Patric Müller and Thorsten Pöschel, FAU Erlangen-Nürnberg
Lehrstuhl für Multiscale Simulation of Particulate Systems

- Patchy particles are characterized by heterogeneous surface properties.
- The resulting anisotropic chemical and physical behavior makes patchy nano- and microparticles interesting for novel applications.
- Recently a one-pot colloidal method for the facile synthesis of gold/silver patches on silica/polystyrene nanospheres has been described \(^1\), \(^2\), \(^3\).
- The corresponding patch growth process is not completely understood.

**Aims**

- Understand and control the deposition of patches on nanospheres from the fluid phase
- Sound model for the deposition process
- Efficient simulation of the deposition process
- Deposition on complex shaped surfaces

**Approach**

**Diffusion Limited Aggregation**

**Model**

1. **Precipitation**
   - Formation of clusters in the surrounding fluid phase
   - Clusters adhere to the surface of the core particle

2. **Diffusion**
   - Clusters undergo Brownian motion on the curved surface of the core particle

3. **Agglomeration**
   - a) Upon contact, clusters stick together with a certain probability
   - b) Epitaxial growth: local relaxation of clusters

**Preliminary Simulation Results**

- Experiments display fast diffusion limited and slow integration limited aggregation leading to either dendritic or continuous cup-like structures \(^2\).
- Depending on the simulation parameters our model is able to describe both regimes of aggregation and the associated patch morphology.

**References:**

1) Klupp Taylor et al. *Langmuir* 2010, 26, 13564-13571
2) Bao et al. *Advanced Materials* 2011, 23, 2644-2649
3) Bao et al. *Nanoscale* 2014, 6, 3954