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Modeling reaction kinetics of twin polymerization via differential scanning calorimetry

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The recently introduced method of twin polymerization is a synthesis route to produce nanoporous hybrid materials, containing organic and inorganic structure domains of 0.5 to 3 nm in a large variety of different compositions. Although first theoretical and experimental investigation has been performed, the open question still remains: How does the structure formation process of twin polymerization, yielding these interweaved organic-inorganic nanoporous hybrid materials, takes place in detail? Understanding the occurring effects and processes of the structure formation opens up the possibility to design (organic and/or inorganic) nanoporous materials with desired properties for industry. E.g. nanoporous materials are of great interest in applications like gas filter systems, catalyst or fuel cells. Here, we present a possibility to derive kinetic reaction parameters as the activation energy barrier or the reaction rate constant by fitting differential scanning calorimetry data via an equation system obtained from reaction kinetics.

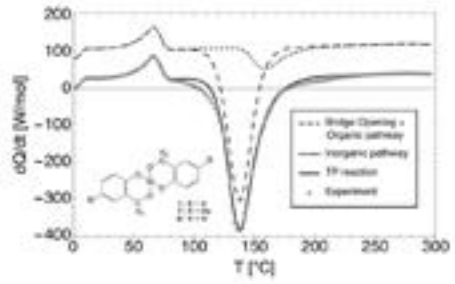

Figure 1: A possible reaction kinetics for the experimental DSC data represented via a two-step twin polymerization process.

Recent Publications

1. Hoffmann KH, Prehl J (2018) Modeling the structure formation process of twin polymerization, Reaction Kinetics, Mechanism and Catalysis 123:367-383.
2. Prehl J, Schönfelder T, Friedrich J, Hoffmann KH (2017) Site dependent atom type ReaxFF for the proton-catalyzed twin polymerization. Journal of Physical Chemistry C 121:15984- 15992.
3. Lang J, Prehl J (2017) An embarrassingly parallel algorithm for random walk simulations on random fractal structures. Journal of Computational Science 19:1-10.
4. Prehl J, Boldt F, Hoffmann KH, Essex C (2016) Symmetric fractional diffusion and entopy production. Entropy 18:275.
5. Tchernook I, Prehl J, Friedrich J (2015) Quantum chemical investigation of the counter anion in the acid catalyzed initiation of 2,2'-spirobi[4H-1,3,2-benzodioxasiline] polymerization. Polymer 60:241-251.
6. Schönfelder T, Friedrich J, Prehl J, Seeger S, Spange S, Hoffmann KH (2014) Reactive force field for electrophilic substitution at an aromatic system in twin polymerization. Chemical Physics 440:119-126.

Biography

Janett Prehl has her expertise in theoretical physics with focus on modelling anomalous diffusion and complex systems. She got her Ph.D. in 2010 from the Technische Universität Chemnitz and works there as research assistant since 2009. In 2014 she got the possibility to work within the research unit FOR 1497 "Organic-Inorganic Nanocomposition through Twin Polymerization" financed by the German Research Foundation (DFG) with her own project "Simulation of structure formation, morphology and functionality of twin polymerization". There she investigates the full structure formation process of twin polymerization on different length scales, from the atomic length scale via quantum chemical calculations and molecular dynamics simulations up to the mesoscopic length scale via Monte Carlo methods as the reactive bond fluctuation model.

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