European Physical Society: Condensed Matter Division



## **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 siliconoxide 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*, <u>Room 3</u>, The Netherlands on September 4<sup>th</sup>-5<sup>th</sup>, 2016.

#### **Colloquium Organizers:**

#### Danny E.P. Vanpoucke

Hasselt University Danny.Vanpoucke@UHasselt.be



Bartłomiej M. Szyja Wrocław University of Technology b.m.szyja@pwr.edu.pl

Wrocław University of Technology

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**Ionut Tranca** *Eindhoven University of Technology* i.tranca@tue.nl



## Sunday September 4<sup>th</sup>

#### Room 3, 14h50-18h00

## **Session 1a: On Zeolites**

#### Chair: Ana Palčić

- 14h55Prof. Dr. Emiel Hensen<br/>Towards rational design of nanostructured Zeolites(TU Eindhoven, The Netherlands)
- **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 AI T-sites in zeolites
- 15h55- Tea & Coffee break

## Session 1b: On Zeolites, MOFs & COFs

Chair: Bartłomiej M. Szyja

- 16h25Dr. Ana Palčić(Ruđjer Bošković Insitute,Croatia)Heteroatoms in zeolite yielding systems
- 16h55Dr. Matthias Vandichel(UGent, Belgium)Understanding defects in Zr-MOFs and their role in catalysis
- 17h25Dr. 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 alkaliexchanged faujasite catalysts
   17h55- With the Densitie
- 18h55 Welcome Reception

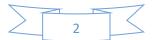
## Monday September 5<sup>th</sup>

#### 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-Tea & Coffee break 11h35



## 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.
- 15h45Ágnes Szécsényi(TU Delft, The Netherlands)On the nature of active sites and mechanism of selective methane<br/>oxidation with H2O2 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 largescale 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



## Colloquium-Sponsor:

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