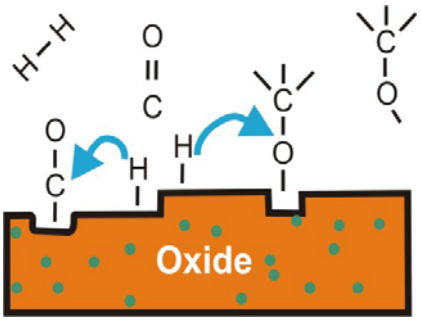
Ruhr-Universität Bochum



SFB 558
„Metall-Substrat-Wechselwirkungen in der heterogenen Katalyse“

Einladung
zum Vortrag von

Prof. Dr. Peter Kratzer
Universität Duisburg-Essen
(Gast von Prof. Marx)

”Chemical reactions and surface diffusion of hydrogen on the Si(001) surface - a test ground for methodologies”

Abstract: Identification of the reaction pathway of H_2 with the Si(001) surface is a problem that has been treated extensively by quantum chemists during the last decade. In my talk, I will review the results obtained with different methodologies, including post-Hartee-Fock methods (MP2, CCSD[T]), density functional theory, and the Quantum Monte Carlo method. Comparing the results enables us to assess the scope and validity of these methods. Moreover, I will present recent results on surface diffusion of hydrogen on stepped Si surfaces, where calculated diffusion barriers can be compared to accurate experimental diffusion rates derived from the analysis of STM images.

Termin:	**25.04.2006**
Zeit:	**11.15 h**
Ort:	**HNC 5/99**

Gäste sind herzlich willkommen.