

Oorgdagar 2011 – A Marcus Wallenberg Symposium

First national inorganic chemistry meeting organised by the Swedish Chemical Society
Stenungsbaden, Stenungsund, June 13-15 2011

13 June

11.30 **Registration and lunch**

Session I

Chair person: *Lars Öhrström*

13.00 Welcome
Lars Öhrström, Chalmers

13.10 Inorganic chemistry in Sweden
Sven Lidin, Lund University, Sweden

Session II Inorganic chemistry and energy

Chair person: *Sven Lidin*

13.35 Artificial Photosynthesis - Molecular Catalysts for Light Driven Water Splitting
Licheng Sun, Royal Institute of Technology

14.15 Comparison of structure and proton conductivity of 50 mol % In and Sc doped
BaTiO₃
Seikh Rahman, Chalmers

14.35 Ruthenium Fulvalene Compounds for Solar Thermal Energy Storage and
Conversion
Kasper Moth-Poulsen, Chalmers

14.55 **Coffee & Check in**

Session III

Chair person: *Elisabeth Ahlberg*

15.30 Metal Rich Molecules Filling the Gap between Complexes and Clusters
Roland Fischer, Ruhr University Bochum

16.10 Structural controls on surface hydroxyl reactivity in iron hydroxides
Jean-François Boily, Umeå University

16.30 Crystal chemistry of Complex Metallic Alloys
Cesar Pay Gomez, Uppsala University

16.50 Structure determination by electron crystallography
Xiadong Zou, Stockholm University

17.15-18.30

Session IV Poster Flash Presentations

Chair person: *Ola Wendt*

- Poster No 1 Sputtering of Amorphous Metal Carbide Thin Films
Matilda Andersson, Uppsala University
- Poster No 2 Palladium chemistry in the advanced reprocessing of spent nuclear fuel
Emma Aneheim, Chalmers
- Poster No 3 Alkylation of Amines with Alcohols Catalyzed by a Novel Iridium-Carben Complex
Agnieszka Bartoszewicz, Stockholm University
- Poster No 4 Lithium ion intercalation in $\text{Li}_{0.5}\text{Ni}_{0.25}\text{TiOPO}_4$
Rickard Eriksson, Uppsala University
- Poster No 5 Atomic Layer Deposition for Energy Related Applications
Mattis Fondell, Uppsala University
- Poster No 6 Time resolved *in situ* UV-vis absorption spectroscopy on growing ZnO quantum dots in correlation to steady state fluorescence and x-ray diffraction measurements
Jesper Jacobsson, Uppsala University
- Poster No 8 Proton conducting pyrochlore electrolytes for intermediate temperature fuel cells
Christopher Knee, University of Gothenburg
- Poster No 10 The complexation of Cm(III) with CyMe4-BTBP investigated using TRLFS
Elin Löfström-Engdahl, Chalmers
- Poster No 11 Multifunctional NbC based nanocomposite thin films
Nils Nedfors, Uppsala University
- Poster No 12 Mono- and Bi-Nuclear Pathways of Catalytic Water Oxidation: an Involvement of Lewis Acid-Lewis Base Cooperation and Radical Coupling
Timofei Privalov, Stockholm University
- Poster No 13 Nanostructured cathodes for lithium ion microbatteries
David Rehnlund, Uppsala University
- Poster No 14 Direct vs. indirect mechanisms for electron injection in DSSC
Rocio Sanchez, Royal Institute of Technology
- Poster No 15 Structure and Property Investigations of the $\text{La}_2\text{Co}_{1+z}(\text{Ti}_{1-x}\text{Mgx})_{1-z}\text{O}_6$ Perovskite System
Samrand Shafeie, Stockholm University
- Poster No 16 LiFeSO_4F as cathode material for Li-ion batteries
Adam Sobkowiak, Uppsala University
- Poster No 17 W-S-C-(Ti) Films for Tribological Applications
Jill Sundberg, Uppsala University

Poster No 18	Crystal Growth <i>Göran Svensson, Gorans kemi</i>
Poster No 19	Constructing metal organic frameworks with alkaline earth bisphosphonates <i>Matti Tuikka, University of Eastern Finland</i>
Poster No 20	Theoretical study on catalytic activity of water oxidation catalysts based on Ruthenium complex <i>Ying Wang, Royal Institute of Technology</i>
Poster No 21	Bioinspired and biomimetic energy conversion <i>Shuainan Zhao, Uppsala University</i>
Poster No 22	Simulation of the energy barrier for diamond growth processes, without and with dopants <i>Yiming Zou, Uppsala University</i>
19.00	Dinner
20.30- 21.30	Annual meeting of the Inorganic chemistry section within the Swedish Chemical Society

MARCUS WALLENBERG'S STIFTELSE
FÖR INTERNATIONELLT VETENSKAPLIGT SAMARBETE

GRUNDAD AV SKANDINAVISKA ENSKILDA BANKEN



SVENSKA KEMISTSAMFUNDET
Swedish Chemical Society

MATERIALS SCIENCE
A CHALMERS
AREA OF ADVANCE



14 June

Session V Teaching of Inorganic Chemistry

Chair persons: *Lennart Sjölin, and Göran Svensson,*

08.30 Multiple Representations of Chemical Models
George Lisensky, Beloit College

Session VI

Inorganic Chemistry at the MSc and BSc levels at Swedish Universities
(This session will be held in Swedish)

Chair persons: *Lennart Sjölin and Göran Svensson*

09.00 Introduction: *Lennart Sjölin*
Stockholm University: *Lars Eriksson*
University of Gothenburg: *Lennart Sjölin*
Chalmers: *Lars Öhrström*
Uppsala University: *Ulf Jansson*
Lund University: *Sven Lidin*
Umeå University: *Madeleine Ramstedt*
Linköping University: *Fredrik Söderlind*

10.00 **Coffee**

Session VII Organometallics and Catalysis

Chair person: *Vadim Kessler*

10.15 Iridium-catalysed Carbon-Heteroatom Bond Formation via Transfer Hydrogenation
Belén Martín-Matute, Stockholm University, Sweden

10.45 Pyrazolyl Copper and Zinc Complexes as D,L-Lactide and ϵ -Caprolactone Ring Opening Polymerization Catalysts
James Darkwa, University of Johannesburg

11.15 Reactivity of NHC Au(I)-C σ -bonds with electrophiles
Magnus T. Johnson, Lund University

11.35 DFT Studies of the Heck Reaction
Sten Nilsson Lill, University of Gothenburg

11.55 **Lunch**

Session VIII Organometallics and Catalysis

Chair person: Belén Martín-Matute

- 12.50 Halogen Bonding Interactions Between I₂ and Ruthenium Bipyridine Complexes
Matti Haukka, University of Eastern Finland
- 13.20 Oxidation of propenol on nanostructured Ni and NiZn electrodes in alkaline solution
Gert Göransson, University of Gothenburg
- 13.40 Theoretical Studies on Stability and Activity of Ru Catalysts
Mårten Ahlquist, Royal Institute of Technology
-

Session IX

Chair person: Madeleine Ramstedt

- 14.00 Inorganic Chemistry through the Computational Looking-Glass
Kersti Hermansson, Uppsala University
- 14.40 Metallophilic Interactions in 1D Rhodium Structures
Elina Laurila, University of Eastern Finland
- 15.00 Mechanistic aspects of the hydrogen transfer reactions with the main group and transition-metal catalysts
Timofei Privalov, Stockholm University
- 15.20 Absolute Asymmetric Synthesis
Mikael Håkansson, University of Gothenburg
-

15.40-17.15 Coffee and Session X Poster Session

Chair person: Zareen Abbas

- 15.45 Presenters of odd numbered posters
- 16.30 Presenters of even numbered posters
-

Session XI A vision from the Stenungsund Chemical Industry

Chair person: Christopher Knee

- 17.15 Sustainable Chemistry 2030: a vision for the chemical cluster in Stenungsund
Robert Onsander, Senior Adviser for the chemical industrial cluster in Western Sweden
-

- 20.00 **Conference dinner**
-

15 June

Session XII Porous Materials

Chair person: *Xiaodong Zou*

- 08.30 The Flexible Fluoride Ion; Porous Metal Fluorophosphates
Mark Weller, University of Southampton
- 09.15 Soft Chemistry Synthesis of Metal Oxide Materials with Controlled Porosity and Dimensionality
Vadim Kessler, Swedish Agricultural Univ
- 09.35 The Motions of Water in the Zeolite Chabazite, a Molecular Dynamics Study
Philippe A. Bopp, University Bordeaux 1
-

09.55 **Coffee**

Session XIV

Metal Ions in Medicine

Chair person: *Mikael Håkansson*

- 10.15 Bioactive Metal Ion Complexes as Antimicrobials
Madeleine Ramstedt Inv, Umeå University
- 10.45 Development of New Half Sandwich Chloroquine Analogues With Antimalarial Properties
Lotta Glans, Lund University
-

Session XV Minerals, Mining and Chemistry

Chair person: *Lars Öhrström*

- 11.15 Sweden's supply of strategic elements, the role of chemistry
Anders Hallberg, Geological Survey of Sweden
- 11.45 Extraction of base metals and byproducts at Boliden Mineral AB, Rönnskär
Michael Borell &, Jonas Bäckström Boliden Mineral AB
-

12.10 **Concluding Remarks**
Lars Öhrström & Sven Lidin

12.15 **Lunch**

Departure
