

## UniCat Colloquium

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- Lecturer: **Prof. Martha Grover**, School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, USA
- Title: **Microstructure design of inorganic materials using process systems engineering**
- Abstract: The micro and nanostructure of inorganic materials often dominates their function, relative to the properties of the bulk single crystal material. Grain boundaries in metal oxide thin films are critical for ion transport in a fuel cell electrolyte, and the surface area and faceting of transition metal nanoparticles determines their catalytic activity. Because these grain boundaries and dispersed phases are non-equilibrium structures, the final material is in a metastable state that is often highly dependent upon the process recipe and process conditions. Microstructure optimization in these batch processes is often accomplished using a strictly empirical approach, due to the lack of predictive models for microstructure dynamics. Here an alternative approach is presented and discussed, using the principles and tools of process systems engineering. Statistical and mechanistic models are used synergistically for *in situ* estimation and process recipe optimization. Mechanistic models are constructed, and then subsequently simplified using automated methods drawn from model reduction and machine learning. These methods are applied in two experimental case studies in surface deposition: metal organic chemical vapor deposition of polycrystalline thin films and supercritical carbon dioxide deposition of transition metal nanoparticles on carbon nanotubes.
- Date: **Wednesday, August 24, 2011**
- Time: **2:00 pm - around 3:30 pm**
- Location: **TU Berlin; Institute of Chemistry  
Straße des 17. Juni 115; 10623 Berlin  
Building C; Lecture Hall C 243**
- Organiser: **Prof. Günter Wozny (TUB)**

Coffee and tea will be served thirty minutes prior to the lecture start.  
**Guests are cordially invited to attend!**

Prof. Dr. Matthias Driess, Chair of the Cluster of Excellence UniCat