücken** — ●ULRIKE TROPFMANN, CAROLINE GOLLUB und REGINA DE VIVIE-RIEDLE — Ludwig-Maximilians-Universität, Department Chemie, Butenandtstr. 11, 81377 München

Das Verständnis von intramolekularen Energietransportprozessen ist von grundlegendem Interesse für Fragestellungen, wie Schwingungsumverteilung und damit gekoppelte Reaktionen in komplexen

(bio)molekularen Systemen, oder Elektronen-Transport in molekularen Drähten. Wir untersuchen IVR-Prozesse in eindimensionalen molekularen Brücken am Beispiel linearer  $(C\equiv C)_n$ -Brücken mit den CC-Streckschwingungen als Transport-Moden. Unser Modell-System ist das Octatetraim-Molekül. Ausgehend von numerischen Quantendynamik-Simulationen auf ab initio berechneten Potentialflächen wird ein modularer Ansatz zur Beschreibung der IVR-Prozesse im Bild der Lokalmode vorgestellt. Die Güte dieser Beschreibung wird anhand des Vergleichs mit volldimensionalen Rechnungen abgeschätzt und eine Anwendbarkeit auf höherdimensionale Systeme (längere Ketten) diskutiert. Ziel dieser Arbeiten ist es, den Informationstransfer über Schwingungsumverteilung in molekularen Brücken zu beschreiben und über Laseranregung zu kontrollieren.

MO 21.4 Di 11:55 H12

**Molekulare Schalter als Brücken in Elektronentransfer-Systemen** — ●DOROTHEE GEPPERT und REGINA DE VIVIE-RIEDLE — LMU München, Department Chemie, Butenandtstr. 11, 81377 München

Wir untersuchen Donor-Brücke-Akzeptor-Systeme, durch die ein Energie- oder Elektronentransfer möglich ist. Ein Fulgid als verbrückende Einheit kann, initiiert durch Photochemie, zwischen zwei stabilen Zuständen wechseln, von denen nur ein Isomer einen Elektronentransfer zulässt. Mit quantenchemischen und -dynamischen Methoden wird dieser Schaltprozess genauer untersucht.

Für einen effektiven Schaltprozess muss die über elektronisch angeregte Zustände verlaufende Isomerisierung schnell und vollständig ablaufen. Wir schlagen dafür den Einsatz von geformten Laserpulsen vor, die wir mittels Optimal Control Theory erhalten. Dabei kommen verschiedene Kontrollstrategien zum Einsatz, die an der Isomerisierungsreaktion der funktionalen Untergruppe der Fulgide illustriert werden [1]. Die verschiedenen benutzten Zielzustandsdefinitionen führen zu unterschiedlichen Reaktionspfaden. Während ein intermediäres Target das Wellenpaket durch die konischen Durchschnitte führt, ergibt sich mit einer Zieldefinition im Grundzustand ein Pump-Dump-Reaktionsweg. In diesem Fall lassen sich die optimierten Laserpulse drastisch vereinfachen.

[1] D. Geppert, L. Seyfarth, and R. de Vivie-Riedle, *APB* 79 (2004) 987-992.

MO 21.5 Di 12:10 H12

**Towards Dispersion Free Exciton Diffusion: Ultrafast Förster Transfer in Doped Polymer Films** — ●STEFAN LOCHBRUNNER und MARTIN SCHLOSSER — LS für BioMolekulare Optik, Ludwig-Maximilians-Universität München

In optoelectronic applications of organic thin film systems the absorbed energy is transported by exciton diffusion to the active interface where charge separation occurs. In unordered materials like in most polymers the sites exhibit electronic states with a large energy dispersion and the excitons are trapped at low energy sites. Therefore we propose as active sites chromophores which are incorporated in the polymer matrix but interact only weakly with the polymeric environment. Their electronic states have similar energies and no trapping of the excitons should occur allowing for a dispersion and loss free long range energy transport by Förster transfer between them. To test the approach we performed femtosecond absorption experiments on PMMA films highly doped with perylene bisimide dyes and characterized the energy transfer between the chromophores. We find a stretched exponential time dependence characteristic for Förster energy transfer between immobilized chromophores with a transfer time of 1.5 ps for an average distance of 2.3 nm resulting in a high mobility of the optically generated excitons. We can also collect the energy with high efficiency on dye molecules which exhibit an absorption spectrum that is red shifted compared to the perylene dyes responsible for the exciton diffusion. This opens a design route for artificial light harvesting complexes.

MO 21.6 Di 12:25 H12

**Ultrafast Electronic Dynamics in Ordered Pentacene Films** — ●TOBIAS BITTKAU<sup>1</sup>, STEFAN LOCHBRUNNER<sup>1</sup>, IDA KOZMA<sup>1</sup>, MARTIN HUTH<sup>2</sup>, STEFAN SCHIEFER<sup>2</sup>, and BERT NICKEL<sup>2</sup> — <sup>1</sup>Lehrstuhl für BioMolekulare Optik, LMU München — <sup>2</sup>Department für Physik und CeNS, LMU München

Micro crystalline thin films of organic molecules are frequently used in organic electronics applications, especially for field effect transistors. In case of low defect densities such films can exhibit band transport. Pentacene films for example have a highly ordered, characteristic herring bone structure which seems to be responsible for the extraordinary high exciton mobility in these films. Since charge and energy transport properties are directly linked to the electronic structure and dynamics of the systems, we started investigating electronic excitations in ordered pentacene films with ultrafast absorption spectroscopy. Contrary to time resolved luminescence experiments, this technique allows also for the observation of non radiating species like polarons. We observe that the excitation induced bleach has a complex recovery kinetics consisting of a 400 fs, a 5 ps, and a some hundred ps component. The localization of the excitation and its dissociation into charged species is discussed with respect to spectral signatures appearing around 630 nm. In addition, we find an unexpected long lasting memory of the excitation polarization which points to highly anisotropic excitation exchange processes.