IRES FACULTY PROJECT BANK

to forge new collaborations

October 31, 2018

The inaugural IRES faculty are listed here, http://sustech.ucsb.edu/projects/ires, whose membership can be expanded upon interest and application. Please find details about the IRES program and how to apply in http://sustech.ucsb.edu/projects.

"Electrocatalytic biomass valorization – from material design to reactor concepts"

RWTH Host Faculty: Regina Palkovits

Affiliation: Institut für Technische und Makromolekulare Chemie, RWTH

Description: Non-edible biomass is a promising feedstock of chemical industry. Electrocatalytic reactions enable to integrate renewable energy into the transformation of biomass as renewable carbon source. Starting from major biomass-based platform molecules, highly valuable chemical products such as acrylates, diols or diacids for polymer industry are accessible. Challenges for efficient technologies are (1) electro-catalysts of sufficient selectivity and activity at minimum energy requirement (overpotential) as well as (2) an operation under continuous conditions. The student will experience the design of novel electro-catalysts, metal-doped graphene, metal oxide covered titanium, etc., the testing of these electrodes in reactions such as adipic acid production based on succinic acid and the design of continuous reactor systems using 3-D printing.

Potential Collaborators: Susanna Scott (reaction, catalyst engineering), Songi Han (characterization of solvent distribution dynamics and nanoporous materials), Louis Bouchard (transport measurement, NMR imaging)

RWTH Student Mentor(s): Jerome Meyers (PhD till ~ fall 2021), Nils Kurig (PhD till ~ fall 2021)

"Solid molecular catalysts for small molecule activation"

RWTH Host Faculty: Regina Palkovits

Affiliation: Institut für Technische und Makromolekulare Chemie, RWTH

Description: Highly crosslinked polymers constructed from functional monomers as basic building units enable molecular metal coordination resembling homogeneous catalysts. At the same time, these materials possess high chemical, thermal, mechanical stability and intrinsic porosity—beneficial properties of heterogeneous catalysts. These materials inspire novel strategies for selective CO_2 activation at molecularly defined active sites in continuous liquid flow or even in gas-phase reactions. Examples include covalent organic frameworks (COFs) or polymers with intrinsic microporosity (PIMs) designed to contain nitrogen or phosphorus coordination sites for metal complexation, e.g. of Ru, Ir, Co or even Fe. These materials have already demonstrated to us their potential to activate CO_2 to make formate in the liquid phase. In the future other targets will be tackled including base-free conditions, methanol as products and the potential to transfer the technology into continuous gas-phase applications. The student will experience a research project covering the preparation of tailored porous materials, their characterization of physicochemical properties with state-of-the-art techniques, and potentially, learn about their applications in catalytic transformations.

Potential Collaborators: Susanna Scott (reaction, catalyst engineering), Songi Han (characterization of solvent distribution dynamics and nanoporous materials), Louis Bouchard (transport measurement, NMR imaging)

RWTH Student Mentor(s): Anna Kann (PhD till ~ fall 2020), Andrée Iemhoff (PhD till ~ summer 2021)

“Wetting of porous media for complex homogeneous and immiscible fluids”

RWTH Host Faculty: Matthias Wessling

Affiliation: Institut für Chemische Verfahrenstechnik (Chemical and Process Engineering)

Description: Wetting of porous media is a physico-chemical process relevant for many energy-related challenges such as oil and gas extraction from rock formation, heterogeneous catalysis as well as electrochemical processes. We address the fundamental question how the geometry of a porous system influences the wetting behavior when one phase inside the porosity is replaced by the second immiscible phase. We particularly focus on the interplay of geometry and surface properties of the unit cells building up the geometry. The unit cells will be micro- and nanofabricated in our 3D-FabLab at RWTH. Surface modifications of these super-lattices of unit cells explore the parameter domains of hydropholicity/amphiphilicity/hydrophobicity as well as surface charge. The two-phase behavior is systematically evaluated by 3D NMR imaging.

Potential Collaborators: Bernard Bluemich (NMR spectroscopy, diffusion and relaxation measurements), Songi Han (EPR and Overhauser DNP to study transport of mixed solvents)

RWTh Student Mentor(s): Anna Kalde, Denis Wypysek

“Molecular catalysts based on base metals for the activation of small molecules”

RWTH Host Faculty: Jun Okuda

Affiliation: Institut für Anorganische Chemie, RWTH

Description:

So-called small molecules such as dihydrogen, carbon dioxide, carbon monoxide, dinitrogen and nitrous oxide are highly inert substrates which require specifically designed metal centers to allow efficient transformations. This project focus on the synthesis, structural characterization and reactivity as well as catalysis studies of soluble, ligand-stabilized metal complexes. In line with the environmental requirements to avoid toxic, expensive precious metals, focus is laid on main group metals such as alkali and alkaline earth metals (some of them NMR active) which recently have revealed a remarkably rich coordination chemistry reminiscent of d- and f-block elements. Specific topics relate to the mechanistic study of unconventional reduction of carbon dioxide to give C-C bonded products and catalytic fixation of dinitrogen to give amine derivatives. Such reactions also bear resemblance to so-called prebiotic chemistry in the context of the origin of life processes that resulted in the formation of bioorganic molecules.

The student will experience a research project covering the synthesis of molecularly defined orgnanometallic precursors, structural characterization using state-of-the-art spectroscopic and diffraction techniques, and perform catalytic transformations involving small molecules.

Potential Collaborators: Susanna Scott (reaction, catalyst engineering), Gabriel Menard (organometallic catalysis), Louis Bouchard (transport measurement, NMR imaging), Paula Diaconescu (switchable catalysis), John Arnold (organometallic chemistry)

RWTH Student Mentor(s): Florian Ritter (PhD till ~ fall 2020), Sebastian Schrader (PhD till ~ fall 2021)

“Microporous materials for solar cooling”

RWTH Host Faculty: André Bardow

Affiliation: Lehrstuhl für Technische Thermodynamik, RWTH

Description: Current technologies for heating and cooling require substantial amounts of electricity. However, electricity can be replaced by sustainable energy sources such as solar heat or waste heat in thermally-driven heating and cooling processes. A promising class of thermally-driven processes is based on adsorption. The key element of these processes is microporous material employed for adsorption. Today, commercial materials are employed that have been designed for other purposes, while the tailoring of novel materials for the heating and cooling processes seems highly promising. In this project, we will therefore explore novel classes of materials, including MOFs. These materials should provide both high uptake and fast kinetics to allow for efficient and compact devices. To guide the material development, we will characterize these materials in dedicated setups. Uptake and release will be analyzed to quantify the potential application for cooling, heating, drying or energy storage. The generated data will be used to design real-world applications of the novel materials.

Potential Collaborators: Jeff Reimer (make/supply MOF), Bernhard Blümich (NMR measurements)

RWTH Student Mentor(s): Jan Seiler, Mirko Engelpracht

“Multicomponent diffusion in liquids”

RWTH Host Faculty: André Bardow

Affiliation: Lehrstuhl für Technische Thermodynamik, RWTH

Description: Diffusion is slow – and therefore important: In many processes, diffusion is the rate-limiting step defining the overall speed. Thus, knowledge of diffusion coefficients is required to understand and optimize such processes. However, data on diffusion coefficients is usually lacking. The reason is again: diffusion is slow and diffusion experiments are therefore usually tedious. The situation worsens for multicomponent mixtures which are commonly encountered in real life, but are even more cumbersome to study. To overcome the deficiencies of previous diffusion experiments, we will employ microfluidic measurements techniques. Microfluidics has small dimensions that can lead to faster diffusion, depending on the channel design. In addition, microfluidic chips are optically accessible allowing the use of optical measurement techniques. We will therefore employ Raman spectroscopy to resolve the concentrations of all species in multicomponent mixtures. By combining microfluidics with Raman microspectroscopy, we can perform fast and easy diffusion measurements in multicomponent mixtures. These characterization measurements will be complemented by magnetic resonance based transport and diffusion measurements, as well as modeling. This enable the study of real-life mixtures relevant to processes in the chemical industry and biology.

Potential Collaborators: Jeff Reimer (measure self-diffusion), Louis Bouchard (diffusion model), Songi Han (mixed solvent diffusion properties near surface vs bulk)

RWTH Student Mentor(s): Carsten Flake, David Müller

“Life-Cycle Assessment of Carbon capture with metal-organic frameworks”

RWTH Host Faculty: André Bardow

Affiliation: Lehrstuhl für Technische Thermodynamik, RWTH

Description: Achieving the climate targets of the Paris agreement requires carbon capture and storage (CCS). This is now consensus of the Integrated Assessment Models predicting sustainable pathways for the future. However, while carbon capture can help to mitigate climate change, CCS also leads to additional environmental impacts. Thus, there are trade-offs to consider. In particular, first generation capture technologies have an enormous energy penalty leading to major demands in resources. Adsorption of CO2 in

metal-organic frameworks (MOF) has been proposed as a potential breakthrough technology lowering the energy requirement for CO2 capture and even enabling efficient CO2 capture from air. In this work, we will quantify the potential of CO2 capture by MOFs using life-cycle assessment (LCA). LCA determines environmental impacts along the life cycle from cradle-to-grave.

Potential Collaborators: Jeff Reimer (provide MOFs and data), Benhard Blümich (measure MOF data), Sangwon Suh

RWTH Student Mentor(s): Sarah Deutz, Leonard Müller

"Tailor-made Molecular Catalysts for Polymer Recycling"

RWTH Host Faculty: Jürgen Klankermayer

Affiliation: Institut für Technische und Makromolekulare Chemie, RWTH Aachen University

Description:

A wide range of synthetic polymers is currently produced and designed to meet the various needs and requirements of industry and consumers. The raw materials for these durable products are predominantly centered on petroleum resources and only recently the possibility to use bio-based alternatives is being industrially explored. Moreover, the steadily increasing production and usage of these polymers is largely unsustainable, as efficient recycling strategies for these non-biodegradable materials remain elusive. This results in a tremendous growth of waste plastics and the environmental pollution with the respective material is becoming an enormous environmental problem. Consequently, the European Environmental Agency is fostering research towards a "Circular economy" based on effective recycling strategies as core task. The recycling strategies envisage a selective process in which polymer wastes are depolymerized back to their starting monomer, which is subsequently purified and reused to yield polymeric materials with comparable quality or educts and building blocks for new value-added polymeric materials.

The student will experience a research project covering the synthesis of molecularly defined orgnanometallic catalysts and their application in tailored reactions systems for effective catalytic depolymerisation of the most abundant consumer products.

Potential Collaborators: Susanna Scott (reaction engineering, catalyst engineering), John Arnold (organometallic chemistry), Jeff Reimer (reaction engineering)

RWTH Student Mentor(s): Jasmine Idel (PhD Student), Dr. Kassem Beydoun (Post-Doc)

"Utilization of Carbon Dioxide in Organic Synthesis"

RWTH Host Faculty: Jürgen Klankermayer

Affiliation: Institut für Technische und Makromolekulare Chemie, RWTH Aachen University

Description:

The utilization of carbon dioxide as C1 building block in organic synthesis is a topic of longstanding interest and great current dynamic. Whereas there are well-established organometallic catalytic systems for its hydrogenation to formic acid and recent examples for the hydrogenation to methanol, the application as starting material in organic synthesis remains highly challenging. Cyclic oxygenates are known to be attractive candidates for fuels or fuel additives due to their ability to reduce soot formation during the combustion in diesel engines, but their synthesis is largely unsustainable. Novel tailored catalytic system open a sustainable synthetic pathway to these liquid energy carriers via the combined utilization of bio-based feedstock and CO_2 as carbon sources together with "green hydrogen" from water electrolysis ("bio-hybrid fuels").

The student will experience a research project covering the synthesis of molecularly defined orgnanometallic catalysts and their application in tailored reactions systems for selective transformation of carbon dioxide.

Potential Collaborators: Susanna Scott (reaction engineering, catalyst engineering), John Arnold (organometallic chemistry), Jeff Reimer (reaction engineering)

RWTH Student Mentor(s): Dr. Kassem Beydoun (Post-Doc)