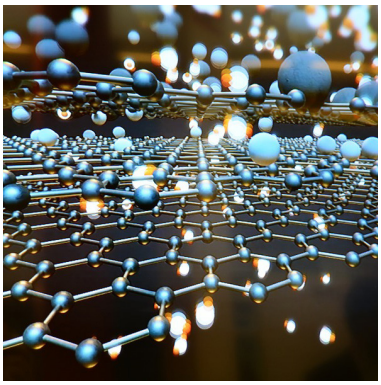
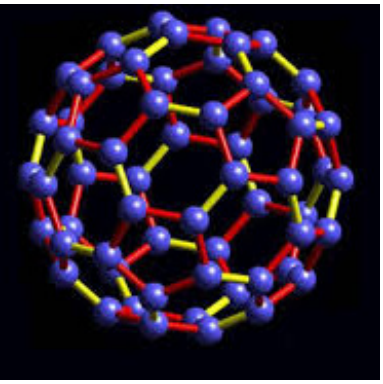
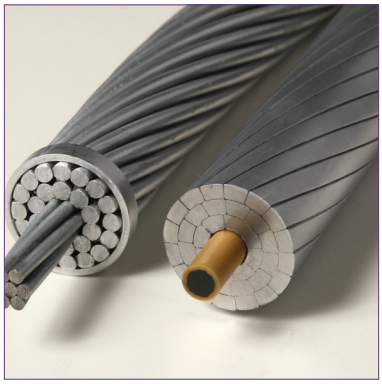
Scientific Tracks & Sessions
March 20, 2019

Materials Chemistry 2019







2nd International Conference on

Materials Science and Materials Chemistry

March 20-21, 2019 | London, UK

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Magnetic framework composites: Energy efficient materials for fine chemicals synthesis and fast adsorbent regeneration

Evgeny Rebrov
University of Warwick, UK

Composite magnetic catalysts and sorbents are leading candidates for catalytic applications under RF heating in flow. The development of supported catalysts with well-defined active structures that catalyse selective chemical transformations and have an additional functionality (e.g. light absorbing, microwave absorbing or magnetic properties) remains a major challenge. Successful development in this area could provide reactors and processes for synthetic routes and chemical products with optimal space-time yields, minimum waste production, minimum energy consumption, and minimum operating costs.

Ferromagnetic materials (like nickel ferrites) are known to generate heat when exposed to an alternating magnetic field in the radiofrequency range (RF). This property can be utilised for induction heating of a composite magnetic catalysts, where magnetic nanoparticles are embedded in the catalyst (sorbent) support. The control of magnetic material structure at the nanoscale is the key to increase performances and improve the energy efficiency under RF heating. Thanks to powerful characterization tools, we can now control critical catalyst parameters such as particle size, composition, shape, and particle-support interfaces. This has boosted numerous studies linking chemical processes, reactor design, nanostructures, and development of advanced kinetic models, paving the way for the rational design of nanostructured catalysts and structured reactors. In this lecture, recent developments in our lab in the area of magnetic framework composites and structured reactors will be discussed highlighting several examples of enhancement of reaction rate and selectivity under RF heating: from fine chemicals synthesis (direct amide synthesis and glucose isomerization in flow) to CO_2 capture and its subsequent transformation to solar fuels and chemicals.

Speaker Biography

Evgeny Rebrov got his PhD in Chemistry from Boreskov Institute of Catalysis in 1999. After 4 years of post-doctoral research work, he became Assistant Professor at Eindhoven University of Technology (the Netherlands). In 2007 he got a fellowship from the British Council-NWO partnership program in science and went to Cambridge University (UK). In 2009, he was appointed Visiting Research Professor at Wright State University (Dayton, Ohio). In 2010, he became Chair of Process and Reactor Engineering at Queen's University Belfast. In 2014, he took his present position at the University of Warwick. He is member of the Young Academy of Europe (YAE) and member of editorial board of AIMS Materials Science journal and member of international scientific committees of three international conferences. Evgeny Rebrov has published > 170 scientific papers in peer-reviewed journals and 9 book chapters (h-index =29). He is also co-founder and CTO at StoliCatalysts Ltd, an innovative award-winning SME, a spin-out of University of Warwick.

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Synthesis of EPDM rubber coconut leaves activated carbon composite for automobile application

Abhijit S Jadhav
AISSMS COE, India

This paper reports on usability of activated carbon obtained from coconut leaves (CL) as a filler to prepare Ethylene-propylene-diene monomer (EPDM) based composite for automobilebased application. The carbon is prepare and activated by phosphoric acid (H_3PO_4) as dehydrating agent and was sieved for mesh size of CL-355, CL-710, CL-500, and CL-53. The stoichiometric ratio of phosphoric acid to biomass is maintained as 3:1 for 300 g of batch size.CL-355 given optimised results for yield, methylene blue number, Iodine number and surface area found greater as compared with the CL-710, CL-500, CL-53. CL- 355. Hence CL-355 mesh size activated carbon was adapted for further study. SEM was studied to know the morphology of activated carbon. Compounding is carried out on a two-roll mill and at 160°C. As compared to commercially available carbon filler, the activated carbon derived from coconut leaves biomass waste responded better to the petrol swelling test. Activated carbon derived from coconut leaves was appeared to be the best for percent swelling and percent deviation in hardness. The composite prepared are of 40 parts per hundred (Phr) basis.

Speaker Biography

Abhijit S Jadhav is a founder faculty member of Department of Chemical Engineering, AISSMS College of Engineering, India. He earned a Bachelor of Chemical Engineering (1994), a Master of Engineering (2008), and is pursuing a PhD (Chemical Engineering) from Birla Institute of Technology, India. He has developed "STOPPER" a composite product from EPDM/Coconut leaves activated carbon in association with Pallavi rubber ltd. India for automobile application. He has conducted several lectures in Industry and colleges. For the past 20 years, Abhijit has taught various Chemical Engineering subjects in AISSMS College. His interests includes: interactive learning; scaffolding lessons for all skill levels; and incorporation of technical innovative ideas within his classroom. He is a member of the organization, "Institution of Engineers", "Indian Institute of Chemical Engineers", "Indian Society of Technical Education".

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Quantum and Monte-Carlo molecular dynamics investigations of the liquid anti-corrosive performance of a series of macrocyclic polyethers with a thiadiazolic core

Aziz Aboulmouhajir, A Mahsoune, K Sadik and **S Byadi**

Hassan II University, Morocco

The corrosion inhibitive performance, in acidic medium, of a series of macrocyclic polyether compounds containing a thiadiazolic core: n-MCTH (n=1-5) which differ by the oxygen number in the macrocyclic polyether part, was studied on the basis of their degree of planarity, their global quantum electronic molecular descriptors and their local electronic proprieties (Fukui indices, Electrostatic molecular potential, Natural population atomic charges, Natural bond orbitals interaction) as well as their deformation capacity to adhere onto the metal surface, by using DFT calculations and Monte-Carlo system dynamics simulation. The proton affinity locating the most favorable site of protonation was evaluated and the competitiveness between neutral and protonated species in vacuo and in aqueous solution was also considered. The molecule 5-MCTH was found more reactive in vacuo and in aqueous phase. Moreover, the Fe-(N9N10)-like interaction involving 5-MCTH was found to be the strongest, in accordance with electrochemical and gravimetric results.

Speaker Biography

Aziz Aboulmouhajir has completed his PhD in Molecular Modeling and spectroscopy, at the age of 25 years from Instelling Antwerpen University in Belgium with High Distinction. He is holder of the STAS Prize of the Royal Academy of Sciences, Letters and Arts of Brussels, in Belgium. For the last ten years, he was head of the Molecular Modeling and Spectroscopy E2MS Team at Chouaib Doukkali University. He is currently professor and director of several thesis projects in Molecular Recognition and spectroscopy in Hassan II University (Morocco).

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Science, technology and innovation (STI) in the age of globalization – including STI in materials sciences and materials chemistry

Aderemi Kuku
National Mathematical Centre, Nigeria

The talk starts with a discussion of the concept of globalization and how this affects the development of many areas of STI which pose global challenges that require to be global tackled and solved across geo-political, linguistic and cultural boundaries. it is noteworthy that these challenges need mathematical sciences for their in-depth study since mathematical sciences constitute the bedrock of all developments in STI. We thus discuss the role of mathematical sciences vis-a-vis other areas of science and technology and identify the four areas of Science and technology--basic sciences, applied sciences, classical or low technologies and high Technologies as concentric layers with diffuse boundaries with inner core of basic sciences and mathematical sciences as its innermost core such that theories from the inner core help to solve problems in applied sciences and technology while problems arising from the outer layers of technology and applied sciences provide the inner core with new structures, new concepts and new methods. We illustrate this phenomenon copiously with many examples from various technologies. Moreover, we identify the role of ICT (Information, Communication, Technology) as a unifying force for the development of STI thus turning the world into a global village. Furthermore, we observe that many developing countries are yet to produce a critical mass in any of the areas of science and technology mentioned above.

Next we focus six of the areas for which we need to pull global resources together to achieve more rapid global development: 1) Health and Well-being, 2) Food security and nutrition; 3) Sustainable Agriculture 4) Climate Change 5) Water and Sanitation. 6) Sustainable Energy and in particular 7) Materials Sciences and Materials Chemistry which constitute the theme of the conference. We will discuss progress so far made in research and smart technologies in these areas and identify the ways forward in this age of globalization to ensure that the benefit of such research and technologies reach all corners of our world.

Speaker Biography

Aderemi Kuku is the immediate past President of the African Academy of Sciences 2014-2017. He was the President of the African Mathematical Union during 1986-1995 and a Distinguished Professor at the National Mathematical Centre, Abuja,Nigeria. He was a Professor of Mathematics at the International Centre for theoretical Physics (ICTP), Trieste, Italy 1995-2003, and a member of the Institute of Advanced Study, Princeton, NJ, USA 2001-2004. He has over fifty years of University research and teaching experience and he is a foundation Fellow of the American Mathematical Society, Fellow of the World Academy of Sciences, European Academy of Arts Science and Humanities, Nigerian Academy of Science, and Foreign Fellow of the Mongolian Academy of Sciences.

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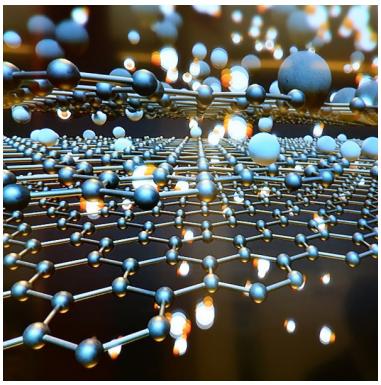

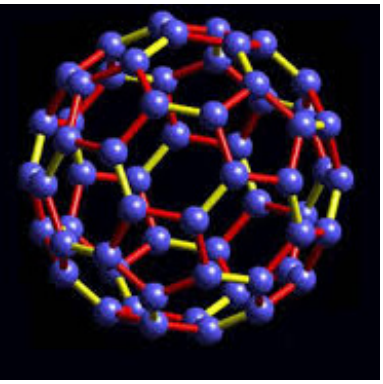

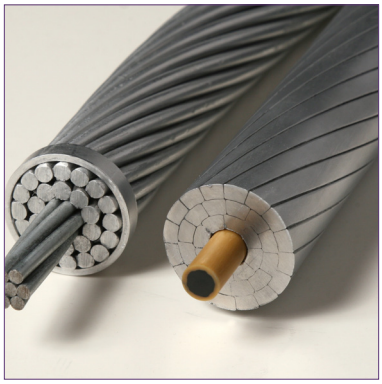

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Role of trioctylphosphine on quantum size effect in Ni nanolattice

Gunadhor S Okram
UGC-DAE Consortium for Scientific Research, India

Nickel nanoparticles are of special interest for their attractive potential applications in magnetic resonance imaging, magnetic fluids, catalysts, magnetic recording media, rechargeable batteries, optoelectronics, conducting paints, magnetic hyperthermia and other biomedical applications. When these nanoparticles are dispersed in a liquid medium for example, they tend to agglomerate/ disperse due to van der Waals or other attractive forces. Similarly, what kind of forces they may need to form their own periodic lattice in solid state and how this will influence their overall properties may be intriguing. We have investigated some of these aspects. They revealed that trioctylphosphine is responsible for their nanolattice formation, how the Ni atoms are arranged in these nanoparticles, how their electronic density of states changes, nearest-neighbour atoms are changed with particle size and why their quantum size effect is unique in heat capacity, not in electronic or magnetic properties. Some of these shall be discussed briefly.

Speaker Biography

Okram has completed PhD from Indian Institute of Technology, Bombay (1995), India. He has worked at several research institutes including National Institute of Materials Science, Tsukuba, Japan (1996-98) as STA Fellow before joining at UGC-DAE Consortium for Scientific Research, Indore, India as Scientist D in 2001. He has delivered over 61 invited lectures at various conferences, published over 210 papers that have been cited 985 times and his publication H-index is 16 and has been serving as a reviewer of several reputed journals.

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Waste to energy generation from distillery waste water

Rajendra S Raut
AISSMS COE, India

Molasses based distilleries are classified as "Red Category" because of the large volume of high strength waste water generated by them. Pollution caused by spent wash is one of the most critical environmental issues. Spent wash is one of the recalcitrant waste having extremely high COD (120000 mg/l), BOD (60000 mg/l), SS, inorganic solids, low pH, strong odour and dark brown colour. The problem of increasing amount of spent wash generation and stringent norms has resulted in development of new technologies for its effective and economical disposal.

Biomethanation is viewed as a complex ecosystem in which physiologically diverse groups of micro-organisms operate and interact with each other in a symbiotic, synergistic, competitive and antagonistic association. The anaerobic microbial food chain consists of mainly three functionally different groups of microorganisms. Following four pathways are involved in anaerobic digestion of organic wastes

• Hydrolysis: Hydrolysis break down macro organic materials such as carbohydrates, proteins and lipids, by incising water molecules into lower molecular weight fatty acids, amino acids and sugars.

• Acidogenesis: Acidogenic bacteria convert fatty acids, amino acids and sugars into organic acids, hydrogen, ammonia and carbon dioxide.

• Acetogenesis: Acetogenic bacteria convert organic acids, hydrogen and carbon dioxide into acetic acid, hydrogen and carbon dioxide.

• Methanogenesis: Methanogenic bacteria convert acetic acid, hydrogen and carbon dioxide into methane and carbon dioxide. Readily available CO_2 is used as an electron accepter. This reaction is slowest and the rate limiting step of the total anaerobic digestion process.

Generated methane gas is used as a fuel and cost saving by using methane in boiler or it is possible to make bottling of gas

Speaker Biography

Rajendra S Raut is a faculty member of Department of Chemical Engineering, AISSMS College of Engineering, India. He earned a Bachelor of Chemical Engineering (2000), a Master of Engineering from Institute of Chemical Technology, Mumbai. He has total 16 years of working experience in Chemical Engineering filed. For the past 6 years, Rajendra has taught various Chemical Engineering subjects for PG and UG in AISSMS College. His interests include: Energy Saving in plants, Energy Conservation, Heat Transfer; Mass Transfer, Alcohol and incorporation of technical innovative ideas within his classroom. He is a member of the organization "Indian Institute of Chemical Engineers".

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Conformational stability, vibrational spectral assignments, UV-Vis, NMR, NBO, HOMO-LUMO and NLO properties of a series of trimethyl-pentane based on DFT calculations

Aziz Aboulmouhajir, M Hachim, K Sadik and **S Byadi**
Hassan II University, Morocco

The structure of a hydrocarbon fuel has a profound impact on its ignition and other combustion properties. Based on experimental studies, the roles of fundamental kinetic properties of these hydrocarbon fuels on ignition rates have become clearer. Trimethyls pentane (TMP) compounds are of particular industrial interest as they are used in commercial gasoline to increase the octane number because their ability to withstand compression and reducing contribution to pollution. Then, it is necessary to identify the right computational method for modeling them, especially their conformational isomerism and their rich infrared and Raman vibrational spectra. In the present work, the theoretical study was carried out by DFT quantum methods for a series of trimethylpentane molecular (2,2,4-, 2,2,3-, 2,3,3- and 2,3,4-TMP), in order to have insight into electronic properties of each studied molecule and to differentiate between its conformers. After the conformational optimization, the rotational barriers between the most stable conformers have been calculated. The Natural bond orbital (NBO) analysis have also been carried out to analyze the effects of intramolecular charge transfer. HOMO and LUMO frontier orbitals, molecular electrostatic potential (MEP), the polarizability (α) and first order hyperpolarizability (β) and related properties were calculated. In addition to NMR and UV simulations, the normal mode calculations of the most stable conformers using a scaled force field in terms of non-redundant local symmetry coordinates have been made to approach the vibrational spectra temperature dependency.

Speaker Biography

Aziz Aboulmouhajir has completed his PhD in Molecular Modeling and spectroscopy, at the age of 25 years from Instelling Antwerpen University in Belgium with High Distinction. He is holder of the STAS Prize of the Royal Academy of Sciences, Letters and Arts of Brussels, in Belgium. For the last ten years, he was head of the Molecular Modeling and Spectroscopy E2MS Team at Chouaib Doukkali University. He is currently professor and director of several thesis projects in Molecular Recognition and spectroscopy in Hassan II University (Morocco).

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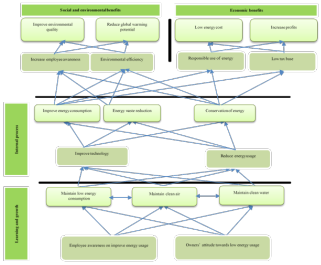
An analysis of barriers for minimizing embedded energy in the construction materials

Sampath P Dayaratne and **G H Samadhi Wickremathillake**
Ace Property and Business Consultants, Sri Lanka

Rapid increase of population, consumer demand increased. As a result, production has increased to meet the consumer demand while operate in the competitive market. At the production stage of brick manufacturing, it is a requirement SMEs to consider the impact to the environment. It is necessary to protect the natural environment for the purpose of organism preservation and conservation. Therefore, it is essential to accelerate transition to generate long term dramatic carbon footprint mitigation measures during production process through the control of embodied energy which is a determining factor. Small and Medium Scale Enterprises have still not considered significance of reduction of usage of energy. Researchers identified consumption of energy being largely associated with the manufacturing process, reduction of embedded energy and emissions are extraordinarily connected to productivity of kW/H of energy consumption. In order to carry out research goal of implementing barriers of reduction of embedded energy usage in bricks, responses to thirty-five questionnaires were collected from brick manufacturing SMEs registered under the Ministry of Industry and Commerce, Sri Lanka. Five unstructured interviews were conducted with relevant professionals in order to ascertain their opinion. These findings can be used as residue of the research process for the development of reduction of embodied energy consumption during production process. Implementation model of embodied energy usage minimizing which is based on the balance scorecard framework to acceleration transition and can be used for policy makers to re-think their planning. These findings could directly benefit any country where bricks manufacture for construction purposes is being put into practice; in order to identify factors that would minimize global warming potentials of brick manufacturing SMEs, while gaining return to the SMEs, providing benefit to the society and to the environment at large through sustainable production



Speaker Biography

Sampath P Dayaratne is the founder member and Managing Director of the Ace Property & Business Consultants (Pvt.) Ltd. His careers are Chartered Valuation Surveyor, human & business development professional, researcher, lecturer and trainer. He has twenty years of working experience in national and international level in both corporate and development sectors. He has published technical research articles in refereed journals, refereed conferences proceedings, numerous other papers and monographs.

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