	Experiment title: All-organic films for electgronic applications: fine-tuning of the solid-state ordering of quaterthiophene derivatives	**Experiment number**: MA-1535
Beamline: BM26	**Date of experiment**: from: 25.05.2012 to: 28.05.2012	**Date of report**:
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Report:

Abstract:

We report on bulk structures of a family of quaterthiophene (4T) derivatives with linear and branched end groups such as α,α′-dihexylquaterthiophene (Hex-4T-Hex), α,α′-didecyl-quaterthiophene (Dec-4T-Dec) and α,α′-bis(2- ethylhexyl)quaterthiophene (EH-4T-EH), tetramethyldisiloxane- based dimers D2-Und-4T-EH and D2-Und-4T-Hex, and carbosilane-siloxane-based tetramers D4-Und-4T-EH and D4- Und-4T-Hex. The dimers and tetramers contain undecylenic (Und) spacers between the disiloxane and 4T- units of the molecule. The impact of the molecular architecture on the bulk structure at different temperatures is addressed with X-ray diffraction and differential scanning calorimetry. For all of the studied quaterthiophene-containing organosilicon multipods the formation of 4T-crystal sublattice is observed. The alkyl periphery plays an important role in the molecular packing and thermal stability of the ordered phase. They can stabilize or destabilize the crystal phase, depending on their length and architecture. The quaterthiophenes with 2-ethylhexyl end groups adopt a zig-zag conformation in the crystalline state at room temperature. This change of

conformation leads to a significant decrease of the polymorphic transition and isotropization temperatures. The efficiency of 4T packing in the sublattice is estimated from the molecular cross-section (S) in the plane normal to the molecular axis. Correlations between S and field-effect charge carrier mobility are established.

Reference:

Denis.V. Anokhin, Matthieu Defaux, Ahmed Mourran, Martin Moeller, Yury N. Luponosov, Oleg V. Borshchev, Artem V. Bakirov, Maxim A. Shcherbina, Sergei N. Chvalun, Timo Meyer-Friedrichsen, Andreas Elschner, Stephan Kirchmeyer, Sergei A. Ponomarenko and Dmitri A. Ivanov. "*Effect of Molecular Structure of α,α′-Dialkylquaterthiophenes and Their Organosilicon Multipods on Ordering, Phase Behavior, and Charge Carrier Mobility"*. **J. Phys. Chem. C** 2012, 116, 22727−22736