

VENUE



GOLDEN TULIP
STRANDHOTEL WESTDUIN

Golden Tulip Strandhotel
Westduin 1
4371 PE Koudekerke/Vlissingen
The Netherlands
Phone +31 118-555 515



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CONFERENCE ORGANIZERS

The ICTAC-14 meeting is a joint Dutch-Belgian organization and more specifically a collaboration between Schuit Institute for Catalysis (<http://www.nrsc-catalysis.nl>) of Eindhoven University of Technology (The Netherlands) and the Center for Molecular Modeling (<http://molmod.ugent.be>) of Ghent University.

TU/e Technische Universiteit
Eindhoven
University of Technology



WWW.ICTAC14.ORG



ICTAC-14

14th International Conference on THEORETICAL ASPECTS OF CATALYSIS

Vlissingen, The Netherlands
June 26 - 30, 2012

FIRST ANNOUNCEMENT

WWW.ICTAC14.ORG

SCOPE

The prediction of catalytic reactivity

The ICTAC-14 is part of a biannual series of conferences that focuses on Theoretical Aspects of Heterogeneous Catalysis. This conference is an important platform to discuss the state of the art and progress in the field of computational catalysis.

With the current advances in computational capabilities, it has now become possible to realistically model the relation between the structure/composition of the active site of the catalyst and catalytic performance. For this reason the use of computational techniques has become indispensable to study mechanistic aspects of heterogeneous catalysis. Computational studies have provided a large amount of new data which are of great interest to the science and use of molecular heterogeneous catalysis.

Based on the data obtained from quantum-chemical studies on reaction intermediates and corresponding transition states, the mechanism of several important heterogeneous reactions has been unraveled and related to the active state of the catalyst surface. New technological challenges as the need for renewable energy create many new opportunities for the investigation of novel catalytic systems.

Structure and particle size dependence, the effect of microporous structure and structural reorganization are important catalyst parameters that are becoming also accessible to computation. Multiscale approaches that enable to couple reaction kinetics with adsorption and diffusion have to be further developed.

With the increasing predictability of catalytic simulations, theory becomes able to predict the most optimal catalyst for a certain catalytic process. Modeling can also assist in understanding the synthesis processes of the materials. There are many opportunities for new method development and their proper applications and such aspects will be highlighted during this symposium.

Ample opportunity will be provided to exchange ideas on above mentioned topics through a number of plenary, invited and contributed oral contributions. In addition two evening sessions are completely devoted to poster sessions, to stimulate discussions in an informal manner.

MAIN TOPICS

TRANSITION METAL CATALYSIS

NANOPOROUS MATERIALS: ZEOLITES – MOFS

SYNTHESIS MODELING

ELECTRO CATALYSIS – ENERGY STORAGE

THEORETICAL METHODS

(MULTISCALE MODELING, FORCE FIELD DEVELOPMENT,...)

INVITED SPEAKERS

PLENARY SPEAKERS

Jens Nørskov (Stanford University, USA)

Jürgen Hafner (University of Vienna, Austria)

Philippe Sautet (ENS / University of Lyon, France)

Xinhe Bao (Dalian University, China)

Matthew Neurock (University of Virginia, USA)

Richard Catlow (University College London, UK)

Geert-Jan Kroes (Universiteit Leiden, The Netherlands)

Dion Vlachos (University of Delaware, USA)

Michiel Sprik (University of Cambridge, UK)

Karsten Reuter (Technical University of Munich, Germany)

Joachim Sauer (Humboldt University Berlin, Germany)

Rochus Schmid (Ruhr University Bochum, Germany)

INVITED LECTURERS

Peijun Hu (Queen's University Belfast, North Ireland)

German Sastre (Polytechnic Univ. of Valencia, Spain)

Piero Ugliengo (University of Turin, Italy)

Stian Svelle (University of Oslo, Norway)

Marc-Olivier Coppens (Rensselaer Polytechnic Institute, USA)

Momoji Kubo (Tohoku University, Japan)

Titus van Erp (KU Leuven, Belgium)

Timo Jacob (University of Ulm, Germany)

IMPORTANT DATES

1st September 2011 Start early registration + Call for abstracts (*oral contributions / posters*)

1st December 2011 Deadline for abstracts (*oral contributions*)

1st February 2012 Acceptance oral contributions

15th February 2012 Deadline for abstracts (*posters*)

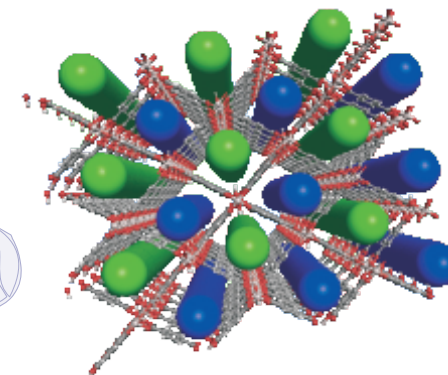
1st March 2012 Acceptance posters

15th April 2012 Deadline for early registration

15th May 2012 Deadline for final registration

ABSTRACT SUBMISSION

Call for abstract submissions for oral contributions and/or poster presentations will start from 1st September 2011.



CONFERENCE WEBSITE

All information about ICTAC-14 is available on the conference website www.ictac14.org, and will be updated regularly.