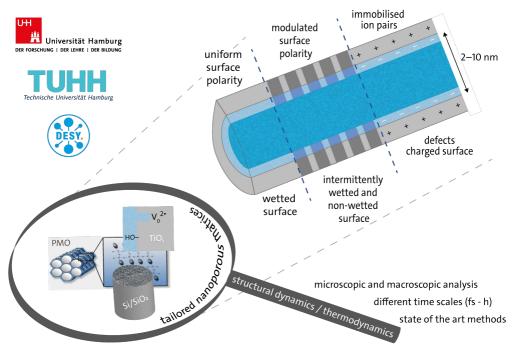
### Landesforschungsförderung Hamburg Control of the special properties of water in nanopores



Despite the enormous relevance of water and aqueous solutions, little is known about the underlying processes and the influence of limited geometries on the thermodynamics and structural dynamics of water/hydrogen bonds. This is particularly surprising, since there are already many findings in this respect for simple molecular fluids, such as linear hydrocarbons. Molecular dynamics studies, among other things, indicate significant changes in the electrical polarizability of water in interface-determined geometries, especially in nanopores.

Within the framework of this research project, this gap is now to be closed. To this end, tailormade nanoporous materials with specifically adjustable pore characteristics (diameter and shape) and surface chemistry are to be developed as model compounds.

The cooperation of the three institutions (UHH, TUHH and DESY) will then make it possible to investigate the materials and the complex interplay of the influence of pure geometric constraints and the interaction of the water dipoles and the hydrogen bond network with the pore walls in detail and on different length and time scales. Thus, a systematic investigation of these influences and the relationships between the thermo- and structural dynamic properties of water in nanopores is possible.

For instance, investigations of the water dynamics over 18 decades in temporal resolution (fs-h) are planned using high-power radiation sources and in cooperation with the planned Centre for Molecular Water Research (CMWS). The enormously relevant influence of dissolved electrolytes on the change of phase equilibria (in comparison between the volume vs. nanostructured system) will also be investigated.



### For further information about the PI's and subprojects please turn the side...

# **List of Projects**

#### Nanoporous matrices: Tailored synthesis

 Subproject 1: "Water and Aqueous Electrolytes in Periodic Mesoporous Organosilicas (PMOS) with different Surface Chemistry"
Variation of Geometric Constraints and Surface Chemistry / Polarity

Variation of Geometric Constraints and Surface Chemistry / Polarity

PI: Prof. Dr. M. Fröba (UHH, Department of Chemistry), michael.froeba@chemie.uni-hamburg.de

 Subproject 2: "Confinement of Water in Mesoporous Functional Metal Oxides" Influence of Lewis and Brønsted acidity and appropriate doping

PI: Jun.-Prof. Dr. S. Mascotto (UHH, Department of Chemistry), simone.mascotto@chemie.uni-hamburg.de

• Subproject 3: "Water and Aqueous Electrolytes in Mesoporous Solids: Phase Behaviour, Hydrodynamic Transport and Dielectric Behaviour" Electrochemical synthesis of suitable materials (mesoporous silicon and silica) with well-defined pore

geometry and pore wall chemistry

PI: Prof. Dr. P. Huber (TUHH, Institute of Materials Physics and Technology), patrick.huber@tuhh.de

#### Thermodynamics / macroscopic analysis

 Subproject 3: "Water and Aqueous Electrolytes in Mesoporous Solids: Phase Behaviour, Hydrodynamic Transport and Dielectric Behaviour"

Studies on hydrodynamics and the dielectric behaviour of materials in laboratory experiments

PI: Prof. Dr. P. Huber (TUHH, Institute of Materials Physics and Technology), patrick.huber@tuhh.de

• Subproject 6: "Phase Equilibria of Aqueous Electrolyte Systems in Mesopores" Systematic investigation of the phase equilibria for the different materials/electrolyte systems

PI: Prof. Dr. M. Steiger (UHH, Department of Chemistry) michael.steiger@chemie.uni-hamburg.de

#### Structural dynamics / microscopic analysis

 Subproject 4: "X-Ray Scattering Experiments – Structure and Dynamics on a Molecular Length Scale" Investigation of the molecular structure of water and electrolyte solutions in the nanopores of the matrices

PI: Dr. F. Lehmkühler (DESY), felix.lehmkuehler@desy.de

• Subproject 5: "Structural Dynamics and Chemical Exchange of Water and Solutes in Mesoporous Solids" Investigation of water dynamics and the dynamics of chemical reactions as a function of matrix material properties

PI: Prof. Dr. N. Huse (UHH, Department of Physics), nils.huse@uni-hamburg.de

Further information about the project and open positions - soon on our website: https://www.chemie.uni-hamburg.de/en/forschung/lff-h2o



## **Open PhD positions, starting July 1st 2020! Get in contact!**