4. Applications and Benchmarking of MOF Materials

Evaluation of DEFNET materials for applications in catalysis, separation and benchmarking will be done against the zeolites. **Gas sorption and separation applications** based on the defect engineered MOFs will be studied.

Training program

The research and training schemes in DEFNET closely interconnect the disciplines of materials chemistry, physics, chemical engineering, and materials modelling into one consortium which will provide ESRs with a fundamental understanding and excellent education in the most exciting and emerging field of (functional) molecular framework materials science. A rich portfolio of competences and transferable skills within and outside the academic sector will be offered.

The research and training of **15 Early Stage Researchers (ESR/PhD)** in DEFNET covers diverse fields and the training activities are based on **6 workshops** on materials synthesis, characterisation, theory and applications. **Two schools** with an integrated transferable skills training program in "**academic skills**" and "**entrepreneurship**" will be offered with the aim of a bottom-up approach in the self-development of young researchers. The DEFNET network is designed to actively promote the careers of the fellows, ESR secondments to other academic and non-academic partners and joint PhD supervision schemes will be adopted.

A broad curriculum will be adopted for the training of ESRs in the MOF field by offering training in synthesis, characterisation, theory and modelling methods, as well as in transferable skills.

DEFNET

A unique international collaborative research platform based on excellence

The collaborative research and innovative doctoral training program in DEFNET is a unique effort involving Trans-European research driven universities and institutes together with small and large innovative industries. DEFNET enables industry and academia to work together in an international, multi-disciplinary context in the exciting and currently advancing field of molecular network materials (MOFs) science and engineering.

PhD Positions

DEFNET offers Marie Sklodowska-Curie fellowships for 15 ESRs (PhDs for 36 months). All the details including eligibility, recruitment conditions, application procedures, research projects and training program are available on the network's web page.

www.defnet-etn.eu

Starting Date: 01.01.2015
Duration: 4 years (2015 -2018)

Coordination

Inorganic Chemistry II,
Organometallics and Materials
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Marie Sklodowska-Curie Actions

DEFNET

DEFect NETwork Materials Science and Engineering

European Training Network (ETN)

Funded by the European Commission

www.defnet-etn.eu

Beneficiaries

DEFNET consortium consists of **9 beneficiaries** and **7 partner organisations**

Ruhr-University-Bochum, Germany
Organometallics & Materials
Industrial Chemistry

KU Leuven University, Belgium
Centre for Surface Chemistry and Catalysis

ITQ-CSIC, Valencia, Spain
Institute of Chemical Technology

CNRS-Aix Marseille University, France
Gas Storage and Separation Group, Laboratory MADIREL

Utrecht University, Netherlands
Inorganic Chemistry and Catalysis

University of Ghent, Belgium
Centre for Molecular Modelling

University of Oxford, UK
Inorganic Chemistry Laboratory

RUBOTHERM GmbH, Germany

Scientific Computing & Modelling, Netherlands

Partner Organisations

Evonik, AG, Germany

CEPSA, Spain

Solvay, Belgium

Clariant AG, Germany

Linde AG, Germany

BA Tobacco, UK

Diamond Light Source, UK

Scientific Excellence and Goals

DEFNET (**DEFect NETwork materials science and engineering**) is the first integrated European Training Network (ETN) at the intersection of chemistry, physics and engineering which deals with the structural and functional complexity of **molecular network materials** such as **metal organic frameworks (MOFs)**. It provides a unique research and training platform for early stage researchers (ESRs) in chemistry, materials science and engineering. by connecting synthesis, materials characterization, theory and materials simulation with application and technology. DEFNET will investigate local and long range defects, heterogeneity, disorder and correlated phenomena. **Understanding and controlling defect structures** is essential for advanced functionality suited for catalysis, gas capture, and separation. **DEFNET materials based on MOFs** hold promise for innovative functionalities which cannot be achieved by other materials and benchmarking is done against zeolites, which are well established for catalysis and sorption applications.

Research Programme

The research and training in DEFNET are well structured into 8 work packages (research, training, outreach, management) which will provide the ESRs with a fundamental knowledge and excellent education in the most exciting and emerging field of molecular framework materials science (MOFs).

Scientific Work Packages

1. Synthesis and methods of defect engineering
Defective or fragmented linkers (lacking a ligating group or bearing weaker ligator; even simply monodentate carboxylates) or other metal ions than the parent ones will be employed during MOF synthesis and which will yield defective linker doped networks or metal ion substituted networks.

2. Experimental characterisation of structure, defects and disorder
A unique set of complementary materials characterization (spectroscopic, microscopic, diffraction, scattering and calorimetric) methods will be utilized within the consortium for the research of MOFs and for the training of ESRs

3. Theoretical modelling and materials simulations
Force Field (MM, molecular modelling) techniques combined with ab-initio quantum chemical calculations (DFT) leading to tailored QM/MM methods will be developed and calculations will be performed for local (point) defects in the volume (as reactive and/or adsorption centres), in order to interpret/predict spectroscopic data, sorption behaviour and reactivity, and as well for understanding correlation of such defects and long range disorders in MOFs.