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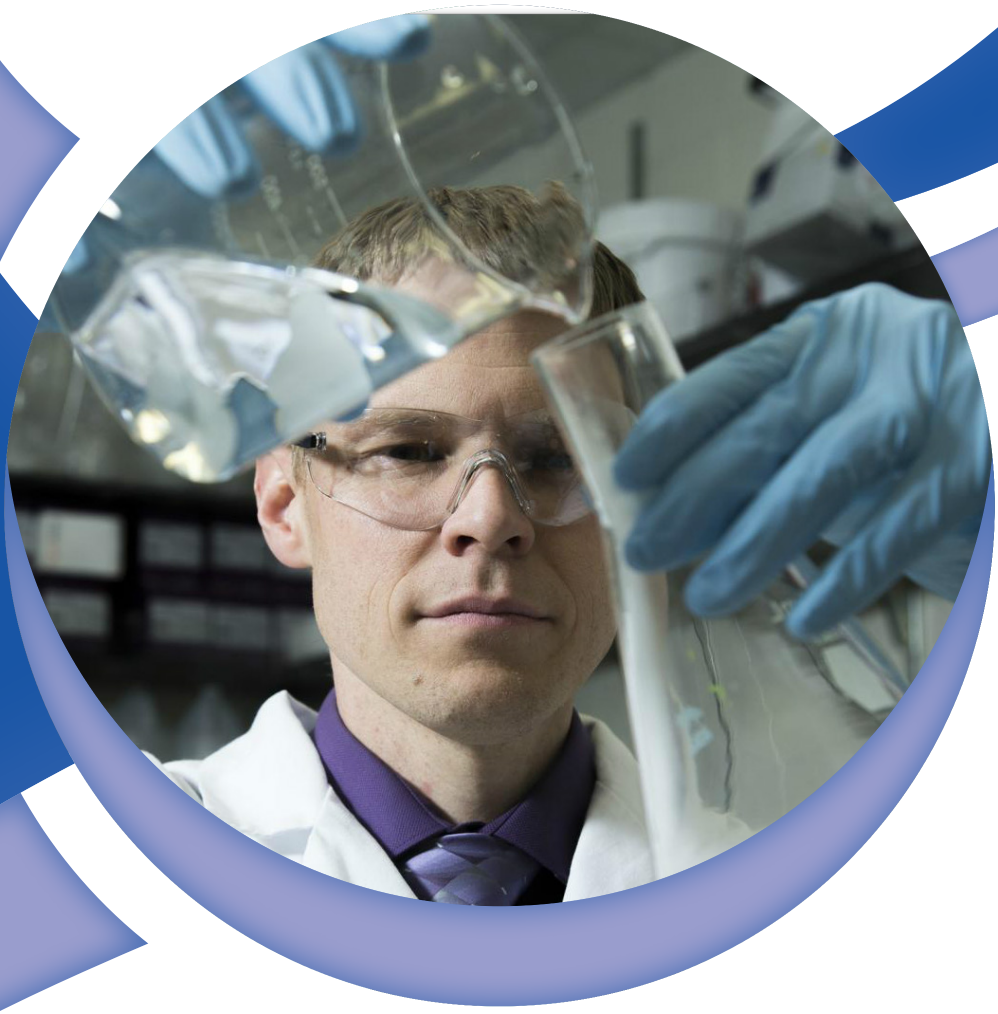

5th World Congress on

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Modeling of 1,4-naphthoquinone derivatives solubility in supercritical carbon dioxide with a density-based correlation and molecular connectivity indices

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The yellow organic solid naphthalene-1,4-dione (1,4-naphtoquinone) is the central chemical structure of natural and synthetized derivatives that present beneficial biological activity for the human health, e.g., 1,4-naphtoquinone pharmacophore is known to impart anticancer activity in drugs like streptonigrin, actinomycins, mitomycins, etc. The study related to the biological and other valuable effects of derivatives from naphthalene-1,4-dione requires their chemical synthesis and their recovery and/or purification. Carbon dioxide (CO_2) at supercritical conditions, i.e., above its critical temperature (T_c=304.1 K) and critical pressure (p_c=7.38 MPa) (SC-CO_2), could be a selective inert solvent, useful to isolate a high-purity derivative while avoiding its thermal damage, and easily removed by decompression to obtain the derivative completely free of solvent. The development and scale-up of a process using SC-CO_2 as solvent to recover derivatives needs experimental data and models for the physicochemical properties, particularly the solubility (mole fraction) of the derivative in SC-CO_2, which is the most relevant thermodynamic constraint. The objective of this work is to summarize and model experimental solubility data of 1,4-naphthoquinone derivatives in SC-CO_2 measured by our research team with a novel semi-empirical model, based on the equation of Chrastil, that incorporates molecular connectivity indices to correlate and predict the solubility for a family of compounds in a single equation with SC-CO_2 density and five indices calculated from solute structure. Our results indicate that the solubility of 1,4-naphthoquinone and eight derivatives can be correlated within one order of magnitude (root mean square deviation≤44%).

Biography

Juan C de la Fuente has completed his PhD in the Chemical Engineering Pilot Plant (PLAPIQUI) from Universidad Nacional del Sur (Bahia Blanca, Argentina) and Postdoctoral Studies at the Technical University of Delt, Netherlands. He is In-Charge of the Laboratory of Process Thermodynamics at the Federico Santa María Technical University, Chile. He has published more than 50 papers in reputed journals related to experimental and modeling of high-pressure phase equilibria.

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High performance phosphite ligands containing various numbers of structural units for n-regioselective hydroformylation of olefins

Baoxin Zhang, Detlef Selent and Armin Börner
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In comparison to phosphines, phosphite is stubborner ligands towards oxidation and therefore finds numerous catalytic applications at each scale. Especially in Rh-catalyzed regioselective hydroformylation of internal olefins, they are indispensable in the isomerization in favor of linear products. Starting from a prototype of all monophosphites tris(2,4-di-tert-butylphenyl) phosphite, which has already been applied in an industrial scale, a new type of polyphosphites containing two and four the similar structural units were prepared. Their catalytic performances as well as hydrolytic stabilities were compared. In Rh-catalyzed hydroformylation of n-octenes, when the phosphite unit of the ligands was increased, the best yield was obtained from the reaction with the biphosphite. The n-selectivity is improved with the increased phosphite moiety, whilst the activity decreases. The regioselectivity is kinetically controlled. Lowering syngas pressure benefits the n-selectivity but decreases the catalyst activity. Besides, the hydrolysis pathway of one of the prepared biphosphites was clarified with in situ NMR spectroscopy. Surprisingly, its first step degradation was conducted simultaneously through three routes. The biphosphite cannot build a metal complex in a chelating manner. Instead, a binuclear Rh-complex was formed, which can further stabilize the ligand towards hydrolysis.

Biography

Baoxin Zhang has completed his PhD majoring Organometallic Chemistry from Technical University of Darmstadt in Germany. He is currently a Research Fellow at Leibniz Institute for Catalysis (LIKAT) in Rostock. In the laboratory of Evonik Advanced Catalysis, he is doing research in homogeneous catalysis for hydroformylation and development of phosphorus ligands.

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Visible-light-assisted peroxymonosulfate activation and novel mechanism for degradation of contaminants over g-C_3N_4 coordinating with iron(II) phthalocyanine catalyst

Tiefeng Xu, Fei Wu, Wangyang Lu, Nan Li and Wenxing Chen
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Recently, Peroxymonosulfate (PMS)-based Advanced Oxidation Processes (AOPs) have received increasing attention because of their capability and adaptability in decontamination. The couple of solar light and PMS activation is an environmentally friendly and efficient strategy for environmental remediation. Herein, the iron hexadecachlorophthalocyanine (FePcCl16) was used to coordinate with graphitic carbon nitride (g-C_3N_4), which was functionalized by pyridine-based ligand Isonicotinic Acid (INA) to prepare a distinctive catalyst, g-C_3N_4-INA-FePcCl16. The experimental results revealed that g-C_3N_4-INA-FePcCl16 can activate PMS efficiently for the elimination of Carbamazepine (CBZ) under visible light irradiation over a wide pH range. Upon irradiation with visible light, CBZ was destroyed by the solider g-C_3N_4 with generated sulfate ($SO_4^{\bullet-}$) and hydroxyl (•OH) radicals, on the other hand, high-valent iron (Fe (IV)=O) species accompanied by $SO_4^{\bullet-}$ and •OH radicals were produced by excited-state FePcCl16 (*FePcCl16) during oxidation, which is different from a traditional PMS activation system. The axial pyridine-based ligand was protected under the FePcCl16 macrocyclic structure shield. Noteworthy, in the absence of visible light, g-C_3N_4-INA-FePcCl16 showed a higher catalytic performance than pure g-C_3N_4, FePcCl16 and a mechanical mixture of the two. This study allows for the construction of an effective and environmental catalytic system, which can be applied to purify water that contains refractory pollutants.

Biography

Tiefeng Xu has graduated in Textile Fiber Materials & Processing Technology, Zhejiang Sci-Tech University, China. Her research interests are focused on photoelectrochemistry, photocatalysis and photoreactors.

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Carlos Zambra et al., J Chem Eng Process Technol 2018, Volume 9
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Increases of the polyphenols concentration in the aqueous phase of the olive oil wastes by biocatalysis

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The intake of natural antioxidants and waste valorization are issues of great importance for improving human health and achieve a modern and efficient industry. Powerful natural antioxidants can be found in high concentrations in liquid waste from the olive oil industry. In this work, the effect of enzymes to increase the polyphenol concentration of the aqueous phase from olive oil wastes (alperujo) was studied. The high concentration of fiber in this waste suggest that biocatalysts with cellulases would useful for obtain an increase of the polyphenols concentration. Two commercial enzymes were used in different rate and concentrations. The total polyphenol content and the presence of free carbonyl group (reducing sugars) was determined by colorimetric methods with the Folin-Ciocalteu and the 3,5-Dinitrosalicylic acid (DNS) reagent, respectively. A liquid-liquid process enzymatic assisted was carry out by one hour at 50 °C and increased the phenolic content up to 1000% compared with the same test without enzymes. Use enzymes improve significantly the polyphenol concentration of the aqueous phase in olive oil wastes. The enzymes can be used to catalyze polyphenols extraction process from the olive oil wastes and thus to make the process more efficiently and economically sustainable.

Biography

Carlos Zambra has his expertise developing mathematical models and numerical simulations. His main interests are in the problems that involve chemical and biochemical reactions and new process such as liquid-liquid extractions, membrane perstraction, pervaporation and membrane distillation.

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Isiaka A Owolabi et al., J Chem Eng Process Technol 2018, Volume 9
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A new type of amino amide organocatalyzed enantioselective crossed aldol reaction of ketones with aromatic aldehydes

Isiaka A Owolabi[1], Madhu Chennapuram[1], Chigusa Seki[1], Yuko Okuyama[2], Eunsang Kwon[3], Koji Uwai[1] and Hiroto Nakano[1]
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A new type of amino amide organocatalysts A was designed and synthesized from commercially available amino acids and polycyclic aromatic amines. The prepared multifunctional organocatalysts A explored as a new class of catalysts with distinctive properties such as easy synthesis, stable in air, and the potential for convenient alteration of the steric sites. Their catalytic activities were examined in enantioselective crossed aldol reaction of various acyclic and cyclic ketones 2 with aromatic aldehydes 3 to afford the corresponding chiral anti-aldol adducts 4 that is a versatile precursor for the synthesis of chiral biologically active compounds and drug molecules.

Biography

Isiaka Alade Owolabi received his MTech. degree in 2015 from Tshwane University of Technology, Pretotia South Africa. He later joined the Graduate School of Engineering, Synthetic Organic Chemistry Laboratory at Muroran Institute of Technology as a Ph.D. student under supervision of Prof. Hiroto Nakano in 2016. His research interest is organocatalytic asymmetric organization.

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Enzyme-catalyzed synthesis of sugar esters in glucose-based deep eutectic solvents with high pressure CO_2

Dong-Woo Shin and Yoon-Mo Koo
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Sugar based esters have been widely used as non-toxix, non-ionic and highly biodegradable surfactants in food, medical and cosmetic industries. The conventional chemical or enzymatic sythesis of these esters were carried out in organic solvents with a certain degree of environmental concerns. Various novel solvents such as ionic liquids and supercritical fluids have been investigated for synthesis of sugar esters with an intention of an productivity enhancement. However, these solvents also have obvious limitations such as high price, toxicity and requirement sophitcated facilities. In this study, Deep Eutectic Solvents (DES) derived from choline chloride (ChCl) and various Hydrogen Bond Donors (HBD) were investigated for the lipase-catalyzed synthesis of sugar fatty acid esters. In order to overcome the high viscosity of DES system, high pressure CO_2 was tried as co-solvent for sugar ester synthesis. The results showed that the synthesis productivity in glucose-based DES was higher than that of the conventional solvent due to the enhancement of substrate solubilty and lipase activity in DES solvent.

Biography

Dong-Woo Shin is currently a PhD student at Department of Biological Engineering, Inha University. His studies focus on the enzymed-catalyzed reactions in ionic liquids, DES and supercritical solvents.

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Deoximation reaction by immobilized ionic liquid catalyst

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Oximes are used for purification of carbonyl compounds as well as to protect carbonyl compounds in the synthesis of carbonyl compounds. Oximes can be also synthesized from noncarbonyl compounds. Various methods, including acid-catalytic hydrolysis, reductive deoximation and oxidative deoximation have been developed for these preparations of oximes, ketones and aldehydes as its byproducts. However, these conventional methods pose environmental concerns regarding release of chemical pollutants. Therefore, the development of clean and highly efficient catalytic process for deoximation reactions is needed. In this study, immobilized ionic liquid resin (Im-IL-resin) which has carboxylic functional group was synthesized and evaluated for the deoximation reaction. The synthesized resins were characterized by FT-IR, SEM and TGA. Im-IL-resin and commercial Amberlyst-15 resin were compared for the deoximation both in batch and column reactor. Although deoximation yield using Im-IL-resin was similar to that of commercial acidic catalytic resin, Amberlyst-15, the deoximation reaction rate obtained was at least two times higher than that of Amberlyst-15 in batch reaction. In addition, the products could be efficiently separated in reactive column packed with Im-IL-resin whereas the products were not able to be separated with commercial Amberlyst-15 resin.

Biography

Chul Shin has graduated from Inha University with BE degree in Biological Engineering in 2017. He is currently enrolled in Master's program at Department of Biological Engineering, Inha University.

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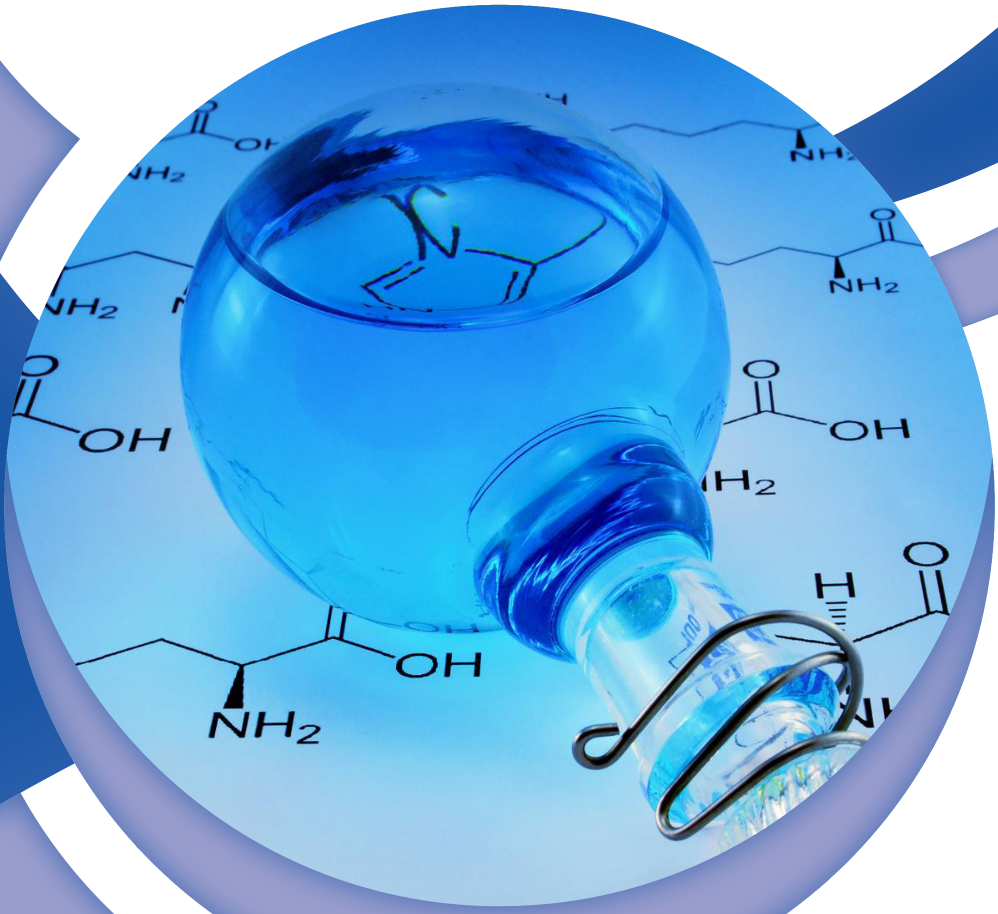

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Stable zirconia based catalyst for production of biofuels from waste cooking oil with high free fatty acid contents

Rabya Aslam
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Waste cooking oil is valuable and cheap feedstock for the production of bio-fuels as compared to virgin edible oil. It can not only help to reduce environmental impacts of waste cooking oil but also can contribute to the future energy demand. Both alkaline and acidic catalyst may be used for trans-esterification of waste cooking oil to biofuel. In most cases, sodium hydroxide and potassium hydroxide are used as alkaline catalyst and mineral acids are used as acidic catalysts in homogeneous reaction, because of their higher reaction rates, availability and low cost. However, recovery of catalyst is difficult in this process. Moreover, in the case of waste cooking oil which contains relatively high percentage of free fatty acid, alkaline catalysts are prone to the saponification reaction which reduces the biodiesel conversions. In order to cope up with low biofuel conversion, slow reaction rates, activity of solid catalysts are evaluated in this work. The activity of in house synthesized zirconia is studied by varying reaction conditions such as time, temperature, alcohol to oil ratio. Effect of modification of zirconia to increase its alkaline nature is also studied by impregnating Sr, Ca, and Mg metal on zirconia. It was found the alkaline modified zirconia results in better yield as compared to simple zirconia. Additionally, the synthesized biodiesel was fully characterized with respect to density, kinematic density, iodine values, acid values, carbon residue, pour points, flash points, etc. and was compared with literature.

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