Condensed Matter Science in Porous Frameworks:

On Zeolites, Metal- and Covalent-Organic Frameworks

Metal-Organic Frameworks, Covalent-Organic Frameworks and Zeolites are three classes of highly porous materials which have received an exponentially growing interest over the last decade. While the first two consist of molecular linkers connected through metal(-oxide) or non-metal nodes, the later consists of silicon-oxide based clusters and have a uniform well defined framework. Due to their modular nature, they are highly tunable allowing for the active design of materials having specific catalytic properties, luminescent or magnetic behaviour. The presence of mechanical properties (such as breathing) is another interesting aspect of some of these materials, while the combination of different properties makes them of interest for sensor-applications. In addition, fine tuning the porosity allows for the use of these materials in sorption and separation processes.

Developments in computational methods and the evolution of computational resources have made these materials also accessible for theoretical approaches, leading to new insights in these materials and the ability to guide the experimental design towards new porous frameworks.

Experimental research on newly synthesized porous frameworks and investigations of the tunability of these frameworks will be presented, as well as theoretical research providing new and deeper fundamental understanding of porous frameworks at the level of their underlying physics and chemistry. The colloquium will consist of three sessions focussing on MOFs, COFs and Zeolites respectively, and aims for equal contributions from theoretical and experimental researchers.

Time and Place:

The colloquium is part of the **CMD26 – Condensed Matter Conference**, taking place in the ***Martiniplaza Conference Centre in Groningen, Room 3***, The Netherlands on **September 4th-5th, 2016**.

Colloquium Organizers:

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Sunday September 4th — Room 3, 14h50-18h00

Session 1a: On Zeolites

Chair: Ana Palčić

14h55 **Prof. Dr. Emiel Hensen** (*TU Eindhoven, The Netherlands*)
Towards rational design of nanostructured Zeolites

15h25 **Dr. Takehito Nakano** (*Osaka University, Japan*)
Antiferromagnetic ordering and insulator-to-metal transition in alkali metal nanoclusters arrayed in sodalite

15h40 **Dr. Gilles De Wijs** (*Radboud University, The Netherlands*)
Ordering and assignment of Al T-sites in zeolites

15h55-16h25 **Tea & Coffee break**

Session 1b: On Zeolites, MOFs & COFs

Chair: Bartłomiej M. Szyja

16h25 **Dr. Ana Palčić** (*Ruđjer Bošković Insitute,Croatia*)
Heteroatoms in zeolite yielding systems

16h55 **Dr. Matthias Vandichel** (*UGent, Belgium*)
Understanding defects in Zr-MOFs and their role in catalysis

17h25 **Dr. Ming Liu** (*University of Liverpool, UK*)
3-D protonic conductivity in porous organic cage solids

17h40 **Ir. Roderigh Rohling** (*TU Eindhoven, The Netherlands*)
Molecular recognition and confinement-driven reactivity in low-silica alkali-exchanged faujasite catalysts

17h55-18h55 **Welcome Reception**

Monday September 5th — Room 3, 10h05-18h00

Session 2a: On MOFs

Chair: Matthias Vandichel

10h10 **Prof. Dr. Dirk De Vos** (*KU Leuven, Belgium*)
Breathing Ti- and Zr-MOFs based on trans-1,4-cyclohexanedicarboxylate linkers

10h40 **Dr. Danny Vanpoucke** (*UHasselt, Belgium*)
Understanding Breathing Metal-Organic Frameworks: Linking Theory to Experiment.

10h55 **Dr. Stefania Tanase-Grecea** (*U. Amsterdam, The Netherlands*)
Building metal-organic frameworks from lanthanide ions and octacyanometallate building-blocks

11h10-11h35 **Tea & Coffee break**

Session 2b: On MOFs & COFs

Chair: Ionut Tranca

11h40 **Prof. Dr. Donglin Jiang** (*JAIST, Japan*)
Structural Diversity and Functional Design of Covalent Organic Frameworks

12h10 **Dr. Diana Tranca** (*TU Dresden, Germany*)
Immobilizing Molecular Metal Dithiolene-Diamine Complexes into Carbon-Rich, Single-Layer

12h25 **Marcin Miklitz** (*Imperial College London, UK*)
Towards screening of hypothetical porous organic molecules: A computational study of Xe/Kr selectivity

12h40-14h55 **Lunch Break & Poster Session**

Session 2c: On Zeolites & MOFs

Chair: Donglin Jiang

15h00 **Prof. Dr. Rochus Schmid** (*Ruhr University Bochum, Germany*)
Force Fields for Structure Prediction of MOFs

15h30 **Prof. Dr. Monique Van der Veen** (*TU Delft, The Netherlands*)
Inducing non-centrosymmetry in metal-organic frameworks: mechanisms and domain formation.

15h45 **Ágnes Szécsényi** (*TU Delft, The Netherlands*)
On the nature of active sites and mechanism of selective methane oxidation with H_2O_2 over Fe-ZSM-5 catalyst: a periodic DFT study

16h00-16h25 **Tea & Coffee break**

Session 2d: On Zeolites, MOFs & COFs

Chair: Danny E. P. Vanpoucke

16h30 **Prof. Dr. Jorge Gascon** (*TU Delft, The Netherlands*)
Metal and Covalent Organic Frameworks as platforms for the development of Heterogeneous Catalysts: Opportunities in C1

17h00 **Prof. Dr. Jarosław Handzlik** (*Kraków University of Technology, Poland*)
Transition Metal-oxides on porous supports — structure and catalytic properties from DFT Calculations

17h30 **Dr. Katrine Svane** (*University of Bath, UK*)
Missing linkers in metal-organic frameworks: from point defects to large-scale disorder

17h45 **Dr. Marcus Rose** (*RWTH Aachen, Germany*)
Porous organic frameworks in liquid phase adsorption: How does hydrophobicity improve

18h00 **End of the Colloquium on Porous Frameworks**

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