



V-CHEM2023

4th Edition of

Catalysis, Chemical Engineering & Technology

Virtual

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About V-CHEM2023

After the success of the 3rd edition now we are announcing the '4th Edition of Catalysis, Chemical Engineering and Technology Virtual' which will be held on "17-18 November 2023".

The aim of the V-CHEM2023 is to provide a promote quality research community of researchers, developers, scientists, and students from research areas of Catalysis and Chemical Engineering to share their research experiences and indulge in interactive discussions and technical sessions in the field of Catalysis, Chemical Engineering and Technology.

The event will be useful in finding the right partners, looking at new projects, discovering reality, and interacting with other catalysis and chemical experts, to understand their challenges and how they solve problems. It will be a good platform to exchange ideas and experiences and learn from each other. Hopefully, this meeting will bridge new collaborations with like-minded people. In addition to the conference's academic and professional pursuits, we hope you will have valuable professional development at this summit.

We're looking forward to an excellent meeting with scientists from different countries around the world and sharing new and exciting results in V-CHEM2023

ABSTRACTS BOOK

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New Codification Approach in Order to Predict and Access the Phase Behavior Profile of a Generical Chemical System

G. V. S. M. Carrera^{1*}, A. V. M. Nunes¹, J. M. S. S. Esperança¹, T. Casimiro¹, A. Aguiar-Ricardo¹

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Abstract

The global environmental, social and economic framework claims for straightforward approaches in order to design and build-up of sustainable chemical processes. Extractions, distillations and reactions are examples where the virtual infinite combinations of chemicals, its proportions and temperature/pressure (TP), hinders the access to optimized conditions by trial and error. The use of chemoinformatic approaches aids on that matter. The use of a new tailor-made codification approach and an appropriate algorithm unveils structural characteristics, at given TP responsible for a certain phase behavior profile. A generical chemical system in Liquid-Liquid equilibrium integrates an ionic liquid (IL) and two organic molecules.

The MOLMAP [1] codification technology comprises the pattern of activation of all the atoms, of a generical chemical system, in a *Kohonen* network, accounting its respective proportions. Each atom's position in the network depends on its atomic property's profile. The Random Forest (RF) algorithm, is used to build a relationship between a chemical system's configuration and the phase behavior profile, input and output, respectively. RF learns with examples (datapoints). A datapoint corresponds to a certain chemical, from a given mixture, at particular TP. Two complementary models were built (IL-rich and IL-poor phases). Both model's predictive ability, evaluated with an independent test set, is excellent with R^2 and MAE of 0.95 and 0.042 (IL-poor) and 0.94 and 0.048 (IL-rich). This approach anticipates interesting perspectives on chemical processes design.

[1] Carrera, G. V. S. M.; Inês, J.; Bernardes, C. E. S.; Klimenko, K.; Shimizu, K; Lopes, J. N. C., *ChemPhysChem*, 2021, 22, 2190-2200.

Biography

Gonçalo Carrera initiated his PhD in 2004 in NOVA University (FCT/UNL), after the completion of his Diploma studies in Applied Chemistry. The PhD comprised chemoinformatic/organic-chemistry profiles (2009). The postdoctoral activity was initiated at that stage in the context of a European ERA-CHEM project and proceed with a postdoctoral individual grant by Portuguese Foundation for Science and Technology (FCT/MCTES). The author is currently an FCT/UNL researcher and was awarded as principal investigator with an FCT/MCTES project (2018-2021). He has published 28 peer-review papers, 3 book chapters and 12 other publications, including a cover-feature. He has presented/participated with/in 18 oral communications.

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Towards More Environmentally Friendly Chemical Synthesis Using Alternative Solvents

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Abstract

For over more than 40 years now, since launching of the first industrial plant utilizing carbon dioxide as a solvent to extract caffeine from coffee, the field of supercritical fluids has been developing at a very high pace. The high sensitivity of the density, thus also many thermophysical properties, of supercritical fluids with only slight changes in operating conditions (pressure or temperature) has led to their many technological applications, spreading over various areas of research.

In the light of global concerns over climate change, carbon dioxide utilization, preferably combined with other sustainable solutions, gains further advantage. Over the years, application of alternative solvents, solo or in mixed systems, for greener chemical processes has attracted considerable attention. Here, examples of the greener organic synthesis will be presented, showing advantages of coupling dense carbon dioxide with other environmentally friendly solvents such as ionic liquids or eutectic mixtures. Carbon dioxide will be employed in a role of a substrate, reaction medium, or solvent in downstream processing for product separation.

Biography

Małgorzata Ewa Zakrzewska has two MSc degrees from the Gdańsk University of Technology, Poland, and PhD degree from the NOVA School of Science and Technology, Portugal. Currently, she is a researcher at the Associated Laboratory for Green Chemistry (LAQV) of the Network of Chemistry and Technology (REQUIMTE), at NOVA, and leads an exploratory project in a chemical engineering field, funded by the Portuguese National Funding Agency for Science, Research and Technology. Over the years, she participated in 7 national and 2 European projects, and co-authored 25 publications. She has served as an invited editor in four special issues for reputed journals.

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Comparative Study of In-Situ Catalytic Pyrolysis of Rice Husk for Syngas Production: Kinetics Modelling and Product Gas Analysis

Bridgid Chin Lai Fui

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Abstract

The concerning rate of global non-renewable or fossil energy resource depletion has been driving us in the direction of green energy. In order to meet the energy needs of a constantly expanding global population and industry, we are forced to pay considerable attention to renewable resources in light of the on-going and impending global energy crisis. Since rice husk that contributes 20% of the mass percentage possess low energy and bulk density, this makes the rice husk not a viable feedstock for direct combustion. Hence, catalytic pyrolysis is an alternative solution to convert this feedstock to renewable energy sources. In this study, the pyrolysis of rice husk in the presence of three different types of catalysts (nickel, natural zeolite, and coal bottom ash) for syngas production were investigated by thermogravimetric analysis coupled with mass spectrometer. The catalyst to rice husk ratio of 0.1 was pyrolyzed at different heating rates of 10, 20, 30, and 50 K.min⁻¹ in the temperature range of 323 K–1173 K. Furthermore, X-ray diffraction (XRD), Brunauer-Emmett-Teller (BET), field emission scanning electron microscope (FESEM) and X-ray fluorescence (XRF) were employed to understand the physiochemical properties and activities of the catalysts before and after pyrolysis of rice husk. Lastly, four different types of kinetic models such as first-order Coats-Redfern equation, Friedman, Flynn-Wall-Ozawa (FWO) and Kissinger-Akahira-Sunose (KAS) were employed to determine the activation energy (E_A). The kinetic analysis revealed that the E_A values reduced when catalysts were introduced into rice husk as compared to absence of catalysts in the pyrolysis process.

Biography

Dr. Bridgid Chin is an Associate Professor for Chemical and Energy Engineering Department for Curtin University Malaysia. She has successfully obtained her PhD from Universiti Teknologi PETRONAS (UTP) in year 2015. She is recognized for her creative contributions within the field of green technology particularly on the conversion of biomass and municipal solid wastes to renewable energy via thermochemical conversion which firmly focused on solving real-world problems particularly on mitigating climate change and developing clean energy. She has also published more than 60 international journal publications and presented several papers in national and international conferences.

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Research Progress in Catalytic Conversion of Low-Carbon Alcohols and Hydrocarbons to Aromatics and Gasoline

Keming Ji and Tao Li

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Abstract

Low carbon alcohols and hydrocarbons, represented by methanol and propane, are important products and by-products of coal and petrochemical industry. They come from a wide range of sources and are cheap and easily available. How to prepare high-value products such as aromatics and gasoline through further chemical conversion processes such as polymerization and cyclization has considerable economic benefits, and related research and application prospects are broad. In our study, by constructing different metal modified ZSM-5 molecular sieve catalysts, the acid strength and acidity type of the catalysts were modulated, thereby affecting the catalytic reaction network and product distribution of propane aromatization, resulting in different olefin and aromatic composition in the products. In another study, we screened and optimized the modified ZSM-5 catalyst. Through a large number of boundary condition tests and stepwise scaling up tests, we obtained a finalized methanol to gasoline catalyst. Using methanol as the raw material, we produced high-quality gasoline products, and the device operated stably for a long time. The above research is supported by the Youth Science Research Project of the Shanxi Basic Research Program (202103021223460).

Biography

Keming Ji (1987-), PhD, senior engineer, worked in Institute of Coal Chemistry, Chinese Academy of Sciences. The reporter has long been engaged in research in the fields of energy chemical engineering, and heterogeneous catalysis. He has published 23 papers in well-known journals, authorized 15 patents, and undertaken and participated in 8 projects with a total project amount of 1.4 million US dollars.

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Mesoporous Cathode Films for Electrochromic Smart Windows

Chi-Ping Li and Cheng-Yen Tsai

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Abstract

Template-assisted sol gel chemistry provides a versatile approach to introduce order and porosity into nanostructured materials. However conventional evaporation induced self-assembly techniques are not easily scaled to produce films with sufficient thickness over large areas at the throughput required by electrochromic windows. The principles of sol gel chemistry may be deployed using ultrasonic spray deposition (USD) for scalable synthesis of nanocrystalline WO₃ films with unrivalled electrochromic performance are demonstrated. Systematic manipulation of sol chemistry enabled the production of mesoporous films with high specific surface area (>100 m²/g), mean pore sizes of ~5 nm, and narrow pore size distributions. Film thickness is found to be proportional to the sol concentration and number of spray passes, and various combinations are shown to produce films capable of modulating >98% of incident solar radiation in the visible spectrum (450–900 nm). Elimination of haze enables full transmission in the bleached state, while the broadband coloration is attributed to the exceptionally high charge density (>120 mC/cm²). The materials have good switching speeds which improve with specific surface area, and the long term durability is promising.

Biography

Dr. Chi-Ping Li received his PhD of Materials Science from Colorado School of Mines (USA) in 2014 and followed by postdoctoral research in National Renewable Energy Laboratory (NREL, USA) in 2015. He joined Department of Chemical Engineering in National United University in Taiwan as an assistant professor in 2018. His research interests are mainly focused on synthesis of nanostructured films, nanocomposite and nanoparticles. Those materials are used in electrochromic windows, lithium batteries, organic photovoltaics and LED encapsulants. His goal is to overcome the challenges and produce great but low cost materials in the fields of green and renewable energy.

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Photodegradation of a Model Pollutant in a Slurry Photocatalytic Membrane Reactor with Vertical Filter and External Membrane.

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Department of Environmental Engineering (DIAM), University of Calabria, Via P. Bucci, Cubo 44/A, Rende (CS), Italy.

Abstract

Wastewater treatment plays a strategic role in mitigating the potable water shortage that is crucial for economic and health reasons, considering the worldwide population growth. A new photocatalytic membrane reactor configuration, based on a vertical filter and an external nanofiltration (NF) membrane, was designed built and tested [1]. The hydraulic and photocatalyst separation behavior of the vertical filter, the ability of a nanofiltration membrane to retain the gemfibrozil (GEM) and the overall performance of the GEM photodegradation in a batch operation mode have been studied. This system allows the recycle in the photoreactor of the pollutants to produce a treated water with quality higher than a submerged membrane. Indeed, the membrane is external to the photoreactor therefore, it cannot be degraded by light irradiation. The advantage of using a vertical filter inside the reactor consists in retaining the photocatalyst particles while ensuring greater flux compared to a submerged membrane (200 vs 40 L m⁻² h⁻¹ average values).

The obtained results showed a rejection of 40-50% using a Fortilife NF membrane at pH 8 with less filter clogging than pH 9.7 (90% rejection). The obtained overall performance (80% reduction of gemfibrozil concentration) can be further improved with a modification of the various operating parameters.

References:

[1] Molinari R., Limonti C., Lavorato C., Siciliano A., Argurio P. Upgrade of a slurry photocatalytic membrane reactor based on a vertical filter and an external membrane and testing in the photodegradation of a model pollutant in water, *Chemical Engineering Journal*, 451, 1, 2023, 138577.

Biography

Cristina Lavorato has completed her PhD in Chemical Engineering and Materials from University of Calabria, Italy, in collaboration with the Polytechnic University of Valencia, Spain. She continued her research activity as postdoctoral fellow and research fellow in Department of Environmental Engineering, University of Calabria, Italy. She has published various papers in reputed journals. She received award for her research activity by the Anassilaos association and the best paper award in recognition of a paper: "The Evolution of Photocatalytic Membrane Reactors over the Last 20 Years: A State of the Art Perspective" from the *Catalysts* journal.

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Nanoporous Composites for Environment, Catalysis, and Medicine

Raffaele Ricco¹

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Abstract

Nanoporous materials encompass a broad category categorized as microporous (below 2 nm), mesoporous (2 to 50 nm), and macroporous (above 50 nm). Porosity in materials is crucial in three key areas: the environment, catalysis, and medicine. Nanoporous materials can capture a wide range of harmful organic and inorganic substances that contaminate soil and water. Porous substrates significantly increase surface area for enhanced reactant contact in catalysis. Additionally, porous particles serve as reservoirs for therapeutic compounds in drug delivery.

Microporous materials, specifically, have gained popularity due to their ability to accommodate small molecules. Over the past decade, porous coordination polymers (PCPs), commonly known as Metal-Organic Frameworks (MOFs), have emerged as a highly exciting class of porous materials. MOFs offer exceptional surface areas (exceeding 1000 m²/g), customizable porosity, and the flexibility to incorporate inorganic nodes and organic linkers. Importantly, they can host guests larger than their pore size through self-assembly, facilitating the creation of composites with unique properties.

MOFs have found applications in environmental remediation, such as detoxifying water from hazardous transition metals, serving as scaffolds for advanced, recoverable metal and bio-catalysts, and acting as platforms for drug delivery, gene transfection, therapeutics storage, and antibody-based sensing.

This communication highlights innovative applications of nanoporous MOF-based composites and offers a forward-looking perspective on the future of this dynamic field, which continues to unfold its full potential.

Biography

Raffaele Ricco has completed his PhD from the University of Padova, Italy, and worked at CSIRO (Australia), and TU Graz (Austria), before becoming Assistant Professor at the Asian Institute of Technology (AIT) in Thailand, teaching in the academic program on Bio-Nano Materials and acting as chair of the Medical Engineering program. In the last decade he has worked in the field of Metal-Organic Frameworks, publishing more than 50 papers in international journals.

Revolutionizing Penicillin Antibiotic Detection in Milk: Analysing the Performance and Eco-Friendly Attributes of Amino-Functionalized Magnetic Silica Nanocomposites in Magnetic Micro-Solid Phase Extraction

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Abstract

This study explored the synthesis and application of amino-functionalised magnetic silica ($\text{Fe}_3\text{O}_4@\text{mSiO}_2\text{-NH}_2$) nanocomposite as a selective sorbent for the extraction of penicillin antibiotics (PENs) from milk samples via magnetic micro-solid phase extraction (M- μ -SPE). The physicochemical characteristics of the 10 synthesized sorbent were evaluated through important spectroscopy analyses. The adopted M- μ -SPE conditions were: 25 mg of $\text{Fe}_3\text{O}_4@\text{mSiO}_2\text{-NH}_2$; pH 4; 3 min of extraction time; 1 min of desorption time; acetonitrile as the desorption solvent; 10 % of salt addition; and 30 mL sample. Under the optimum conditions, the developed method demonstrated satisfactory from 10 to 500 $\mu\text{g/L}$ ($r^2 \geq 0.9986$), low limits of detection (2.5-3.1 $\mu\text{g/L}$), high analytes recovery (85.2-106.7%), and good precision ($\text{RSDs} \leq 8\%$, $n=5$). The proposed method is rapid, simple, inexpensive, and shows good sensitivity when compared to previously developed methods. This study provides new insight into the development of a new sorbent for PENs and new microscale sample preparation for monitoring PENs in complex milk matrices.

Biography

Dr Noorfatimah Yahaya was trained as an analytical chemist in the field of separation science, specifically in developing green sample preparation and extraction techniques combined with chromatography/electrophoresis to analyze emerging pollutants and important pharmaceutical compounds. Several advanced materials, such as molecularly imprinted polymers, biopolymers, silica, carbon-based sorbents, and magnetic nanoparticles have been conceived in her research. Presently, she is an Associate Professor in the Department of Toxicology at the Advanced Medical and Dental Institute of Universiti Sains Malaysia. Over the years, she and her students have made substantial contributions to analytical and bioanalytical method development and the application of mass spectrometry in conjunction with green separation technologies.

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Polyterpene Oxidation Assisted by Molybdenum Catalysts Derived From Acyl-Hydrazone Ligands

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Jana Pisk¹

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²Department of Chemistry, Institut Universitaire de Technologie Paul Sabatier, University of Toulouse, Av. G. Pompidou, BP20258, CEDEX, F-81104 Castres, France.

³LCC-CNRS, Université de Toulouse, CNRS, UPS, CEDEX 4, F-31077 Toulouse, France.

Abstract

In front of climate change, depletion of fossil resources and the current geopolitical crisis, Europe is trying to find sober ways to use energy and fossil resources. This policy is being pursued in all areas, including academic research. Chemical processes often require the use of organic solvents, mainly derived from fossil resources. There is an urgent need to find ways to synthesize chemicals, i.e. both inorganic and organic compounds, using solvent-free processes. For this reason, the catalysts presented here are prepared not only by the classical solvent-based method but, more importantly, by mechanochemical synthesis that minimizes the use of solvents. Molybdenum-based catalysts have been recognized as active and selective in epoxidation reactions, and our further aim was to test them in polyterpene oxidations.^{1,2} Polyterpenes are very interesting substrates applied in the pharmaceutical and fragrance industries. For example, terpenic alcohols are abundant, renewable, and attractive raw materials used for the synthesis of fine chemicals, fragrances, perfumes, and agrochemicals. Recently, the catalytic activity of Mo and V compounds for the linalool oxidation reactions was investigated.³ The choice of benign oxidizing agents, such as *tert*-butyl hydroperoxide, and minimal catalyst loading are in line with green chemistry principles, emphasizing the use of environmentally friendly reagents and the reduction of waste and energy consumption in chemical processes.

Overall, this research demonstrates a commitment to finding innovative and sustainable solutions in chemistry, highlighting the importance of adopting green chemistry practices and exploring renewable resources to meet the needs of various industries.

¹ J. Pisk, D. Agustin, V. Vrdoljak, R. Poli, *Advanced synthesis & catalysis*, **353** (2011), 16, 2910.

² J. Pisk, D. Agustin, V. Vrdoljak, *Catalysis communications*, **142** (2020), 106027

³ A. A. H. Haidar, D. Agustin, *Tetrahedron Green Chem*, **2** (2023), 100029.

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Biography

J. Pisk received her doctorate in chemistry in 2012. In 2010, she spent a year at LCC Toulouse and IUT P. Sabatier Toulouse III, France, where she learned the basics of catalysis. She was a Marie Curie Cofund fellow and postdoctoral researcher at LCC, Toulouse (project “Diligent search for chemical bio-sources: solvent-free homogeneous and heterogeneous oxidation processes catalyzed by polyoxometalates”). She has been an assistant professor at the Faculty of Science, Zagreb, since 2018 and will be an associate professor from 2023. Her main interest is the coordination chemistry of molybdenum and vanadium and the study of the catalytic properties of the obtained materials.

Origin of the Apparent Particle-Size Limit in Gamma-alumina:

Karl Sohlberg^{1,2}

¹*Department of Chemistry, Drexel University, Philadelphia, PA, USA.*

²*Department of Materials Science and Engineering, Drexel University.*

Abstract

Gamma alumina has long been a material of enormous technological significance, being produced in high volumes for use as an adsorbent, catalytic support, and catalyst. Consequently, its structure and durability have been of sustained interest. Full resolution of the atomic-scale structure of gamma alumina has been stymied by the absence of large single crystals for X-ray analysis. Particle sizes in samples of gamma-alumina are routinely sub-micron. Attempts to form larger particles invariably fail. Extended structures of the material have only been produced in the form of thin films, generated by annealing a layer of amorphous alumina on a sapphire substrate. The apparent limitation of gamma alumina to very tiny particle size appears to defy the principle of Ostwald ripening; whereby small particles aggregate and coalesce into larger particles to minimize surface energy. This talk will describe new insight into the physical origin of the limit on particle size. It is well known that gamma alumina is an intrinsically defective material, containing cation vacancies and/or hydrogen atoms to maintain the balance of valence. First principles calculations show that the migration of defects from the bulk to the surface is energetically preferred. Using the results of these first principles calculations as input, analytic modeling shows that, compared to a single particle, two or more smaller particles of the same total volume realize greater stabilization from the migration of defects to the surface because of the greater surface area. This energetic benefit of smaller particles negates the energetic benefit that drives Ostwald ripening.

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Biography

Karl Sohlberg is an Associate Prof. of Chemistry at Drexel University. His broad research area is theoretical and computational materials chemistry, with specific research programs in molecular nano-devices and complex catalytic materials. Before joining the Drexel faculty in 2000, he was an Oak Ridge Associated Universities postdoctoral fellow at Oak Ridge National Lab. Earlier, he held postdoctoral appointments at The Johns Hopkins University and Brigham Young University. He received his Ph.D. in physical chemistry from the University of Delaware under the direction of Krzysztof Szalewicz. At Drexel, he teaches molecular modeling, quantum chemistry, and mathematical and computer skills for chemists.

Functionalized Magnetic Biocomposite for Efficient Adsorption of Anionic azo dye: Spectroscopic and Kinetic Studies

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²*Department of Science, Faculty of Education, Dicle University, 21280 Diyarbakır, Turkey.*

Abstract

A novel magnetic biocomposite (MBC) was fabricated using raw biomass (pomegranate waste) and metal chlorides by co-precipitation method. The resulting product, MBC was characterized by Fourier transform infrared spectra (FTIR), X-ray diffraction (XRD), and vibrating sample magnetometer (VSM). The adsorption performance of the MBC was tested with removal of anionic azo dye (congo red) from aqueous solution. Adsorption kinetics experiments were carried out and the data were well fitted by a pseudo-first-order equation. The results revealed that the MBC could efficiently adsorb the azo dyes from aqueous solution, and the spent adsorbent could be recovered completely by magnetic separation process. Therefore, the prepared magnetic biocomposite could thus be used as promising adsorbent for the removal of azo dyes from polluted water.

Biography

Dr. Hasan SAYGILI is currently working as an Assoc. Prof. in the Chemistry and Chemical Process Technology Department, Vocational School of Technical Sciences, Batman University, Turkey. He has an experience in the field of carbon-based materials for environmental applications. He holds a PhD in activated carbon production from biowastes from Dicle University, Turkey. His primary research interests include carbon nanomaterials, waste minimization, environmental pollution, hydrothermal carbonization, cleaner production technology and wastewater treatment. He has published 26 SCI papers.

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Biofuels from Algae and Microorganism

Gaweł Sołowski¹

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Abstract

The European sustainability plan for 2030 assumes conversion from fossil fuels into renewable sources. Therefore many countries besides Europe published many plans of using microbial and algae as relevant parts, also. Both methods often combine themselves for optimization. Butanol and ethanol can be obtained by acetone-butanol-ethanol bacteria but more solutions are from algae, while hydrogen is from dark fermentation. Algae are lipid-rich plants and after biophotolysis and biosorption can be then fed for dark fermentation. In dark fermentation, the rest are partially converted by anaerobic bacteria into hydrogen and unconverted for biodiesel.

Biography

Gaweł Sołowski completed his Master's Degree at the Silesian University of Technology at Gliwice in 2014. He has been a Ph.D. student at the Institute of Fluid Machinery of the Polish Academy of Science since 2014. He has been serving as an assistant editor in Open Chemistry in de Gruyter Open and published 61 publications including 26 in reputed journals. From 2022 he works as a specialist at Bingol University in Turkey. He is a specialist in dark fermentation and polymer membranes. He is also interested in phytomedicine.

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The Co-N Bond Cleavage in The Adenosyncobalamin Cofactor in Advance to Glutamate Mutase and Methylmalonyl-Coa Mutase Processes

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^aDepartment of Chemistry, Columbia University, Broadway 3000, New York, New York 10027, USA.

^bNatural Sciences Department, Hostos Community College, 500 Grand Concourse, Bronx, New York 10451, USA.

Abstract

CASSCF geometry optimization of the vitamin B12 active forms plus substrates joint models have been performed. These joint models include the adenosylcobalamin or methylcobalamin cofactors of the vitamin B12, the substrate negative ion model of the studied processes' active substrates, and the histidine molecule.

The rupture of the Co-N axial bond and the removal of the axial ligand dimethylbenzimidazole take place under the joint influence of the histidine molecule, on the one hand, and of the negative ion of each bioactive substrate, which is participating in the enzymatic process. The process of the Co-N axial bond breaking occurs under the influence of partial electron density transfer from the highest occupied molecular orbitals HOMO1, HOMO2, and HOMO3, which are composed only of the atomic orbitals of the negative ion atoms of the substrates to the lowest unoccupied molecular orbitals LUMO1, LUMO2, and LUMO3, which represent antibonding molecular π -orbitals, composed from the atomic orbitals of the corrin ring and dimethylbenzimidazole ligand in the case of the adenosylcobalamin cofactor dependent processes. As a result, the Co-N axial bond is permanently elongated during the CASSCF geometry optimization until its complete rupture and until the removal of the dimethylbenzimidazole ligand from the central cobalt atom and the corrin ring is complete. The rupture of the Co-N axial bond in the adenosylcobalamin cofactors in Glutamate Mutase, Methylmalonyl-CoA Mutase, and Methionine Synthase processes occurs in the absence of an energy barrier.

Biography

Teodor Dumitrescu is a student who is passionate about Bio and Theoretical Chemistry. He performs research under the supervision of Dr. Tudor Spataru at Columbia University.



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