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Unifying Concepts in Catalysis

UniCat Colloquium

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Lecturer: **Prof. Jürgen Gauss**, Department of Physical Chemistry - Theoretical Chemistry, Johannes Gutenberg-Universität Mainz, Germany

Title: **Chemical Relevance of High-Accuracy Quantum-Chemical Calculations: New Molecules, Rotational Spectroscopy, and Relativistic Effects**

Abstract: The talk features recent methodological developments for high-accuracy quantum-chemical calculations and demonstrates how these calculations can be used in chemical applications. Examples are given that deal with computational thermochemistry as well as theoretical predictions in the field of rotational spectroscopy. In the latter case, it is shown how the interplay of theory and experiment enables the detection of new molecules (e.g., HSSOH, HPSi, OSiS, cyclic SiS2). A further aspect that is discussed is the importance of relativistic effects for the accurate prediction of the hyperfine parameters relevant to rotational spectroscopy.

Date: **Wednesday, January 11, 2012**

Time: **5:15 pm - around 6:45 pm**

Location: **TU Berlin, Department of Chemistry**
Straße des 17. Juni 115, 10623 Berlin
Building C
Lecture Hall C 243

Organiser: **Prof. Helmut Schwarz (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