



Colloquium Announcement

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

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Modeling HIOS – Approaching the Device Level

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Chemically Tailored 2D Materials for Electronic and Energy Technologies

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Modeling HIOS – Approaching the Device Level

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Around the start of the 3rd funding period of the CRC 951, the modeling of hybrid inorganic/organic systems for optoelectronics (HIOS) has changed its focus from principal questions such as whether SPASING with organic gain materials is possible [1] and how to quantize a dissipative (e.g. plasmonic) system [2] to more applied problems that are situated in the realm of modeling entire functional elements all the way to complete (and potentially optimized) device designs.

In this talk, a report on the status of our optimization technique [3] and the modeling of active devices such as plasmonically enhanced DBR-cavity lasers with organic gain [4] will be provided. In addition, recent progress in the modeling of electron energy loss spectra from certain plasmonic elements that eventually will be combined into a HIOS chiral plasmonic sensor will be discussed.

[1] G. Kewes, K. Herrmann, R. Rodriguez-Oliveros, A. Kuhlicke, O. Benson, and K. Busch, *Limitations of Particle-Based Spasers*, Phys. Rev. Lett. **118**, 237402 (2017)

[2] S. Franke, S. Hughes, M.K. Dezfouli, P.T. Kristensen, K. Busch, A. Knorr, and M. Richter, *Quantization of Quasinormal Modes for Open Cavities and Plasmonic Cavity Quantum Electrodynamics*, Phys. Rev. Lett. **122**, 213901 (2019)

[3] T. Kiel, P. Varytis, B. Beverungen, P.T. Kristensen, and K. Busch, *Enhanced Faraday rotation by dielectric metasurfaces with Bayesian shape-optimized scatterers*, Opt. Lett. **46**, 1720 (2021)

[4] M. Kliem, T. Kiel, M. Kück, S. Meister, A. Mischok, H. Fröb, K. Busch, and K. Leo, *Defect-State Lasing in Photonic Lattices of Metal-Organic Microcavities*, Advanced Photonics Research **2**, 2000116 (2021)

Chemically Tailored 2D Materials for Electronic and Energy Technologies

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Layered two-dimensional (2D) materials interact primarily via van der Waals bonding, which has created new opportunities for heterostructures that are not constrained by epitaxial growth. However, it is important to acknowledge that van der Waals interactions are not limited to interplanar interactions in 2D materials. In principle, any passivated, dangling bond-free surface interacts with another via non-covalent forces. Consequently, layered 2D materials can be integrated with a diverse range of other materials, including those of different dimensionality, to form mixed-dimensional van der Waals heterostructures [1]. Furthermore, chemical functionalization provides additional opportunities for tailoring the properties of 2D materials [2] and the degree of coupling across heterointerfaces [3]. In order to efficiently explore the vast phase space for mixed-dimensional heterostructures, our laboratory employs solution-based additive assembly. In particular, constituent nanomaterials (e.g., carbon nanotubes, graphene, transition metal dichalcogenides, black phosphorus, boron nitride, and indium selenide) are isolated in solution, and then deposited into thin films with scalable additive manufacturing methods (e.g., inkjet, gravure, and screen printing) [4]. By achieving high levels of nanomaterial monodispersity and printing fidelity, a variety of electronic and energy applications can be enhanced including photodetectors, optical emitters, supercapacitors, and batteries [5-7]. Furthermore, by integrating multiple nanomaterials into heterostructures, unprecedented device function can be realized including anti-ambipolar transistors, gate-tunable Gaussian heterojunction transistors, and neuromorphic memtransistors [8-10]. In addition to technological implications for electronic and energy technologies, this talk will explore several fundamental issues including band alignment, doping, trap states, and charge/energy transfer across van der Waals heterointerfaces.

- [1] D. Jariwala, *et al.*, *Nature Materials*, **16**, 170 (2017).
- [2] S. Li., *et al.*, *ACS Nano*, **14**, 3509 (2020).
- [3] S. Padgaonkar, *et al.*, *Accounts of Chemical Research*, **53**, 763 (2020).
- [4] G. Hu, *et al.*, *Chemical Society Reviews*, **47**, 3265 (2018).
- [5] W. J. Hyun, *et al.*, *ACS Nano*, **13**, 9664 (2019).
- [6] W. J. Hyun, *et al.*, *Advanced Energy Materials*, **10**, 2002135 (2020).
- [7] K.-Y. Park, *et al.*, *Advanced Energy Materials*, **10**, 2001216 (2020).
- [8] M. E. Beck and M. C. Hersam, *ACS Nano*, **14**, 6498 (2020).
- [9] M. E. Beck, *et al.*, *Nature Communications*, **11**, 1565 (2020).
- [10] V. K. Sangwan and M. C. Hersam, *Nature Nanotechnology*, **15**, 517 (2020).