



## Seminar “IRTG Soft Matter Science”

### **Well-defined, defect-free and end-functionalized poly(3-hexylthiophene) via externally initiated Grignard metathesis polymerization**

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In semi-crystalline conjugated polymers such as poly(3-hexylthiophene) P3HT, microstructure and degree of crystallinity are important factors that determine the electronic properties. One important method to prepare P3HT is the Kumada catalyst transfer polymerization (KCTP), which uses Ni(dppp)Cl<sub>2</sub> as the catalyst. Owing to the mechanism of the KCTP method, one tail-to-tail (TT) defect per chain is formed and incorporated into the polymer. While it was until now assumed that the TT-defect is exclusively located at the beginning of the polymer chain, it is now clear that the major fraction of P3HT carries the TT-defect somewhere within the chain. Here we report the synthesis and characterization of defect-free P3HT via the external initiation using new nickel initiators. This method enables regioregularities of 100% via the elimination of the TT initiating dimer, quantitative incorporation of the 3-hexylthiophene starting group and accurate control over molecular weight and polydispersity. The external initiation with more complex initiator precursors is also used to synthesize endfunctionalized polymers, and the mechanism of initiation, propagation and termination reactions is studied by <sup>1</sup>H-NMR endgroup analysis.

**Monday, May 16, 16h00**  
**“Hörsaal Makromolekulare Chemie”,**  
**Stefan-Meier-Str. 31, Freiburg**

You are welcome to meet Dr. Sommer, do not hesitate to contact Christelle Vergnat ([softmattergraduate@physik.uni-freiburg.de](mailto:softmattergraduate@physik.uni-freiburg.de))