RCMS Research Center for Materials Science, Nagoya University

Nagoya University

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Platform: Nano-Energy

Theoretical Chemistry Colloquium

May 12, 2015 (Tue), 16:00-17:00

RCMS, 2nd floor, Chemistry Gallery

Understanding and Designing Heterogeneous Catalysts from First Principles

Prof. Dr. Andreas Heyden
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University of South Carolina, Columbia, SC, USA

Abstract: In the last ~15 years computational catalysis started to significantly impact catalysis research by providing a new tool for testing experimental hypotheses and by screening a large number of materials in silico. In this seminar, I will present two case studies illustrating the strengths and challenges of computational catalysis. For these topics, I will highlight the importance of solvent effects in catalysis and present recent tools for including solvation effects in computational studies.

CHEMISTRY Nagoya University

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