INTERESTING RESEARCH GROUPS – Q2 / 2020

Name of the Group/Institution:

Process Engineering For Sustainable Systems (ProcESS) / KU LEUVEN

Head of the Group:

Prof. Tom Van Gerven

Research profile:

The ProcESS section is dedicated to contribute to sustainable chemical processing by developing intensified and integrated flow sheets, using continuous reactors and separators, with alternative energy forms. Process intensification and integration are key to the overall approach of our research as we aim at the design of new unit processes as well as their integration with other unit operations (hybrid and multifunctional devices) and in complete flow sheets. Research focuses on process intensification, membrane technology and transport phenomena in multiphase systems.

Research topics related to PI:

- Process Intensification by ultrasound and light
- Transport Phenomena and Multiphase Systems
- Membrane Technology
- Smart responsive separation with hybrid processes

Relevance for industrial challenges and trends:

Our research expertise on sustainable processing, water and solid waste technology, and determination of (in)organic components in liquid or solid media is of advantage to external parties. We provide services to industry by developing dedicated processing solutions, performing chemical analyses and providing consultancy.

Recent achievements:

- Intensified SOlvent extraction for critical MEtal Recovery
- Sonication and Microwave Processing of Material Feedstock

Recent publications:

- Mendoza, Heidy Ramirez; Jordens, Jeroen; Pereira, Mafalda Valdez Lancinha; Lutz, Cecile; Van Gerven, Tom; 2020. **Effects of ultrasonic irradiation on crystallization kinetics, morphological and structural properties of zeolite FAU**. Ultrasonics Sonochemistry; 2020; Vol. 64; doi.org/10.1016/j.ultsonch.2020.105010
- Dong Zhengya; Delacour Claire; Mc Carogher Keiran; Udepurkar Aniket Pradip; Kuhn Simon, **Continuous Ultrasonic Reactors: Design, Mechanism and Application**, Materials, 2020, Volume13 Issue2, DOI: 10.3390/ma13020344

Website or contact:

https://cit.kuleuven.be/process

Name of the Group/Institution:

Catalysis Center for Energy Innovation (CCEI) / Univ. of Delaware, USA

Head of the Group:

Prof. Dionisos G. Vlachos

Research profile:

CCEI's research enables the U.S. to meet the energy challenges of the future by developing catalytic technologies for sustainable energy applications through a spectrum of processes envisioned in a future biorefinery. Our research focuses on the conversion of lignocellulosic (non-food based) biomass and its derivatives to fuels, chemicals, and other bioproducts. CCEI explores also feedstock diversification to render biorefineries profitable. In parallel, our work entails (1) synthesis and characterization of novel catalysts, (2) development and application of multiscale modeling, (3) catalyst evaluation, (4) mechanistic and kinetics insights of macromolecular chemistry occurring in complex environments of micro- and meso-pores and often in solvents, (5) workforce development, and (6) technology transfer.

Research topics related to PI:

- Microchemical devices for power generation
- Intensified production of renewable fuels and chemicals

Relevance for industrial challenges and trends:

The Group develops a range of new catalysts and catalytic technologies that will convert inedible biomass—wood, switchgrass and other organic waste—into sugars and oils that can be used in fuels and chemicals.

Recent achievements:

A continuous-flow microreactor with a single-mode MW applicator and the corresponding computational fluid dynamics model to simulate the temperature profile …

Recent publications:

- Chen, Tai-Ying; Baker-Fales, Montgomery; Vlachos, Dionisios G., **Operation and Optimization of Microwave-Heated Continuous-Flow Microfluidics**, Industrial & Engineering Chemistry Research, 2020, Volume59 Issue22 Pages10418-10427 DOI:10.1021/acs.iecr.0c01650

Website or contact:

https://ccei.udel.edu/about/

Name of the Group/Institution:

Design and synthesis of inorganic materials (DESINe)/University of Hasselt, Belgium

Head of the Group:

Prof. dr. Marlies Van Bael

Research profile:

The main activity is the study of environmentally friendly, chemical methods for the synthesis of high-tech, nanostructured inorganic materials. Solution based synthesis routes, including aqueous and non-aqueous sol(ution)-gel methods, hydro/solvothermal routes, combustion synthesis, co-precipitation, thermal decomposition synthesis etc. are created for the preparation of ferroelectric, piezoelectric, conductive and dielectric metal oxide powders and thin films, strategically important for future developments in nanoelectronics, solar cells and energy storage in batteries, as well as power to X. Applications situate in the field of MOSFETs, DRAMs, FERAMs, MEMS, biosensors and transparent electrodes, photovoltaics, lithium ion, sodium ion and lithium sulphur batteries, as well as catalysts for CO2 reduction and hydrogen generation.

Research topics related to PI:

- Solar systems in the Power-to-X context

Relevance for industrial challenges and trends:

Sustainability. The Group develops new materials that can be used in green production of fuels and chemicals

Recent achievements:

A minireactor using sunlight as direct energy source for CO_2 and synthesis gas conversion, developed in collaboration with TNO.

Recent publications:

- Sastre, Francesc; Versluis, Caroline; Meulendijks, Nicole; Rodriguez-Fernandez, Jessica; Sweelssen, Jorgen; Elen, Ken ; Van Bael, Marlies K. ; den Hartog, Tim; Verheijen, Marcel A.; Buskens, Pascal, **Sunlight-Fueled, Low-Temperature Ru-Catalyzed Conversion of CO2 and H-2 to CH4 with a High Photon-to-Methane Efficiency**, ACS OMEGA, 2019, 4(4), p. 7369-7377
- Kalipyappan, Periyasamy ; Leyssens, Karen; Samyn, Pieter ; Meynen, Vera; Hardy, An ; Van Bael, Marlies K., **Core-Shell SiO_2@TiO_2 beads for Plasma Catalytic CO2 Dissociation in a Packed bed DBD reactor**, 17th International Conference on Carbon Dioxide Utilization - ICCDU 2019, Aachen-Germany, 23-27 June 2019

Website or contact:

https://www.uhasselt.be/UH/Onderzoeksgroepen/DetOndgr.html?oid=13099
https://www.researchgate.net/profile/Marlies_Van_Bael

Name of the Group/Institution:

James M Tour Group/Rice University (U.S.A.)

Head of the Group:

Prof. James M. Tour

Research profile:

Tour's scientific research areas include nanoelectronics, graphene electronics, silicon oxide electronics, carbon nanovectors for medical applications, green carbon research for enhanced oil recovery and environmentally friendly oil and gas extraction, graphene photovoltaics, carbon supercapacitors, lithium ion batteries, lithium metal batteries, CO2 capture, water splitting to H2 and O2, water purification, carbon nanotube and graphene synthetic modifications, graphene oxide, carbon composites, hydrogen storage on nanoengineered carbon scaffolds, and synthesis of single-molecule nanomachines which includes molecular motors and nanocars and nanomachines that can drill through cell membranes. He has also developed strategies for retarding chemical terrorist attacks. For pre-college education, Tour developed the NanoKids concept for K-12 education in nanoscale science, and also Dance Dance Revolution and Guitar Hero science packages for elementary and middle school education: SciRave (www.scirave.org) which later expanded to a Stemscopes-based SciRave. The SciRave program has risen to be the #1 most widely adopted program in Texas to complement science instruction, and it is currently used by over 450 school districts and 40,000 teachers with over 1 million student downloads.

Research topics related to PI:

- Advanced materials with PI-technologies
- Electricity-based processing

Relevance for industrial challenges and trends:

Sustainability and advanced materials. The Group develops new methods and materials that can be used in green production of fuels and chemicals

Recent achievements:

Making graphene from any carbon source (e.g. waste) in 10 ms via flash Joule heating.

Recent publications:

- Duy X. Luong, Ksenia V. Bets, Wala Ali Algozeeb, Michael G. Stanford, Carter Kittrell, Weiyin Chen, Rodrigo V. Salvatierra, Muqing Ren, Emily A. McHugh, Paul A. Advincula, Zhe Wang, Mahesh Bhatt, Hua Guo, Vladimir Mancevski, Rouzbeh Shahsavari, Boris I. Yakobson & James M. Tour, "**Gram-scale bottom-up flash graphene synthesis**", Nature 2020, 577, 647–651.
- Li, J. T.; Stanford, M. G.; Chen, W.; Presutti, S. E.; Tour, J. M. "**Laminated Laser-Induced Graphene Composites**," ACS Nano 2020, ASAP. DOI: 10.1021/acsnano.0c02835
- Stanford, M. G.; Zhang, C.; Fowlkes, J. D.; Hoffman, A.; Ivanov, I. N.; Rack, R. D.; Tour, J. M. "**High-Resolution Laser-Induced Graphene. Flexible Electronics beyond the Visible Limit**," ACS Appl. Mater. Interfaces 2020, 12, 10902–10907. 10.1021/acsami.0c01377

Website or contact:

http://www.jmtour.com/

Name of the Group/Institution:

Materials Chemistry and Catalysis/University of Southampton (U.K.)

Head of the Group:

Prof. Robert Raja

Research profile:

Porous materials and their composites form a big part of Group's research portfolio, encompassing metal-organic frameworks (MOFs), silica and aluminophosphates across the micro- and mesoporous regimes, respectively. The Group is developing strategies to process MOFs into application-specific configurations inspired by the interfacial interactions that govern biomineralisation processes and have prepared a wide-range of MOF-based composite materials with enhanced properties, including MOF-oxide composites for efficient chromatographic separation of xylene isomers, MOF-based capsules for pH triggered cargo release and size-selective biocatalysis and the use of biopolymers to influence crystal growth and orientation. The design of functional catalytic materials at the nanoscale is also a major area of research, wherein a detailed understanding of the nature of the active sites at the molecular level has led to the predictive design of single-site heterogeneous catalysts for multi-scale petrochemical and environmental technologies; with a multidisciplinary focus on photonics, renewable energy, sustainable nanocomposites and maritime engineering. Strategies to prepare hierarchically porous materials spanning multiple pore size regimes are also under development.

Research topics related to PI:

- Novel microreactors
- Materials and devices for photocatalysis

Relevance for industrial challenges and trends:

Sustainability and advanced materials. The Group develops new methods and materials that can be used in production of solar fuels and chemicals

Recent achievements:

Photocatalytic microreactors that convert water into hydrogen fuel using solar energy. The reactors are based on microstructured optical fibre canes (MOFCs).

Recent publications:

- Matthew E. Potter, Daniel J. Stewart, Alice E. Oakley, Richard P. Boardman, Tom Bradley, Pier J. A. Sazio, and Robert Raja, **Combining Photocatalysis and Optical Fiber Technology toward Improved Microreactor Design for Hydrogen Generation with Metallic Nanoparticles**, ACS Photonics 2020, 7, 3, 714–722.

Website or contact:

https://www.southampton.ac.uk/chemistry/research/groups/functional_inorganic_materials_and_supermolecular_chemistry.page?

Name of the Group/Institution:

Institute for Micro Process Engineering/Karlsruhe Institute of Technology

Head of the Group:

Prof. Dr.-Ing. Roland Dittmeyer

Research profile:

Development of microstructured devices at IMVT is based on the skills of producing nozzles of smallest deflection radii of up to 30 µm by machining with ground, shaped diamonds. These so-called separation nozzles were used for the enrichment of fissile uranium from isotope mixtures. In the late eighties, the mechanical microstructurization technique was used for the first time by the former Institute for Nuclear Process Technology of Kernforschungszentrum Karlsruhe to produce microstructured heat exchangers and reactors (Schubert et al., DE 37 09 278 A1, 1988). In the nineties, development of microstructured devices for process engineering was furthered consistently and eventually resulted in the foundation of IMVT as an independent institute in 2001.

Today, IMVT is one of the leading academic research institutions in the field of micro process engineering worldwide. An international team of 64 employees specialized in various disciplines focuses on the construction and fabrication of microstructured devices, on fundamental studies of transport processes and chemical reactions in microstructures, and on the use of prototypes in selected thermal and chemical processes. Apart from research projects financed from basic funds under the Helmholtz programmes, projects funded by third parties are being executed in cooperation with industry and academic research institutions in Germany and abroad.

Research topics related to PI:

- Novel microreactors and microstructured devices

Relevance for industrial challenges and trends:

Sustainability and modularization. Among other things, the Institute is involved in Power-to-X: Carbon-neutral Fuels from Air and Green Power

Recent achievements:

The world's first integrated Power-to-Liquid (PtL) test facility to synthesize fuels from the air-captured carbon dioxide.

Recent publications:

- Loewert, M.; Zaghini Francesconi, V.; Brübach, L. T.; Pfeifer, P., **Coupling of Fischer-Tropsch reaction kinetics, enhanced vapor-liquid flash calculation and residence time distribution modeling for time-dependent product determination in load-flexible plants**; Chem. Eng. J. 2020, https://doi.org/10.1016/j.cej.2020.126032.
- Kirsch, H.; Lochmahr, N.; Staudt, C.; Pfeifer, P.; Dittmeyer, R., **Production of CO_2-neutral liquid fuels by integrating Fischer-Tropsch synthesis and hydrocracking in a single micro-structured reactor: Performance evaluation of different configurations by factorial design experiments**, Chem. Eng. J., 2020, 3939, 124553.

Website or contact:

http://www.imvt.kit.edu/english/index.php

Name of the Group/Institution:

Membrane Research Lab/Texas University at Austin

Head of the Group:

Prof. Benny Freeman

Research profile:

Benny Freeman's research program explores the relationship between polymer structure, processing and properties. More specifically, his research group studies the effect of polymer structure on the solubility, diffusivity, and permeability of small molecules in polymers and polymer-based materials. These fundamental studies bear directly upon membranes for liquid, gas, and vapor separations; controlled drug delivery devices and techniques; barrier plastics for food and specialty packaging; monomer and solvent removal from formed polymers; and physical aging of glassy polymeric materials and membranes.

Research topics related to PI:

- Novel membranes and membrane materials

Relevance for industrial challenges and trends:

Sustainability. Extended research in CO_2 removal and water purification.

Recent achievements:

New, MOF-based membrane filtration technique that could dramatically reduce the amount of time it takes to extract lithium from the earth, taking the process from months and years to hours (in collaboration with Monash University).

Recent publications:

- Yoon, H.W., T.H. Lee, C.M. Doherty, T.H. Choi, J.S. Roh, H.W. Kim, Y.H. Cho, S.-H. Do, B.D. Freeman, and H.B. Park, **"Origin of CO(2)-philic Sorption by Graphene Oxide Layered Nanosheets and Its Derivatives,"** Journal of Chemical Physics Letters, 11, 2356-2362 (2020).
- Rodriguez, C.G., M. Chwatko, J. Park, C.L. Bentley, B.D. Freeman, and N.A. Lynd, **"Compositionally Controlled Polyether Membranes via Mono (μ-alkoxo) bis (alkylaluminum)-Initiated Chain-Growth Network Epoxide Polymerization: Synthesis and Transport Properties,"** Macromolecules, 53(4), 1191-1198 (2020).
- Lu, Jun, Huachang Zhang, Jue Hou, Xingya Li, Xiaoyi Hu, Yaoxin Hu, Christopher D. Easton, Qinye Li, Chenghua Sun, Aaron W. Thornton, Matthew R. Hill, Xiwang Zhang, Gengping Jiang, Jefferson Zhe Liu, Anita J. Hill, Benny D. Freeman, Lei Jiang, and Huanting Wang, **"Efficient Metal Ion Sieving in Rectifying Subnanochannels Enabled by Metal-Organic Frameworks,"** Nature Materials, 19, 767–774 (2020).

Website or contact:

https://membrane.ces.utexas.edu/

Name of the Group/Institution:

Department of Chemical and Pharmaceutical Sciences / University of Ferrare, Italy

Head of the Group:

Prof. Olga Bortoloni

Research profile:

In the group Organic Chemistry of the department, part of research is focused on the development of Flow Chemistry. This research area involves the design and test of fixed-bed and monolithic microreactors using organo- and bio-catalysts immobilized on silica or polystyrene as packing materials. The development of continuous-flow processes by the microreactor technology allows for the synthesis of high added-value molecules on the milligram-multigram scale with improved efficiency, sustainability, and lower costs compared to traditional batch processes. The goals are as follows: Study of the immobilization strategy of the (bio)organocatalyst; Physicochemical characterization of the (bio)material; Fabrication of fixed-bed microreactors and monolithic columns; Development of new stereoselective carboligation reactions in flow regime; Reaction modeling for process optimization.

Research topics related to PI:

- Flow Chemistry, Batch-to-continuous

Relevance for industrial challenges and trends:

Sustainability and modularization.

Recent achievements:

A versatile one-step photopolymerization approach for the immobilization of enantioselective organocatalysts.

Recent publications:

- De Risi, Carmela; Bortolini, Olga; Brandolese, Arianna; Di Carmine, Graziano; Ragno, Daniele; Massi, Alessandro **A Review. Recent advances in continuous-flow organocatalysis for process intensification**; Reaction Chemistry & Engineering 2020 Volume 5 Issue 6 Pages1017-1052 DOI:10.1039/d0re00076k
- Rico Warias Daniele Ragno Alessandro Massi Detlev Belder, **A visible-light-powered polymerization method for the immobilization of enantioselective organocatalysts into microreactors**, Chem. Eur. J. 2020 DOI: 10.1002/chem.202002063

Website or contact:

http://www.unife.it/international/education/master-courses/chemical-and-pharmaceutical-sciences-1

Name of the Group/Institution:

LSRE-LCM (Department of Chemical Engineering) / University of Porto, Portugal

Head of the Group:

Prof. Madalena Dias

Research profile:

LSRE-LCM is a partnership between LSRE - Laboratory of Separation and Reaction Engineering and LCM - Laboratory of Catalysis and Materials. The Mission of LSRE-LCM is to promote the advance of scientific and technological know-how in the Chemical Engineering areas of Separation and Reaction Processes, Product Engineering, Catalysis and Carbon Materials, Thermodynamics and Environmental Engineering. A wide range of know-how levels is covered by LSRE-LCM activities, from fundamental research to the development of industrial products and processes, including contributions from materials, process and product engineering. research at LSRE-LCM is organized in 4 Research Groups in different strategic areas: CYCLIC ADSORPTION/REACTION PROCESSES; PRODUCT ENGINEERING; THERMODYNAMICS & ENVIRONMENT; CATALYSIS AND CARBON MATERIALS.

Research topics related to PI:

- Multifunctional (reaction-separation) and hybrid separation processes
- SMBR, PermSMBR, PSAR technologies

Relevance for industrial challenges and trends:

- Sustainability and Environment. Advanced multifunctional processes dedicated to wastewater treatment.

Recent achievements:

- Water gas shift for the production of hydrogen
- Isomerization and separation of hexane isomers
- Advanced oxidation technologies combined with direct contact membrane distillation for water treatment.

Recent publications:

- Espindola, Jonathan C.; Vilar, Vitor J. P., **Innovative light-driven chemical/catalytic reactors towards contaminants of emerging concern mitigation: A review**; Chemical Engineering Journal, 2020 Volume 394 Pages124865 Journal; DOI:10.1016/j.cej.2020.124865
- R.V. Kumar, M.O. Barbosa, A.R Ribeiro, S. Morales-Torres, M.F.R. Pereira, A.M.T. Silva, **Advanced oxidation technologies combined with direct contact membrane distillation for treatment of secondary municipal wastewater**; Process Safety and Environmental Protection, 2020, 140, 111-123 https://doi.org/10.1016/j.psep.2020.03.008

Website or contact:

https://sigarra.up.pt/feup/en/uni_geral.unidade_view?pv_unidade=872

Name of the Group/Institution:

CatSEE group (Institute of Physical Chemistry) / Polish Academy of Sciences, Warsaw, Poland

Head of the Group:

Assoc. Prof. Juan Carlos Colmenares Quintero

Research profile:

The “Catalysis for sustainable energy production and environmental protection” Group, (CatSEE), covers the following research topics: catalytic hydrogen transfer, coal liquefaction, catalytic selective hydrogenation and oxidation, mechanisms of (super)acid-(super)base catalysis, petrochemical processes, synthesis-characterization applications of novel nanomaterials, heterogeneous photocatalysis, green chemistry, sonocatalysis, natural products’ synthesis, chemical waste (biomass) valorization, CH4/CO2 chemistry, solar energy, combustion chemistry, fuel cells.

Research topics related to PI:

- Synergistic combinations of alternative energy forms
- Photocatalytic reactors
- Sonocatalytic reactors

Relevance for industrial challenges and trends:

- Sustainability
- Ultrasound and Microwave methods for nanomaterials synthesis and water purification.

Recent achievements:

- Conversion of Lignocellulosic Biomass into Platform Chemicals
- Green Synthesis of Fine Chemicals and Pharmaceuticals by Thermo-, Sono- and Photo-Catalysis.

Recent publications:

- Giannakoudakis, Dimitrios A.; Lomot, Dariusz; Colmenares, Juan Carlos, **When sonochemistry meets heterogeneous photocatalysis: designing a Sonophotoreactor towards sustainable selective oxidation**; Green Chemistry 2020 DOI:10.1039/d0gc00329h
- S.R. Pradhan, V. Nair, D.A. Giannakoudakis, D. Lisovytskiy, and J.C. Colmenares, **Design and Development of TiO2 coated microflow reactor for photocatalytic partial oxidation of benzyl alcohol**; Molecular Catalysis , 486 (2020), 110884 https://doi.org/10.1016/j.mcat.2020.110884

Website or contact:

http://ichf.edu.pl/home_en.html