Hybrid Inorganic/Organic Systems for Opto-Electronics

Collaborative Research Centre 951

Colloquium Announcement

of the Collaborative Research Centre 951
"Hybrid Inorganic/Organic Systems for Opto-Electronics"

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From Simple Triarylamines to Functional Heteroaromatic Scaffolds

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Morphology, growth and dynamics of organic molecules at structured surfaces

Time: Thursday, April 25, 2019, 3 pm c.t.

Place: Erwin-Schrödinger-Zentrum, Rudower Chaussee 26, Room 0'119.

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From Simple Triarylamines to Functional Heteroaromatic Scaffolds

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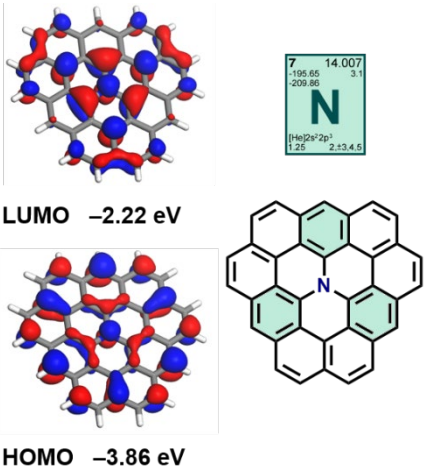
Triarylamines have in the meanwhile become ubiquitous in the area of organic electronics owing to their appreciable electron donor and hole transport properties.[1] However, in most cases rather straightforward derivatizations of the triphenylamine scaffold were used to achieve the desired materials. We have realized that various structurally relatively simple triarylamines[2] may serve as versatile building blocks for the construction of novel nitrogen-containing polycyclic aromatic hydrocarbons (PAHs) with appealing electronic and materials characteristics.[3-5]



In general, the incorporation of heteroatoms directly into the sp^2-carbon framework provides a powerful tool to manipulate the optoelectronic properties and supramolecular behaviour of PAHs.[6] Nitrogen is particularly appealing in this context as it can readily adopt a planar sp^2-hybridized geometry to enable for efficient electronic communication with the surrounding π system. The resulting nitrogen-containing PAHs are highly attractive objects for experimental and theoretical studies as defined molecular fragments of heteroatom-doped carbon allotropes on one hand and as functional materials for diverse applications on the other. In this talk, our recent synthetic efforts carried out in solution and on surfaces will be presented and fundamental characteristics of the resulting compounds discussed.

References: [1] J. Wu, K. Liu, L. Ma, X. Zhan, *Chem. Rev.* **2016**, *116*, 14675. [2] N. Hammer, T. A. Schaub, U. Meinhardt, M. Kivala, *Chem. Rec.* **2015**, *15*, 1119. [3] N. Hammer, T. E. Shubina, J.-P. Gisselbrecht, F. Hampel, M. Kivala, *J. Org. Chem.* **2015**, *80*, 2418. [4] C. Steiner, J. Gebhardt, M. Ammon, Z. Yang, A. Heidenreich, N. Hammer, A. Görling, M. Kivala, S. Maier, *Nat. Commun.* **2017**, *8*, 14765. [5] C. Steiner, Z. Yang, B. D. Gliemann, U. Meinhardt, M. Gurrath, M. Ammon, B. Meyer, M. Kivala, S. Maier, *Chem. Commun.* **2018**, *54*, 11554. [6] P. O. Dral, M. Kivala, T. Clark, *J. Org. Chem.* **2013**, *78*, 1894.

Morphology, growth and dynamics of organic molecules at structured surfaces

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In this talk I will give an overview of our recent work on organic molecules at structured surfaces using computer simulation methods based on classical models, particularly kinetic Monte Carlo and (atomistic) Molecular Dynamics simulations. Topics include the cluster growth of a simple model of an anisotropic molecule-on-solid system, the role of molecular size, and surface diffusion of polar molecules. We close with ongoing work on the use of an artificial neural network to determine energy barriers in kinetic Monte Carlo simulations.