



Vortragsankündigung

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Es spricht: **Prof. Dr. Keith E. Gubbins**
North Carolina State University, Raleigh

Zeit: **Montag, 29. September 2008**
10:15 Uhr

Ort: **TU Berlin**
Institut für Chemie, Altes Chemiegebäude
Straße des 17. Juni 115
10623 Berlin
Raum C230

Thema: **Surface Nanostructure, Diffusion and**
Catalysis: The Role of Confinement and
Surface Chemistry

Abstract: Chemical reactions are often carried out in nano-structured materials, which can enhance reactions due to interactions with the reacting mixture, high surface area and confinement effects. Diffusion of reactants and products to and from catalyst sites is frequently a limiting factor. Molecular dynamics studies of the effect of tube diameter and chirality for diffusion in single-walled carbon nanotubes are reported. For sufficiently narrow tubes the diffusion is via the single file mechanism, while for larger tubes there is a transition to the faster Fickian diffusion mechanism. The chirality of the carbon tubes has only a small effect at room temperature, but becomes important at lower temperatures.

A study of reactions in confinement is presented, using ab initio and semi-classical methods. We consider several reactions to produce hydrogen, including the decomposition of methane and water on carbon surfaces, with and without the presence of defects and added transition metal atoms. These results provide examples of the influence on reaction mechanism, yield and rate of electrostatic interactions with the supporting material, surface defects and surface curvature.

Organisator: **Prof. Dr. Martin Schön (TUB)**

Gäste sind herzlich willkommen!

Prof. Dr. Matthias Drieß
Sprecher des Exzellenz-Clusters UniCat