chemisch
physikalische
gesellschaft

Gegründet im Jahre 1869 von H. Hlasiwetz,
J. Loschmidt, J. Petzval und J. Stefan

Computational Materials Science
CMS
Center for

EINLADUNG

zum Vortrag von

Prof. Dr. Rutger A. van Santen

Technische Universiteit Eindhoven, The Netherlands

über

Theoretical Catalysis

am

Dienstag, 23. Jänner 2007, um 17.30 Uhr

im Großen Hörsaal des Instituts für Experimentalphysik der Universität Wien
1090 Wien, Strudlhofgasse 4 / Boltzmanngasse 5, 1. Stock

Abstract:
The impact of computational quantum theoretical approaches to catalysis is twofold. Computational analysis is indispensable to deduce from spectroscopic data information on molecular structure. Systematic computational study of catalytically active systems is also generating new knowledge basic to a formulation of a theory of catalysis. Computational studies can be especially used to determine the limits of their validity. We will discuss application to the analysis of reactivity indices and principles as:

- Bond order conservation ideas to estimate bond strengths;
- Brønsted-Eyring-Polanyi rules to estimate transition state energies;
- Sabatier principle predictions of vulcano curve maxima.

Another important catalytic theory currently addressed is the Langmuir view versus that of Taylor on the nature of catalytic centers. Especially Taylor emphasized the importance of specific structural requirements. Illustrative examples will be from transition metal catalysis and relate to ammonia oxidation, methane and CO conversion catalysis.

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