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Tentative Program

2nd International Conference and Exhibition on

Materials Chemistry

July 13-14, 2017 Berlin, Germany

Theme: "Strategic Approach Leading to Unfolding Tactics in the World of Materials Chemistry"



For Available Speaker Slots

materialschemistry@chemistryconference.org

19+ Interactive Sessions	15+ Keynote Lectures	75+ Plenary Lectures	5+ Workshops

Conference Secretariat

2360 Corporate Circle, Suite 400 Henderson, NV 89074-7722, USA

Tel: +1-702-508-5200 Ext: 8047, Fax: +1-650-618-1417, Ph: +1-650-268-9744, Toll free: +1-800-216-6499

Email: materialschemistry@conferenceseries.net; materialschemistry@conferenceseries.com

July 10-11,2017 Berlin, Germany

Program at a Glance

Day 1

Morning Sessions

Reception/Registration	08.00-09.00
	Time	General Session
Least of 3 Keynote/Plenary Talks	09.00-09.15	Inaugural Address
	09.15-09.45	Keynote/Plenary Talk 1
	09.45-10.15	Keynote/Plenary Talk 2
	10.15-10.45	Keynote/Plenary Talk 3
Panel Discussions/Group Photo	
Coffee/Tea Break 10.45-11.00 (Networking)	
11.00-12.40	5 Speakers (20 Mins Each)

Evening Sessions

Lunch Break 12.40-13.30
13.30-15.30 — 6 Speakers (20 Mins Each)
Coffee/Tea Break 15.30-15.45 (Networking)
15.45-17.25 — 5 Speakers (20 Mins Each)

Day 1 — 19 Speakers for

Day 2

Morning Sessions

	Time	Session 1	Session 2
09.00-10.40		5 Speakers (20 Mins Each)	5 Speakers (20 Mins Each)
Coffee/Tea Break 10.40-10.55 (Networking)			
10.55-12.35		5 Speakers (20 Mins Each)	5 Speakers (20 Mins Each)
Lunch Break 12.35-13.25			
13.25-15.05		**5 Speakers (20 Mins Each)**	**5 Speakers (20 Mins Each)**
Poster Sessions			
Coffee/Tea Break 15.05-15.20 (Networking)			
15.20-17.00		**5 Speakers (20 Mins Each)**	**5 Speakers (20 Mins Each)**

Evening Sessions

Day 2 — 40 Speakers on

NOTE: Program Schedule is subject to change with final allotment of the speaker slots

For more Details PS: http://materialschemistry.conferenceseries.com/
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Note: *Workshops and Symposia slots are available. To book slot for Workshop and Symposium send us the proposal.*
Call for Abstract: *http://materialschemistry.conferenceseries.com/call-for-abstracts.php*
Registration: *http://materialschemistry.conferenceseries.com/registration.php*
Abstract Submission: *http://materialschemistry.conferenceseries.com/abstract-submission.php*
E-Poster: *http://materialschemistry.conferenceseries.com/eposter-presentation.php*

Glimpses of Chemistry Conferences



















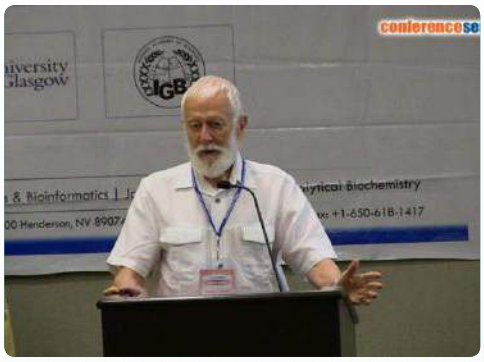






Glimpses of Chemistry Conferences

























Major Scientific Sessions

- Materials Science and Engineering
- Materials Chemistry in Developing Areas
- Formulating Materials Chemistry
- Materials Synthesis and Characterization
- Insilico Materials Chemistry
- Regenerative Materials Chemistry
- Polymer Materials and Technology
- Applied Materials Chemistry
- Materials Chemistry and Physics
- Nanomaterials
- Current Innovations in Materials Chemistry
- Research Aspects of Materials Chemistry
- Role of Graphene in Advanced Materials

Best Poster Award



- You will be given about 5-7 minutes to present your poster including questions and answers. Judges may pose questions during the evaluation of the poster
- Judges will even evaluate the student's enthusiasm towards their study, interest and knowledge in the area of their research
- The winners will be announced at the closing ceremony of the conference. The decision of the winner will be withdrawn if the winner/winners is/are not present at the time of announcement
- Apart from the judging time you may also be present at the poster to share your research with interested delegates



Young Researchers Forum

- Present your research through oral presentations
- Learn about career development and the latest research tools and technologies in your field
- This forum will give pertinent and timely information to those who conduct research and those who use and benefit from research
- Develop a foundation for collaboration among young researchers
- The forum will provide an opportunity for collegial interaction with other young investigators and established senior investigators across the globe
- Interact and share ideas with both peers and mentors

General Queries

materialschemistry@chemistryconference.org

Conference Venue

Berlin, Germany

Contact us
America: Conference Series LLC
Materials Chemistry 2017
2360 Corporate Circle., Suite 400 Henderson,
NV 89074-7722, USA
Phone: +1-888-843-8169, Fax: +1-650-618-1417,
Toll free: +1-800-216-6499
Email: materialschemistry@chemistryconference.org

Contact us
UK: Conference Series LLC
Materials Chemistry 2017
Heathrow Stockley Park Lakeside House
1 Furzeground Way, Heathrow
UB11 1BD, UK
Tel: +1-800-216-6499
Email: materialschemistry@conferenceseries.net

Contact us
Asia-Pacific: Conference Series LLC
Materials Chemistry 2017
Divyasree Building, Raidurg
6th Floor, North Block
Hyderabad 500032, INDIA
Tel: 040-33432334
Email: materialschemistry@conferenceseries.com

Best Tourist Destinations in Berlin



Berlin Cathederal



Berlin Wall



Brandenburg-Gate



Charlottenburg Palace



Memorial to the Murdered Jews of Europe



Museum Island



Neues Museum



Pergamon Museum



Reichstag building

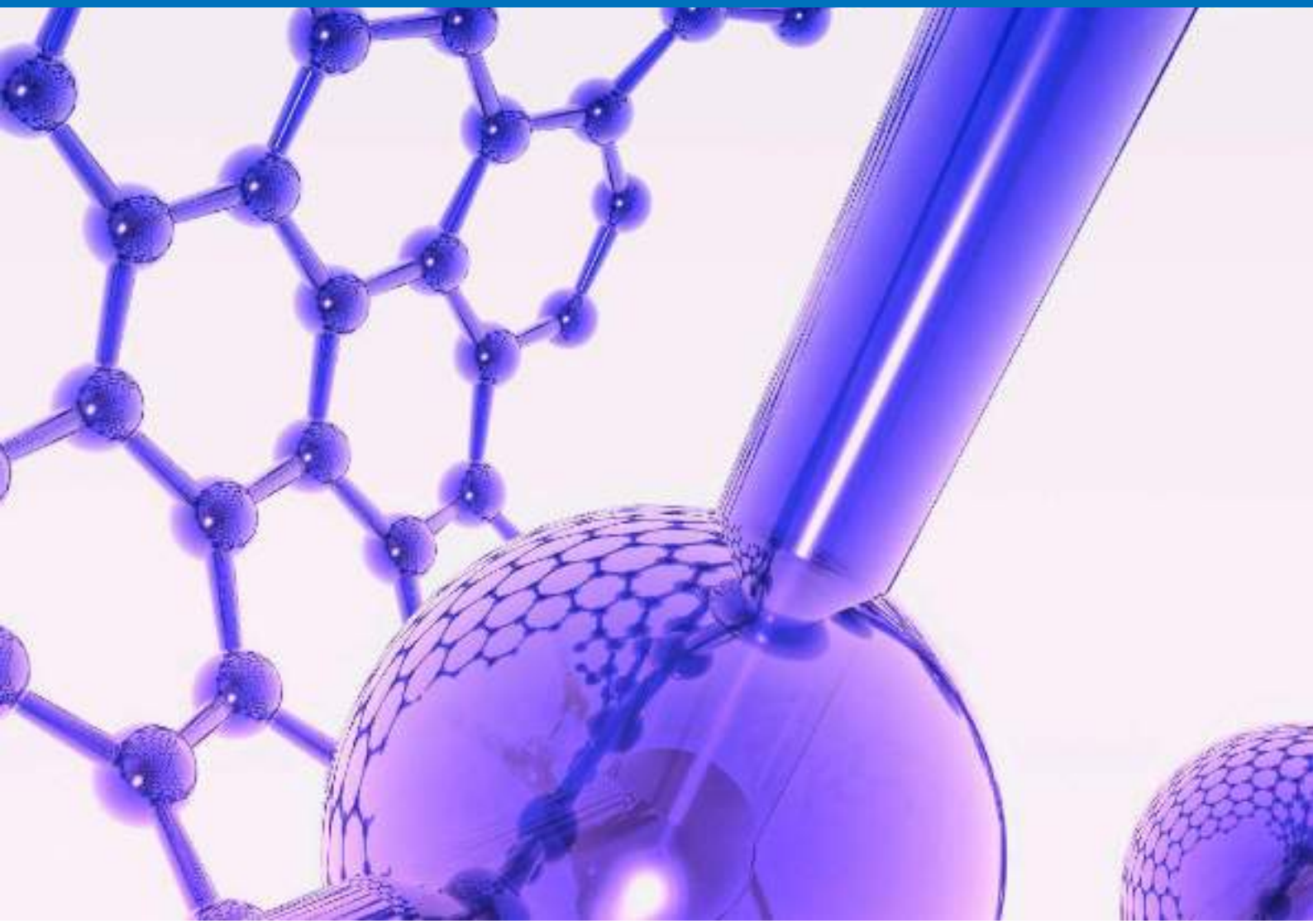
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Scientific Program

International Conference and Exhibition on

Materials Chemistry

March 31-April 01, 2016 Valencia, Spain



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Ph: +1-888-843-8169, Fax: +1-650-618-1417, Toll free: +1-800-216-6499
Email: materialschemistry@insightconferences.com, materialschemistry@conferenceseries.net, materialschemistry@conferenceseries.com

Registrations

Melia Meeting 4 & 5

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Opening Ceremony

Keynote Forum

Introduction

Michael W. Tausch
University of Wuppertal, Germany

Jas Pal Badyal
Durham University, UK

Track 1: Materials Science and Engineering
Track 2: Informatics in Various Fields of Materials

Session Introduction

Session Chair: Urs Meier, Swiss Federal Laboratories for Materials Science and Technology, Switzerland

Session Co-chair: Jijeesh R Nair, Polytechnic University of Turin, Italy

Title: Molecular magnetic switches
Marat M. Khusniyarov, Friedrich-Alexander-University of Erlangen-Nuremberg, Germany
Title: The role of polymer electrolyte in constructing an aging resistant high energy lithium battery for wide temperature application
Jijeesh R Nair, Polytechnic University of Turin, Italy

Group Photo

Coffee Break @ Foyer

Title: The prediction of long-term creep data of fibrous polymer composites based on short term experiments
Urs Meier, Swiss Federal Laboratories for Materials Science and Technology, Switzerland
Title: Group III-Nitride semiconductor nanostructures for novel photonic applications
Yong-Hoon Cho, Korea Advanced Institute of Science and Technology (KAIST), Republic of Korea
Title: Polymer derived boron nitride ceramics for energy applications
Philippe Miele, University of Montpellier, France
Title: Teaching from practice to theory
Mario Pablo Spector, National Technological University, Argentina
Title: Novel biological method for iron rust removal
S.Rajendran, Madurai Kamaraj University, India

Lunch Break @ Restaurant

Young Researchers Forum

Title: Towards more efficient upconverting materials based on $NaYF_4$ nanoparticles: Phase and size controlled synthesis and optical evaluation
Fabrizio Guzzetta, Universitat Jaume I, Spain
Title: High efficiency for photo-polymerizable VCP ester-amide resins: A universal concept providing low volume shrinkage, high reactivity and selectivity
Paul Pineda, University of Bayreuth, Germany
Title: Non-ionic UCST-type polymers: Synthesis and analysis of new thermoresponsive properties in aqueous media
Beatriz A Pineda-Contreras, University of Bayreuth, Germany

Title: Expanding the NMR palette: Insights on artificial charge separators
Brijith Thomas, Leiden Institute of Chemistry, Netherlands

Track 3: Role of Materials Chemistry in Pharmacy
Track 4: Design and Synthesis of Materials

Session Chair: Wlodzimierz Stanczyk, Polish Academy of Sciences, Poland

Session Co-chair: Bruno Bureau, Institut Universitaire de France, France

Title: Synthesis of the first POSS cage - anthracycline nano-conjugates
Wlodzimierz Stanczyk, Polish Academy of Sciences, Poland
Title: Synthesis of fine-controlled subano-metal particles using a dendrimer reactor
Kimihisa Yamamoto, Tokyo Institute of Technology, Japan
Title: Tellurium based glasses for far infrared and thermoelectric applications
Bruno Bureau, Institut Universitaire de France, France
Title: Game-based materials to teaching and learning the periodic table
Antonio Joaquín Franco-Mariscal, University of Malaga, Spain

Coffee Break @ Foyer

Title: Polymers with tunable properties via variable cross-linking conditions
Lee D. Wilson, University of Saskatchewan, Canada
Title: Fibre structures for energy harvesting in wearables
Elias Siores, Bolton University, UK
Title: Advanced functional organic-inorganic nano-composite membranes: Application of membrane technology for removal of contaminants of drinking water
Urfi Ishrat, Taibah University, Saudi Arabia
Title: Microstructure evolution at different cooling rates of a low carbon microalloyed steel
Elena Brandaleze, National Technological University, Argentina
Title: Mechanical response of Ti_3SiC_2 to He/H irradiation: Elaboration from first-principles calculation
Yuexia Wang, Fudan University, China

Day 2 April 01, 2016

Melia Meeting 4 & 5

Keynote Forum

Reshef Tenne
Weizmann Institute, Israel

Der-Jang Liaw
National Taiwan University of Science and Technology, Taiwan

Track 5: Foundational Challenges in Predictive Materials Chemistry
Track 6: Rational Chemical Synthesis on Nanoscale and Nanostructured Materials
Track 7: Polymer Materials and their Technology

Session Chair: Michael W. Tausch, University of Wuppertal, Germany

Session Co-chair: Ruben D. Costa, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Session Introduction

Title: Photoprocesses in science education
Michael W. Tausch, University of Wuppertal, Germany
Title: Hybrid organic-inorganic materials for thin-film lighting technologies
Ruben D. Costa, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Coffee Break @ Foyer

Title: Novel polymer-peptide conjugates and polymer-based peptidomimetics
Marc Devocelle, Royal College of Surgeons in Ireland (RCSI), Ireland
Title: Conjugated copolymers and their optimization for ambipolar field effect transistors
Martin Baumgarten, Max Planck Institute for Polymer Research, Germany
Title: Spectroscopic tools to study and interpret macromolecular dynamics at a molecular scale
Jorge Teno Diaz, Carlos III University of Madrid, Spain
Title: Ultrasonic fabrication of microfluidic polymer chips
Werner Karl Schomburg, RWTH Aachen University, Germany
Title: Synthetic polymers from easily available monossacharides
M. Gracia García-Martín, University of Seville, Spain

Lunch Break: @ Restaurant

Poster Presentations @ Foyer

Title: Inclusion complexes of propiconazole nitrate with substituted β-cyclodextrins II: *In vitro* assessment of antifungal properties
Irina Rosca, Petru Poni Institute of Macromolecular Chemistry, Romania
Title: Inclusion complexes of propiconazole nitrate with substituted β-cyclodextrins: Synthesis, characterization and in silico assessment
Narcisa Laura Marangoci, Petru Poni Institute of Macromolecular Chemistry, Romania
Title: Silver nanoclusters doped in mordenite zeolite as photocatalysts toward pesticides
Imad A Abu-Yousef, American University of Sharjah, UAE
Title: Improving PLA properties through the incorporation of electrospun nanofibers based on PVA and cellulose nanowhiskers
Carol Lopez de Dicastillo, Santiago de Chile University, Chile
Title: Antimicrobial supercritical impregnation of nanocomposites for food packaging
Maria Jose Galotto, Santiago de Chile University, Chile
Title: Preparation and characterization of chitosan-co-hyaluronic acid cryogels
Tugce Kutlusoy, Marmara University, Turkey
Title: Synthesis and characterization of high performance polyimide nanofibers and application on lithium-ion batteries
Emre Aytan, Marmara University, Turkey
Title: Molecularly imprinted polymeric nanoparticle: Preparation and characterization
Merve Yasar, Marmara University, Turkey
Title: Novel macroporous poly-pickering-HIPE composites for heterogeneous photocatalysis
Elif Yüce, Yalova University
Title: Poly-pickering-HIPEs as heterogeneous photocatalysts
Fatma Nur Parın, Yalova University

Track 8 : Applied Materials Chemistry
Track 9 : Current Innovations and Emerging Areas in Materials Chemistry
Track 10 : Research Aspects of Materials Chemistry
Track 11 : Science of Advanced Materials

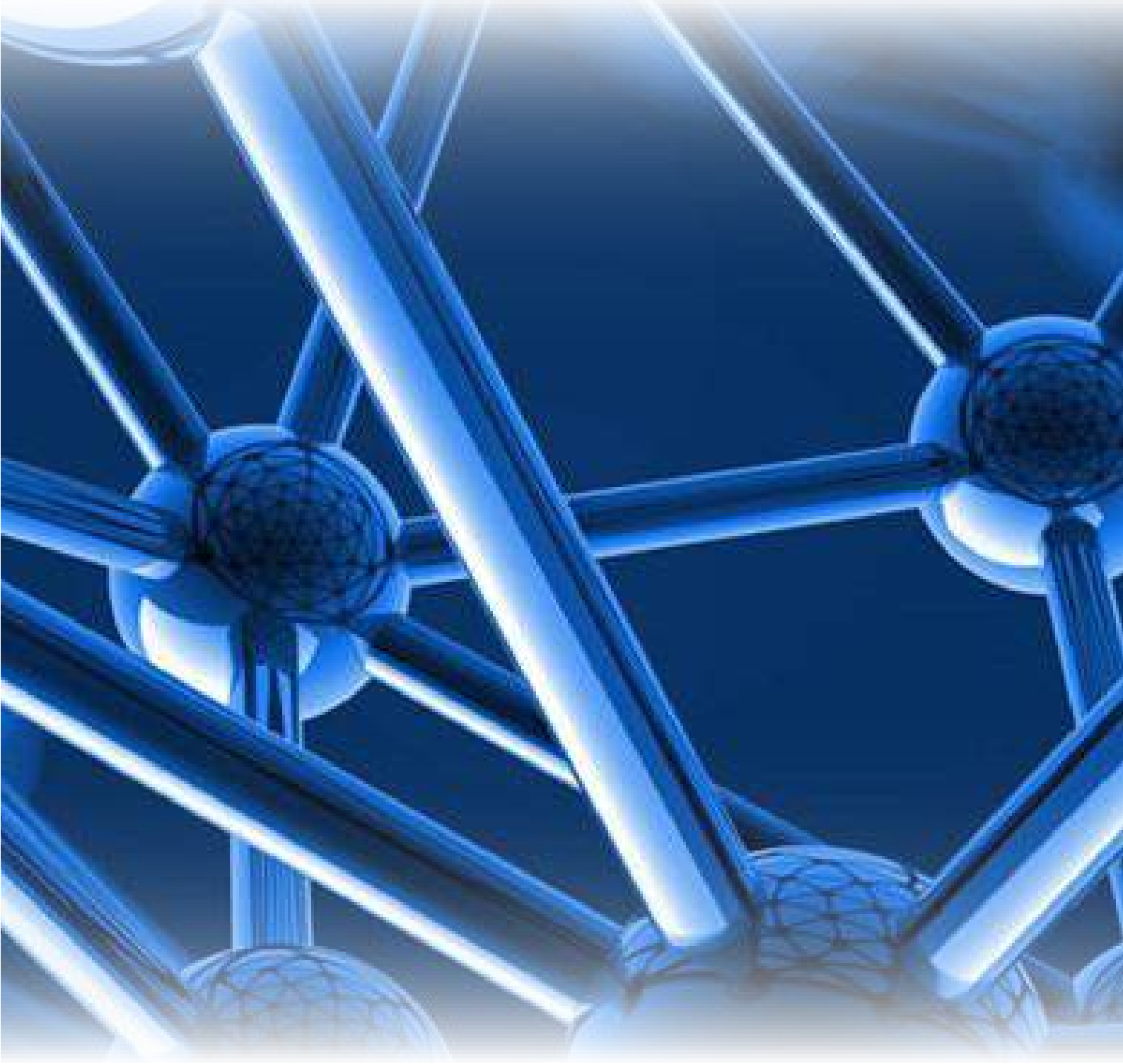
Session Chair: Yan Huang, Brunel University London Institute of Materials and Manufacturing, UK

Session Co-chair: Yo Tanaka, RIKEN, Japan

Title: Solute effect on grain boundary migration in ultrafine/nanostructured materials
Yan Huang, Brunel University London Institute of Materials and Manufacturing, UK
Title: Application of ultra-thin flexible glass sheets to microfluidic devices
Yo Tanaka, RIKEN, Japan
Title: Nanoscale strategies towards development of advanced Mn-based permanent magnets
Felix Jimenez-Villacorta, Materials Science Institute of Madrid (ICMM-CSIC), Spain
Title: Sialon nano-composites matrix reinforced by cubic boron nitride prepared by using spark plasma sintering
Abbas Saeed Hakeem, King Fahd University of Petroleum & Minerals, Saudi Arabia
Title: Segregation of ions in deliquesced droplets of alkali halide nano-crystals on SiO_2
Kenta Arima, Osaka University, Japan
Title: Nanomechanics with nanotubes and fullerene-like-WS_2 (MoS_2)
Reshef Tenne, Weizmann Institute, Israel

Coffee Break @ Foyer

Video Presentation: One-pot waterborne superhydrophobic pigment coatings at high solids with improved scratch and water resistance
Agne Swerin, SP Technical Research Institute of Sweden – Chemistry, Sweden
Title: Fuel briquettes from municipal solid waste through solid state fermentation
S.Rajendran, Saraswathi Narayanan College, India
Title: Microreactors based on nanostructured monolithic materials for electrochromatography separation and catalysis applications
Seydina Ibrahima KEBE, University Paris-East, France
Title: Heterogeneous kinetic uptake studies of conventional and nanomaterials in solution
Lee D. Wilson, University of Saskatchewan, Canada



Bookmark your dates

2nd International Conference and Exhibition on

Materials Chemistry

April 24-26, 2017 Frankfurt, Germany

e-mail: materialschemistry@insightconferences.com; materialschemistry@conferenceseries.net

Website: materialschemistry.conferenceseries.com

Conference Series LLC
2360 Corporate Circle, Suite 400
Henderson, NV 89074-7722, USA
Ph: +1-888-843-8169
Fax: +1-650-618-1417
america@conferenceseries.com

Conference Series Ltd.
Traian Str., No.61, Constanta 900720,
Romania, Tel: 0805-080048
Heathrow Stockley Park Lakeside
House, 1 Furzeground Way, Heathrow,
UB11 1BD, United Kingdom
europe@conferenceseries.com

OMICS International
6th Floor, North Block, Divyasree
Building, Raidurg Hyderabad,
Telangana, INDIA-500032
Tel: +91-40-33432300
asiapacific@conferenceseries.com

Toll free
USA & Canada: +1-800-216-6499
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Scientific Program

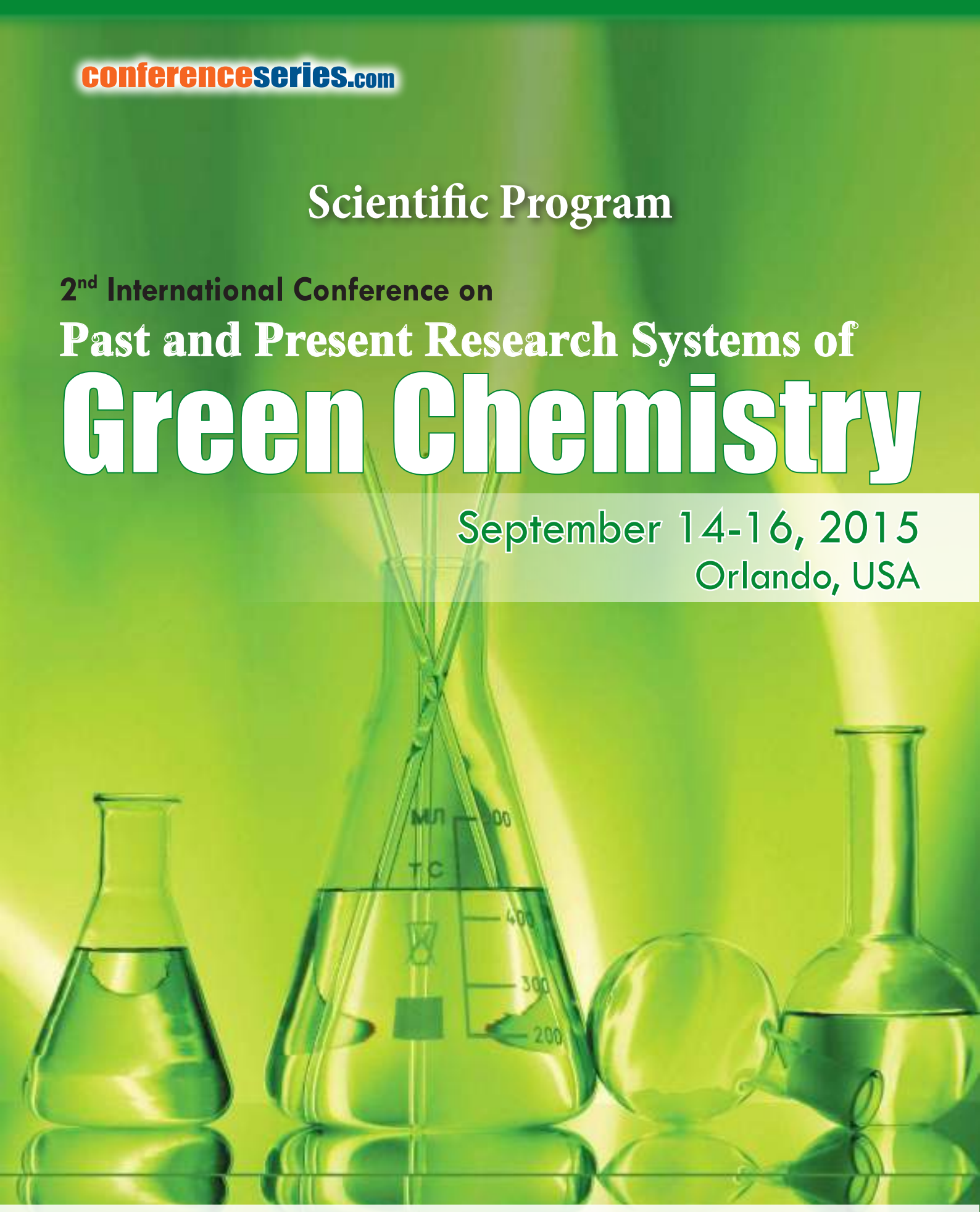
2nd International Conference on

Past and Present Research Systems of

Green Chemistry

September 14-16, 2015

Orlando, USA



Conference Series LLC

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Scientific Program

Day 1 **September 14, 2015**

Continental Ballroom 6-8

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Opening Ceremony

Keynote Forum

Introduction

John Littleton
University of Kentucky, USA

Lothar Brecker
University of Vienna, Austria

Special Session

Title: Green Chemistry: An opportunity for growth and competitive advantage
John C Warner, Warner Babcock Institute for Green Chemistry, USA

Networking & Refreshment Break @ Foyer

Track 1: Basic Principles and New Trends in Green Chemistry
Track 3: Green Synthesis-Designing the Starting Materials
Track 4: Green Catalysis
Track 6: Green Metrics and Measurements

Session Chair: Joseph M Fortunak, Howard University, USA
Session Co-Chair: Dequan Xiao, University of New Haven, USA

Session Introduction

Title: Green pharmaceutical chemistry: Target-directed evolution of plant secondary metabolism
John Littleton, University of Kentucky, USA
Title: Transition metal catalysis for non-directed C-H functionalization
Marion Heidi Emmert, Worcester Polytechnic Institute, USA
Title: Green chemistry and global access to medicines: New chemistry for access to HIV, Malaria, and Hepatitis medicines
Joseph M Fortunak, Howard University, USA
Title: Rapid catalyst screening using a high pressure, Tandem micro-reactor GC/MS
Bob Freeman, Frontier Laboratories Ltd., Japan
Title: Green chemistry in higher education
Amy S Cannon, Beyond Benign, USA
Title: Recent developments of the fixation of atmospheric co_2 by transition metals and lanthanide complexes
Salah S Massoud, University of Louisiana at Lafayette, USA

Lunch Break @ Continental Ballroom 2-4

Title: Exploring the mildest thermodynamic conditions for the inverse design of hydrogenation catalysts
Dequan Xiao, University of New Haven, USA
Title: Efficient cubane catalysts for artificial water-splitting
Sandra Luber, University of Zurich, Switzerland
Title: SnO_2-PbS nanocomposites and hetero structures: Fabrication, structures and applications
Arik Kar, University of Cambridge, UK
Title: The contribution of photochemistry and photocatalysis to Green Chemistry
Angelo Albini, University of Pavia, Italy
Title: Practical catalytic hydrogenation
Xumu Zhang, The State University of New Jersey, USA
Title: Asymmetric heterogeneous catalysts based on copper(II) complexes with bis(oxazoline) ligands
Ana Rosa Silva, Aveiro University, Portugal
Title: Green chemistry in niche applications: Development of "green" photoresists
Frank Wiesbrock, Polymer Competence Center Leoben, Austria

Networking & Refreshment Break @ Foyer

Title: Pulicaria glutinosa plant extract: A green and ecofriendly reducing agent for the preparation of highly reduced graphene oxide
Abdulrahman Al-Warthan, King Saud University, KSA
Title: Leaf extract mediated Green synthesis of silver nanoparticles from *Phyllanthus amarus*: As an antibacterial agent against wide range of microbes
Jaya Parkash Yadav, M.D. University, India
Title: Biogenic preparation of ZnO nanoparticles reduced from *Ocimum tenuiflorum* and their antioxidant activity
B Deva Prasad Raju, Sri Venkateswara University, India
Title: Facile and eco-friendly method for the synthesis of magnesium oxide nanoparticles and their antioxidant properties
Nannepaga John Sushma, Sri Padmavati Women's University, India
Title: Green synthesis of Ag, Au and Au-Ag bimetallic nanoparticles using C. albidum for catalytic application in electro-oxidation of methanol
Kehinde Oluseun Sodeinde, Federal University Oye-Ekiti, Nigeria
Title: Synthesis, antibacterial, cytotoxicity and sensing properties of biopolymer -capped silver nanoparticles
Samuel Oluwatobi Oluwafemi, University of Johannesburg, South Africa
Title: Suzuki-Miyaura Cross coupling reactions in water: New hydrophilic ligand scaffolds from Pincer compounds to cocoa beans
David Morales-Morales, Instituto de Quimica, Mexico

Panel Discussions

Day 2 September15, 2015

Continental Ballroom 6-8

Keynote Forum

Mahdi M Abu-Omar
Purdue University, USA

Craig L Hill
Emory University, USA

Track 2: Green Chemistry-Chemical Applications from Laboratories to Industries
Track 8: Organic Synthesis in Different States
Track 10: Analytical Methodologies
Track 11: Sustainability and Environmental Safety

Session Chair: Mahdi M Abu-Omar, Purdue University, USA

Session Co-Chair: Miguel Yus, University of Alicante, Spain

Session Introduction

Title: Sustainability through catalysis: Making biofuels and chemicals from biomass
Mahdi M Abu-Omar, Purdue University, USA
Title: Natural products as active agents: On the border between sustainable application and risky use
Lothar Brecker, University of Vienna, Austria
Title: Comparing the effect of ecofriendly adsorbents and bioturbators on the concentration pyrene
Febee Louka, University of Louisiana, USA

Networking & Refreshment Break @ Foyer

Title: Green fuel: Selective and water compatible catalysts for solar fuel production
Craig L Hill, Emory University, USA
Title: Atom-economical and sustainable C-N bond formation reactions from alcohols and N-Sources via catalytic hydrogen transfer reactions
Soon H Hong, Seoul National University, South Korea
Title: Atom and step economy in synthetic organic chemistry
Miguel Yus, University of Alicante, Spain
Title: Organolithium chemistry using flow microreactors to Green Chemistry
Aiichiro Nagaki, Kyoto University, Japan
Title: New versatile nanostructured catalysts: From green preparation to environmentally concerned challenges
Capucine Sassoye, UPMC University, France
Title: Sustainable development of infrastructure for electric vehicles
Jennifer L Anthony, Kansas State University, USA

Lunch Break @ Continental Ballroom 2-4

Title: Green capillary electrophoretic stacking of analytes by ionic liquid collapse and its application coupled with ionic liquid based ultrasound assisted liquid extraction to acrylamides determination
Deia Abd El-Hady, University of Jeddah, KSA
Title: Kinetic and thermodynamic profile of solifenacin succinate sorption from wastewater by humic acid-coated TiO_2 nanoparticles: An Approach towards Green Chemistry
Medhat A Shaker, University of Jeddah, KSA

Title: De-polymerization of sugarcane bagasse lignin to value added products in sub and supercritical water
Sunil Joshi, National Chemical Laboratory, India
Title: Towards sustainable surface processing and products through green chemistry and engineering
Kwang-Leong Choy, University College of London, UK
Title: Triazole stabilized transition metal nanoparticles for 4-Nitrophenol reduction
Pengxiang Zhao, China Academy of Enginnering Physics, China
Title: Nanocatalysis and continuous-flow processing: Towards greener and more sustainable chemistry
Mostafa Baghbanzadeh, Harvard University, USA

Networking & Refreshment Break @ Foyer

Title: The study of trace elements uptake by plants from contaminated waters
Olga V Shuvaeva, Novosibirsk State University, Russia
Title: Gelatin wastes for better plant growth
Nabil H Elsayed Khamis, National Research Center, Egypt
Title: Improvements to the biorefinery model through lignin valorization
Ian Klein, Spero Energy, Inc., USA
Title: Detection of human osteosarcoma cell (MG-63) and evaluation of the cytotoxicity of cisplatin using the TiO_2 nanotubes modified wireless magnetoelastic sensing device
Xilin Xiao, University of South China, China
Title: Fabrication of miniaturized capillary waveguide integrated fiber-optic sensor for fluoride determination in water
Yan Xiong, Southwest Petroleum University, China

Poster Presentations @ Continental Ballroom 1-3

Title: An alternative process of reduction of diimines
Ingrid Miranda–Carvajal, National University of Colombia, Colombia
Title: Arsenic adsorption into thermally treated dolomite
Yousef Salameh, American University Beirut, Lebanon
Title: Conversion of crude glycerol, the biodiesel production by-product, into value-add chemical 2,3-butanediol through microbial fermentation
Hsin-Yao Cheng, Green Technology Research Institute, Taiwan
Title: The current progress of cellulosic ethanol development in CPC corporation, Taiwan
Jui-Hui Chen, Green Technology Research Institute, Taiwan
Title: Peanut virginia type (*Arachis hypogaea* L.) as feedstock for biodiesel production: Comparative analysis from methylic and ethylic routes
Euripedes G Silveira Junior, University of Northern of Rio de Janeiro, Brazil
Title: Integrated process of unconventional biodiesel production reusing glycerol: Techno-economic and environmental impact evaluation
Victor Haber Perez, University of Northern of Rio de Janeiro, Brazil
Title: Novel nanoparticles of Ru and Pd supported on bacterial biomass for catalytic hydrogenation of 5-HMF to produce 2,5-DMF
Bayonle Kayode, University of Birmingham, UK
Title: Modeling and simulation of a fuel cell of polymer membrane for the generation of electricity
Claudia Milena Cabrera-Sanmartin, State University of Northern of Rio de Janeiro, Brazil
Title: Study of hydrolysis of sugarcane bagasse in pilot plant for fermentable sugars obtaining for second generation ethanol
Tania F Carneiro, State University of Campinas, Brazil
Title: Extraction and purification of bioactive compounds by combining supercritical fluids and ultrasound and on-line coupling with solid-phase extraction
Mauricio A Rostagno, Universidade Estadual de Campinas , Brazil
Title: Ethanol production in bioreactor assisted by electromagnetic field: Kinetic modeling
Manuel G Mendoza Turizo, University of Northern of Rio de Janeiro, Brazil
Title: Equilibrium and kinetics studies on the biosorption of caffeine by hydrogel beads
Ziu Wing Lo, Borough of Manhattan Community College, USA
Title: Uptake of organic pollutants by solid wastes as an eco-friendly remediation alternative
Kateryna Zhdanova, Borough of Manhattan Community College, USA
Title: Evaluation of deep eutectic solvents as electrolytes for a non-aqueous vanadium redox battery
Laleh Bahadori, University of Malaya, Malaysia
Title: Green route to synthesis of (4-methoxy-phenyl)- phosphonodithioic acid and its Ni & Co complexes
Tomilola Ajayi, University of Kwazulu-natal, South Africa
Title: Isolation and characterization of heavy metal tolerant bacteria for the purpose of bioremediation
Finola Fung-Khee, Borough of Manhattan Community College, USA
Title: Chemoselective reactions of Diaminomaleonitrile (Damn) in water
Jicli Jose Rojas Salgado, Universidad Nacional de Colombia, Colombia

Day 3 September 16, 2015

Continental Ballroom 6-8

Track 5: Green Chemical Solvents
Track 7: New Ideas for Non Toxic By-Products
Track 9: Industrial Applications of Green Chemistry
Track 12: Green Chemistry and Engineering

Session Chair: Feng Xu, Merck Research Laboratories, USA

Session Co-Chair: Carmen Najera, University of Alicante, Spain

Session Co-Chair: Abel E Navarro, Borough of Manhattan Community College, USA

Session Introduction

Title: Green by design for process evolution: Asymmetric syntheses of vibegron
Feng Xu, Merck Research Laboratories, USA
Title: Bioremediation of pollutants from pharmaceutical residual waters with marine algae and derivatives
Abel E Navarro, Borough of Manhattan Community College, USA

Workshop By

Title: Greener Fenton processes for removal of persistent organic pollutants from wastewaters
Andreja Zgajnar Gotvajn, University of Ljubljana, Slovenia

Networking & Refreshment Break @ Foyer

Title: Novel lignocellulosic hydrolysate detoxification using pyrochar from digestate: Application for bioethanol fermentation
Monlau Florian, INRA UMR IATE, France
Title: Thermo-chemical pretreatments for the combined recovery of extractives and bioethanol production from Douglas-fir bark
Cecilia Sambusiti, INRA UMR IATE, France
Title: Environmental impact assessment and bio-treatability potential of deep eutectic solvent based on holing chloride
Andreja Zgajnar Gotvajn, University of Ljubljana, Slovenian
Title: SA Metrics-comparative sustainability metrics for biomass and petrochemical succinic acid production and its catalytic Valorization into ϒ-Butyrolactone
Marcelo E Domine, The Institute of Chemical Technology (ITQ), Spain
Title: Cross-coupling reactions in aqueous media
Carmen Najera, University of Alicante, Spain
Title: Atom economic synthesis of amides
Diego Gamba Sánchez, Universidad de los Andes, Colombia
Title: Production of biofuels and biobased compounds in urban biorefineries: A new paradigm for green chemistry?
Aurore Richel, University of Liege – Gembloux Agro-Bio Tech, Belgium

Lunch Break @ Continental Ballroom 2-4

Title: Alternative ionic liquid-based Lignocellulosic biomass pre-treatment and fractionation towards progress in biorefinery
Ewa Bogel-Łukasik, Universidade Nova de Lisboa, Portugal
Title: Thermodynamics and topological investigations of ternary mixtures containing ionic liquid with organic solvents: Excess molar volumes and excess isentropic compressibilities
Vinod Kumar Sharma, M D University, India
Title: Industrial enzymes used to build green technology for Pre-treatment of textile dyeing
Hui Song, Chinese Academy of Sciences, China
Title: Green chemistry as a tool to prevent pharmaceutical hazards and pollution
Gannu Praveen Kumar, Sahasra Institute of Pharmaceutical Sciences, India
Title: Chromate and arsenate removal by layered double hydroxides-polymer beads
Nguyen Thi Kim Phuong, Institute of Chemical Technology, Vietnam
Title: Shaped carbon nanomaterial supports based heterogeneous catalytic systems for various green routes of chemical synthesis
Vilas M Ravat, Reliance Industries Limited, India

Young Researchers Forum

Title: Conversion of cellulose and lignocellulosic based feedstock over heterogeneous catalysts into liquid polyols
Katarina Fabicovicova, University of Technology Darmstadt, Germany
Title: From batch to continuous conversion of bio-derived platform chemicals: Aqueous phase hydrogenolysis of furfuryl alcohol into 1,2-pentanediol using a trickle bed reactor
Dominik Gotz, Technical University Darmstadt, Germany
Title: Selective extraction and separation of platinum group metals from chloride media using phosphonium based ionic liquid
Viet Tu Nguyen, Korea University of Science and Technology, Korea
Title: A truly green synthesis of α-aminonitriles via Strecker reaction
Juliana M Velazquez, University of Texas Pan American, USA

Award Ceremony

Networking & Refreshment Break @ Foyer



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Opening Ceremony

Keynote Forum

Introduction

Davis L Ford
Texas A&M University, USA

Ashok Kumar Ray
CSIR-National Metallurgical Laboratory, India

Mileva Radonjic
Louisiana State University, USA

S S Amritphale
CSIR-Advanced Materials and Processes Research Institute, India

Group Photo

Coffee Break: @ Atrium

Track 1: Processing Technologies
Track 2: Petroleum Exploration & Field Management

Session Chair: Ildenize Barbosa da Silva Cunha, University of Campinas, Brazil
Session Co-Chair: Bushra Al-Duri, University of Birmingham, UK

Session Introduction

Title: Novel methods for upgrading heavy petroleum products
Russell R Chianelli, University of Texas at El Paso, USA
Title: Mass Spectrometry: A pioneer and renewed tool for petrochemical analysis
Ildenize Barbosa da Silva Cunha, University of Campinas, Brazil
Title: Ethylene–vinyl acetate copolymer-based depressants in marine fuels
Nataliya Kondrasheva, The National Mineral Resources University, Russia
Title: Heterogeneity of fine grained sediment and its hydrocarbon generation and expulsion: An case from Dongying depression
Chen Zhonghong, China University of Petroleum, China
Title: High performance oxygen carriers for chemical looping combustion process by using architectural structure of silica nanoparticles
Yujing Liu, Swiss Federal Laboratories for Materials Science and Technology, Switzerland
Title: Further work on energy-return-on-energy-invested
J C Jones, Kazakh-British Technical University, Kazakhstan

Lunch Break @ Atrium

Title: Plasma processing of fossil fuels
Alexandr Ustimenko, Research Institute of Experimental and Theoretical Physics, Kazakhstan
Title: Production of furans (2,5 dimethylfuran) from furfurals (Hydromethoxyfurfural-HMF) as transport fuel molecules
Bushra Al-Duri, University of Birmingham, UK
Title: Highly active nano-dispersed Ruthenium catalyst for efficient oxidation of p-cymene and cumene C-H bond by molecular oxygen
Peter R Makgwane, Council for Scientific Industrial Research, South Africa

Title: The Ural-African transcontinental oil & gas belt
Valentin Stepanov, The National Mineral Resources University, Russia

Title: Surfactants and other factors input for the control of the reservoir interfacial tension (IFT)
M.S Benzagouta, University Larbi Ben Mhidi OEB, Algeria
Title: Pore volume compressibilities and stress sensitivity of low permeability reservoir rocks in China's oilfield development
Sun He, China University of Petroleum, China
Title: Selective propping of high conductivity fractures
David Dogon, Eindhoven University of Technology, Netherlands
Title: Equilibrium calculations in aqueous carbonation of oil shale waste – sulfur compounds
Kadriann Tamm, Tallinn University of Technology, Estonia

Coffee Break @ Atrium

Track 3: Drilling & Well Completions Challenges
Track 4: Piping and vessel engineering & Transport Phenomena

Session Chair: Byoung Yoon Park, Sandia National Laboratories, USA
Session Co-Chair: Arya Shahdi, Islamic Azad University, Iran

Session Introduction

Title: Interbed modeling to predict wellbore damage for big hill strategic petroleum reserve
Byoung Yoon Park, Sandia National Laboratories, USA
Title: Performance investigation of an experimental shale shaker in filtration of low concentration slurry
Saeid Ghaniyari Benis, The University of Akron, USA
Title: A robust modeling approach for frictional pressure loss calculation of three phase flow in inclined eccentric annuli
Arya Shahdi, Islamic Azad University, Iran
Title: Study on gas hydrate blocking mechanism and precaution in wellbore of deep water drilling
Xiangfang Li, China University of Petroleum, China
Title: Inhibitive properties comparison of different polyetheramines in water-based drilling fluid
Hanyi Zhong, China University of Petroleum, China
Title: A new understanding on low permeability oilfield development
Tang Wei, Research Insititute of Petroleum Exploration and Development (RIPED) of CNPC, China

Cocktails Sponsored by: Journal of Petroleum & Environmental Biotechnology @ Atrium

Day 2 October 28, 2014

Tropicana Ball Room

Track 5: Chemical Applications in Producing Oil and Gas
Track 6: Coal & Natural Gas
Track 7: Challenges and Safety in Petrochemical Industry
Track 8: Energy Economics

Session Chair: Ahmed El-Nahas, El-Menoufia University, Egypt
Session Co-Chair: Xi Liu, Cardiff University, UK

Session Introduction

Title: Nanoparticle stabilized emulsions and foams for EOR and LNG spill mitigation
Zhengdong Cheng, Texas A&M University, USA
Title: Development of porous radiant burners for domestic LPG cooking and industrial applications
P Muthukumar, Indian Institute of Technology Guwahati, India
Title: Porous media for improved polymer electrolyte membrane fuel cells
Aimy Bazylak, University of Toronto, Canada
Title: Use of sulfide/phosphate based sorbents for mercury removal from natural gas: A focus on the Hg stabilization
Carla Luciane Manske Camargo, Federal University of Rio de Janeiro, Brazil
Title: Experimental investigation of polymer adsorption-induced permeability reduction in low permeability reservoirs
Hyemin Park, Hanyang University, Korea

Title: First-principles analysis on enzymatic degradation of nylon
Yasuteru Shigeta, University of Tsukuba, Japan

Coffee Break @ Atrium

Title: Effect of miscibility condition for CO_2 flooding on gravity drainage in 2D vertical system
Jinju Han, Hanyang University, Korea
Title: Thermodynamic and kinetic hydrate inhibition performance of MEG solution and its synergistic inhibition with PVCap
Yutaek Seo, Korea Advanced Institute of Science and Technology, Korea
Title: Dearomatization of straight-run diesel fuel by using adsorbents under magnetic field
Irana Safarli Almas, Institute of Petrochemical Processes of Azerbaijan NAS, Azerbaijan
Title: The use of an ultrasonic technology to increase the productivity of oil wells
Anna Abramova, Institute of General and Inorganic Chemistry of the Russian Academy of Sciences, Russia
Title: Experimental study of pulverized coal oxycombustion and modelling of devolatilization kinetics
Romain Lemaire, Université Lille Nord de France, France
Title: The investigation of catalytic activity of polyoxide catalysts on the base of fiberglass in the reaction of carbon dioxide conversion of methane
Z A Mansurov, Institute of Combustion Problems, Kazakhstan

Lunch Break @ Atrium

Title: LES and RANS of pulverized coal oxy-combustion in swirl burners
Andrzej Boguslawski, Czestochowa University of Technology, Poland
Title: Applicability of non-exhaustive extraction procedures using Tenax® and HPCD to estimate biodegradable contaminant fractions in soil
Kerstin Derz, Fraunhofer Institute for Molecular Biology and Applied Ecology, Germany
Title: E- Neutron scattering studies of catalyst systems at the ISIS neutron spallation Source
Martin Owen Jones, Oxford University, UK
Title: Avoiding gas hydrate problems in Qatar oil and gas industry: Environmentally friendly solvents for gas hydrate inhibition
Nabila Mohamed, Qatar University, Qatar
Title: Insitu transesterification of wet activated sludge under subcritical conditions
Lan Nguyen Phuong Tran, National Taiwan University of Science and Technology, Taiwan
Title: The development of the methods for processing and using of oil sands as the alternative hydrocarbon feedstock
Sultanov F, Al-Farabi Kazakh National University, Kazakhstan

Track 9: Renewable Energy & Feedstock

Session Chair: Abdallah S Berrouk, The Petroleum Institute, UAE
Session Co-Chair: Stella Bezergianni, Centre for Research & Technology Hellas, Greece

Session Introduction

Title: Fast pyrolysis of lignin
Hilkka Kenttamaa, Purdue University, USA
Title: Photosynthetic bioenergy utilizing CO_2: An approach on flue gases utilization for third generation biofuels
Roberto Parra Saldivir, Monterrey Institute of Technology and Higher Education, Mexico

Coffee Break @ Atrium

Title: Decarbonization of transportation fuels via co-hydroprocessing bio-based feedstocks with petroleum fractions
Stella Bezergianni, Centre for Research & Technology Hellas, Greece
Title: Evaluation of methylic and ethylic biodiesels from Pequi oil (*Caryocar Brasiliense* Camb.) as possible diesel substituents
Marcelo Firmino de Oliveira, Universidade de Sao Paulo, Brazil
Title: Combustion heat release models of biodiesels
Abdullah Abuhabaya, King Abdulaziz University, Saudi Arabia
Title: Biodiesel production from *Acrocomiaaculeata* acid oil by (enzyme/enzyme) hydroesterification process: Use of vegetable lipase and fermented solid as low-cost biocatalysts
Erika Cristina G Aguieiras, Federal University of Rio de Janeiro, Brazil
Title: Drying of energy wood by compression
Tuomas Hakonen, Seinäjoki University of Applied Sciences, Finland
Title: Thermochemistry and kinetics of bioalcohols and bioesters as fossil fuel alternatives. Ab initio and DFT studies
Ahmed El-Nahas, El-Menoufia University, Egypt

Title: Thermogravimetric study of powdered laboratory safety examination gloves
Nasrollah Hamidi, South Carolina State University, USA

Poster Presentations @ Atrium

Title: Fischer-Tropsch synthesis reaction in a novel reactor system of cobalt catalyst coated metallic foam and heat-exchanger type reactor
Jung-Il Yang, Korea Institute of Energy Research, Korea
Title: Study of solvent recovery in solvent deasphalting process
Seonju Ahn, Korea University, South Korea
Title: Reforming of methane with carbon dioxide
Kusman Dossumov, Al-Farabi Kazakh National University, Kazakhstan
Title: Green synthesis of Fe nanoparticles for chromate removal
Christiana Mystrioti, National Technical University of Athens, Greece

Title: Investigation of hexavalent chromium removal from polluted soil using electroremediation
Aikaterini Toli, National Technical University of Athens, Greece
Title: Selective viscosifying for conformance control
Joris van Santvoort, Eindhoven University of Technology, The Netherlands
Title: Fracture flow control
Boaz van der Plas, Eindhoven University of Technology, The Netherlands
Title: Vapor-liquid equilibria of the binary system 2-methylfuran + 1-butanol, present in the production of 2,5-dimethylfuran from biomass
Luis A Follegatti-Romero, University of Campinas, Brazil

Title: Production of a solid enzymatic preparation by *Rhizomucor miehei* from a low-cost agroindustrial residue
Jaqueline Greco Duarte, Federal University of Rio de Janeiro, Brazil
Title: Electrical, optical and structural properties of Ga-Al doped ZnO/Copper/Ga-Al doped ZnO multilayer electrode for thin film solar cells
Kyung Hwan Kim, Gachon University, Republic of Korea
Title: Fracture diagnostics of SRV by well testing and micro-seismic method in tight reservoirs, China
Xiaoliang Zhao, China University of Petroleum, China
Title: Determination of dynamic deliverability equation for fractured horizontal well in tight gas reservoir
Xiangji Dou, China University of Petroleum, China
Title: The mechanisms of gas generation during coal deformation
Rongting Xu, University of Chinese Academy of Sciences, China

Title: The effect of water salinity on silica dissolution rate and subsequent formation damage during chemical EOR process
Khaled A. Elraies, Universiti Teknologi PETRONAS, Malaysia
Title: Influence of crude oil type and production technology on bitumen fractional composition
Audrius Vaitkus, Vilnius Gediminas Technical University, Lithuania
Title: Study on chemical properties of some bituminous materials
Nader Nciri, Korea University of Technology and Education, Republic of Korea
Title: Agricultural machinery problems on fuel consumption, exhaust emissions and their normative assessment
Antanas Juostas, Konekesko Lietuva, Lithuania

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Day 3 October 29, 2014

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Track 13: Modeling & Simulation

Track 14: Catalysis Concepts

Session Chair: Renbi Bai, National University of Singapore, Singapore
Session Co-Chair: Joseph Zeaiter, American University Beirut, Lebanon

Session Introduction

Title: Determination of boiling point of petrochemicals by gas chromatography-mass spectrometry and multivariate regression analysis of structural activity relationship
Sayo Fakayode, North Carolina A&T State University, USA
Title: Feedback control over the chlorine disinfection process at a wastewater treatment plant using a smith predictor, a method of characteristics and odometric transformation
Feridun Demir, Osmaniye Korkut Ata University, Turkey

Title: CFD and process simulations of air gasification of plastic wastes in a conical spouted bed gasifier
Abdallah S Berrouk, The Petroleum Institute, UAE

Title: Modelling approaches for the estimation of irreducible water saturation and heterogeneities of the commercial Ashtart reservoir from the Gulf of Gabès, Tunisia
Fatma Taktak, UMS University, Dubai
Title: Liquid phase oxidation of cyclohexane using supported novel metals: Catalytic oxidation or autoxidation?
Xi Liu, Cardiff University, UK
Title: Mathematical modelling of the aqueous phase reforming of sorbitol
Joseph Zeaiter, American University Beirut, Lebanon

Coffee Break @ Atrium

Title: Fixed-bed catalytic wet peroxide oxidation of phenol with titania and Au/titania catalysts in dark
Miron Landau, Ben-Gurion University of the Negev, Israel
Title: Process simulation-based optimization of a commercial amine gas sweetening unit
Abdallah S Berrouk, The Petroleum Institute, UAE
Title: The features of structural transformations of asphaltene molecules during hydro conversion of vacuum residue in the presence of nanosized molybdenum disulfide particles
Olga Zaitceva, Gubkin Russian University of Oil and Gas, Russia
Title: New catalyts for biodiesel of 1st and 2nd generation
Wolfgang F Hoelderich, TCHK Holderich-Consultancy, Germany
Title: Foamability and foam stability of several surfactants solutions: The role of salinity and oil presence
Abdulrahman AlQuraishi, King Abdulaziz City for Science and Technology, Saudi Arabia
Title: A four coefficient model for extending the heptanes-plus fraction for gas condensate systems
Raffie Hosein, The University of The West Indies, West Indies

Lunch Break @ Atrium

Track 11: Chemical Reaction Engineering & Applications
Track 12: Processing Technology & Separation Techniques
Track 15: Reservoir Engineering

Session Chair: Romain Lemaire, Université Lille Nord de France, France
Session Co-Chair: Erik Von Harbou, University of Kaiserslautern, Germany

Session Introduction

Title: Operational behavior and reforming kinetics over Ni/YSZ of a planar type pre-reformer for SOFC systems
Van Nhu Nguyen, Forschungszentrum Jülich GmbH, Germany
Title: Analysis of oil sands bitumen pyrolysis based on thermogravimetry and Py-GC/MS
Sangcheol Shin, Korea University, South Korea
Title: Tuning photocatalytic activity of carbon-based asemblies by their morphology and surface functionalization
Grigoriy A Sereda, University of South Dakota, USA
Title: Non-equilibrium modellingof simulated moving bed processes for separation of Xylenes in petrochemical industry
Ahmet R Ozdural, Hacettepe University, Turkey
Title: Morphological analysis and optimisation of heterogeneously catalysed reactive distillation of complex chemical systems
Erik Von Harbou, University of Kaiserslautern, Germany
Title: Experimental investigation of the transport mechanism of several gases during the CVD post-treatment of nanoporous membranes
Anastasios Labropoulos, NCSR Demokritos, Greece

Coffee Break @ Atrium

Title: Novel hydrophilic and oleophobic hollow fiber membrane for effective and low fouling oil/water separation applications
Renbi Bai, National University of Singapore, Singapore
Title: Experimental analysis of the sooting tendency of different oxygenated molecules used as additives in a diesel surrogate
Romain Lemaire, Université Lille Nord de France, France
Title: Coarse-grained simulations of Multiphase distribution in porous media, with application for oil and for gas hydrates
David Wu, Colorado School of Mines, USA

Title: Behavior of oxidative amorphous alloy $Co_{72}Nb_{24}B_4$ on catalytic cracking of methanol to olefin production
Luciano Nascimento, University Pernambuco-UFPE, Brazil
Title: Use alloy quasicrystalline $Al_{62,2}Cu_{25,3}Fe_{12,5}$ for steam reforming of methanol
Lourdes Cristina Lucena Agostinho Jamshidi, University Pernambuco-UFPE, Brazil

Title: Enhanced oil recovery by injection of nanoemulsion systems
Tereza Neuma de Castro Dantas, Federal University of Rio Grande do Norte, Brazil
Title: Multivariable constrained predictive control of main steam temperature in ultra-supercritical coal-fired power unit
Shi-He Chen, Guangdong Electric Power Research Institute, China

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Salon A

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Opening Ceremony

Keynote Forum

Introduction

James K. Bashkin
University of Missouri-St. Louis, USA

Brian S. J. Blagg
The University of Kansas, USA

Coffeebreak: @ Foyer

Xiang-Qun (Sean) Xie
University of Pittsburgh, USA

Tulay Aygan Atesin
The University of Texas-Pan American, USA

Track 1: Rational Drug Designing

Session Chair: Victor J Hruby, University of Arizona, USA

Session Co-Chair: Alexander Heifetz, Evotec (UK) Ltd., UK

Session Introduction

Title: Design and investigation of multivalent ligands for the detection and treatment of diseases
Victor J Hruby, University of Arizona, USA
Title: Structure-based drug discovery for GPCRs: From receptors to ligands
Alexander Heifetz, Evotec (UK) Ltd., UK
Title: DNA-binding polyamides designed against E1, E2 binding sites of HPV DNA show dramatic anti-HPV activity in cell and tissue culture
James K Bashkin, University of Missouri-St. Louis, USA
Title: Structure-guided design, synthesis, and evaluation of guanine-derived inhibitors of the eIF4E mRNA-cap interaction
Xiaoqi Chen, Amgen, USA

Lunch Break @ Carol & Patio

Title: The design and discovery of CXCR4 chemokine receptor antagonists through incorporation of GPCR-MedChem based fragments
Larry Wilson, Emory University and Emory Institute for Drug Development, USA
Title: Understanding the essential requirements for success in structure-based design
Gregory L Warren, OpenEye Scientific Software, USA
Title: Site Identification by Ligand Competitive Saturation (SILCS): Computational approach for the identification and optimization of ligands targeting proteins, RNA and other macromolecules
Alexander D MacKerell, University of Maryland, USA
Title: Computer-aided design of glucokinase activators
Meihua Tu, Pfizer, USA
Title: Non-competitive regulation of the human proteasome by natural products and natural product inspired scaffolds
Jetze J Tepe, Michigan State University, USA

Coffee Break @ Foyer

Title: Rational design approaches to find novel ligands targeting the aryl hydrocarbon receptor: successful applications and mechanistic studies
William H Bisson, Oregon State University, USA
Title: Modulations of protein-protein interactions of EGFRs: Structure, inhibition, dynamics and its implications in breast cancer
Seetharama D. Satyanarayanajois, University of Louisiana at Monroe, USA
Title: Development of new antibiotics by targeting essential enzymes in bacteria: Structure-based design and simulation studies
Concepción González-Bello, Universidad de Santiago de Compostela, Spain
Title: Design and synthesis of novel pyrimidone analogues as HIV-1 integrase inhibitors
Guisen Zhao, Shandong University, China
Title: Synthesis and anti-candida activity evaluation of new [1,2,4] triazolo[3,4-b][1,3,4] thiadiazines
Mashooq Ahmad Bhat, King Saud University, Kingdom of Saudi Arabia
Title: Newer approaches to the discovery of glitazones
Praveen Thaggikuppe Krishnamurthy, JSS College of Pharmacy, India

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Tahiti

Track 2: Computer-Aided Drug Design and Structure Determination

Session Chair: Istvan J. Enyedy, Biogen Idec, USA

Session Co-Chair: Nicolas Moitessier, McGill University, Canada

Session Introduction

Title: New approaches to "Hit" optimization
Istvan J. Enyedy, Biogen Idec, USA
Title: Accurate binding site models can be derived from low quality PDB files using an empirical geometry based force field
Colin McMartin, Thistlesoft, USA
Integrating computational approaches into high throughput screening for rational drug discovery
Xin Hu, National Center for Advancing Translational Sciences, National Institutes of Health, USA
Title: Using side-chain models derived from atomic resolution X-ray crystallography to develop force fields which can predict global energy minimum geometries
Regine S Bohacek, BostondeNovo, USA

Lunch Break @ Carol & Patio

Title: Forecaster: A computational tool for drug design and discovery developed by experimentalists for experimentalists
Nicolas Moitessier, McGill University, Canada
Title: Genes to Leads: A rational structure guided lead discovery technology that works for both enzymes and protein-protein interaction targets
Kal Ramnarayan, Sapient Discovery, LLC, USA

Title: Discovery of highly-potent and selective inhibitors for the ABCG2 transporter
Achene Boumedjel, Université Joseph Fourier de Grenoble, France
Title: Predictive application of bioisostere transformations to identify novel high quality compound ideas
Matthew Segall, Optibrium Ltd., UK
Title: Novel sildenafil analogues: Possible drugs for increased sensitivity to chemotherapeutic agents
Aina Westrheim Ravna, University of Tromso, Norway

Coffee Break @ Foyer

Title: Structural insights of SIR2 proteins from T. cruzi as promising targets to fight against Chagas disease
Alessandra Nurisso, University of Geneva-University of Lausanne, Switzerland
Title: Stratification of surface lysine residues of bovine testicular hyaluronidase on the base of its 3D structure model: Computer aided drug designing of chondroitin sulphate modified enzyme derivative
Alexander V. Maksimenko, Institute of Experimental Cardiology, Russia

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Day 2 October 16, 2013

Salon B

Track 3: Quantitative Structure-Activity Relationships
Track 4: Drug Development and Delivery System
Track 6: Drug Interactions
Track 8: Pharmacognosy

Session Chair: Tatsuya TAKAGI, Osaka University, Japan
Session Co-Chair: Cesar M Compadre, University of Arkansas for Medical Sciences, USA

Session Introduction

Title: In Silico screening for anti-HPV agents using docking studies
Tatsuya TAKAGI, Osaka University, Japan
Title: The development of the tocoflexols, a series of novel vitamin E analogues with enhanced bioavailability
Cesar M Compadre, University of Arkansas for Medical Sciences, USA
Title: New polymeric "ruthenium-cyclopentadienyl" complexes for drug delivery in cancer therapy
Andreia Valente, Universidade de Lisboa, Portugal
Title: Unraveling the human multidrug resistance p-glycoprotein poly-specificity
Pierre Falson, Institute of Biology and Chemistry of Proteins, France

Coffee Break @ Foyer

Title: PK modulation of haptenylated peptides via non-covalent antibody complexation
Stefan Dengl, Roche Diagnostics GmbH, Germany
Title: Tumour active plant derived compounds in combination with targeted therapy towards overcoming drug resistance in ovarian cancer
Fazlul Huq, The University of Sydney, Australia
Title: Designed monofunctional platinums found to have significant antitumor activity
Laila Arzuman, The University of Sydney, Australia
Title: A phytochemical and biological investigation of aloe grandidentata salm.-Dyck
Taghreed Abdou Ibrahim, King Saud University, Saudi Arabia
Title: Docking guided QSAR study on a series of N-acetamideindolecarboxylic acid derivatives acting as HCV NS 5B polymerase inhibitors
Vaishali M. Patil, Bharat Institute of Technology, India

Track 5: Drug Discovery

Session Chair: Gerard Rosse, Dart Neuroscience, USA
Session Co-Chair: Craig M Williams, University of Queensland, Australia

Session Introduction

Title: Innovative approaches to expand medicinal chemistry space
Gerard Rosse, Dart Neuroscience, USA

Lunch Break @ Carol & Patio

Title: Discovery of a first-in-class topically bioavailable kit inhibitor with clinical activity using computational chemogenomics technology
James Hendrix, nPharmakon LLC, USA
Title: Discovery of a small molecule direct keap1-Nrf2 inhibitor as an anti-oxidant inflammation modulator
Magesh Sadagopan, Otsuka Maryland Medicinal Laboratories, Inc., USA
Title: Can cubane act as a benzene isostere?
Craig M Williams, University of Queensland, Australia
Title: Research and development on novel antitumor agents: Preparation, evaluation, and mechanism of low-molecular-weighted phospha sugar derivatives as IER5/Cdc25B targeted antileukemic agents
Mitsuji YAMASHITA, Shizuoka University, Japan
Title: Modulators of FGF-FGFR-Heparan sulfate complex: identifications of allosteric antagonists and oligosaccharide agonists as potential novel therapeutics
Gilbert Lassalle, Sanofi Aventis, France
Title: Chemistry, bioactivity, and computational prediction of binding modes for sarsolenane and capnosane diterpenes as PTP1B inhibitors from the hainan soft coral Sarcophyton trocheliophorum marenzeller
Yue-Wei Guo, Shanghai Institute of Materia Medica, China

Coffee Break @ Foyer

Title: On the field of metallodrugs-new ruthenium compounds as anti-tumor agents
Ana Isabel Tomaz, Universidade de Lisboa, Portugal
Title: Design, synthesis and antidiabetic, cardiomyopathy studies of cinnamic acid-amino acid hybrid analogs
Subir Samanta, Birla Institute of Technology, India
Title: Synthesis and screening of newer quinazolin-3(h)-4-0ne derivatives for anticonvulsant activity
Jayasekhar P Nair, Oman Medical College, Sultanate of Oman
Title: Drug profile matching- drug discovery by polypharmacology-based interaction profiling
Zoltan Simon, Eotvos Lorand University, Hungary
Title: Novel structural elements for drug discovery: Identification, synthesis and application
Pavel Mykhailiuk, Enamine Ltd., Ukraine

Tahiti

Track 12: Recent Research and Developments

Session Chair: John Spencer, University of Sussex, UK
Session Co-Chair: Carsten Detering, BioSolveIT Inc, USA

Session Introduction

Title: Synthesis and evaluation of some novel thiazolidinedione derivatives as PPAR-α/γ dual agonist
Praveen Thaggikuppe Krishnamurthy, JSS College of Pharmacy, India
Title: Unleash the power of the amygdala: How to incorporate MedChem know-how early on in the CADD lead optimization phase
Carsten Detering, BioSolveIT Inc., USA
Title: Drug discovery: Hit to lead, lead to possible clinical candidates-development of androgen receptor down-regulating agents for the treatment of castration resistant prostate cancer
Purushottamachar Puranik, University of Maryland School of Medicine, USA
Title: Synthesis of privileged structure libraries for biological evaluation
John Spencer, University of Sussex, UK

Coffee Break @ Foyer

Title: Design, synthesis and pharmacological evaluation of novel hybrid compounds to treat sickle cell disease symptoms
Jean Leandro Dos Santos, State University of Sao Paulo, Brazil
Title: Evaluation of serum levels of cadmium and lead in occupationally exposed painters with administration of probiotic (Lactobacillus pentosus kca 1) supplemented yogurt: A pilot study
Osadolor H. B, University of Benin, Nigeria
Title: Lipid pattern in serum of patients with type 2 diabetes mellitus
Ashur S Eljamil, Tripoli University, Libya
Title: What can we expect from new therapeutic strategies in nano-pharmacology and nano-medicine?
Hans-Christian Siebert, Research Institute for Bioinformatics and Nanotechnology (RI-B-NT), Germany
Title: Mitochondria specific antioxidants and their derivatives in the context of the drug development for neuro degeneration and cancer
Gjumrakch Aliev, GALLY International Biomedical Research Consulting LLC, USA

Poster Presentations @ Carol & Patio
Cocktails Sponsored by **Drug Designing: Open Access @ Foyer**

Day 3 October 17, 2013

Salon A

Track 10: Receptors and Inhibitors

Session Chair: Prabagaran Narayanasamy, University of Nebraska Medical Center, USA

Session Co-Chair: Xiang-Qun (Sean) Xie, University of Pittsburgh, USA

Session Introduction

Title: The Hsp90 C-terminal binding site, instructions for and ramifications of inhibition
Brian S. J. Blagg, The University of Kansas, USA
Title: Inhibition of prostanoid receptor EP2: A novel anti-inflammatory therapy for chronic neurodegenerative and autoimmune diseases
Thota Ganesh, Emory University School of Medicine, USA
Title: Selective vitamin K2 biosynthesis inhibitors to treat non-replicating Mycobacterium tuberculosis
Michio Kurosu, University of Tennessee Health Science Center, USA
Title: Inhibitors of fatty acid amide hydrolase (FAAH): SAR and results in pre-clinical pain models
J. Guy Breitenbucher, Dart Neuroscience LLC, USA

Coffee Break @ Foyer

Title: Discovery of novel bicyclic derivatives to stop the growth of mycobacterium tuberculosis by Inhibiting MenA
Prabagaran Narayanasamy, University of Nebraska Medical Center, USA
Title: The synthesis of potential inhibitors of panthothenate synthetase
Kellie L Tuck, Monash University, Australia
Title: Design and synthesis of inhibitors of cysteine protease
Debatosh Majumdar, Glycosyn LLC, USA
Title: Inward rectifier potassium channels as emerging drug targets
Jerod S. Denton, Vanderbilt University School of Medicine, USA
Title: Identification of a new class of SUMO specific protease 2 inhibitors utilizing structure based virtual screening approach
Ashutosh Kumar, Zhang Initiative Research Unit, RIKEN, Japan
Title: Are D-neurons and trace amine-associated receptor, Type 1 involved in mesolimbic dopamine hyperactivity of schizophrenia?
Keiko Ikemoto, Fukushima Medical University, Japan

Lunch Break @ Carol & Patio

Title: Harnessing human N-type Ca2+ channel receptor by identifying the atomic hotspot regions for its blocker design
C. Gopi Mohan, Amrita Vishwa Vidyapeetham University, India
Title: Discovery of small molecule inhibitors of protein-protein interactions using DNA-encoded chemical libraries
Nils Jakob Vest Hansen, Vipergen ApS, Denmark
Title: Post-marketing surveillance of active pharmaceutical ingredients in antimalarial drugs used in Malawi
Ibrahim Chikowe, University of Ghana, Ghana

Award Ceremony

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3rd International Conference on
Medicinal Chemistry & Computer Aided Drug Designing
August 18-20, 2014 Beijing, China

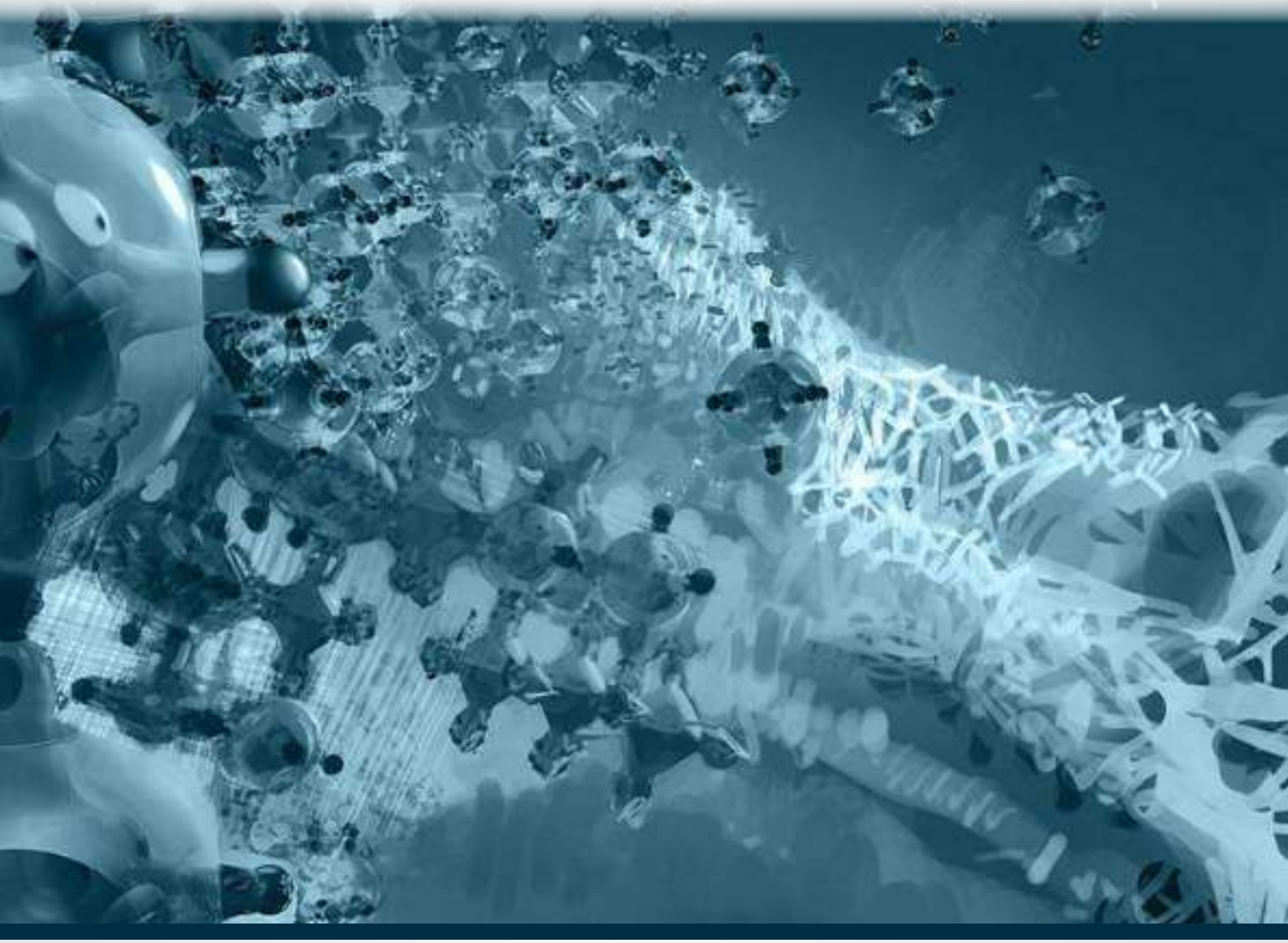
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Day 1 October 22, 2012

Registrations

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Opening Ceremony

Keynote Forum

Introduction

Guy M. Genin
Washington University, USA

Alex V. Vasenkov
CFD Research Corporation, USA

Eugene P. Goldberg
University of Florida, USA

Stephen J Beebe
Old Dominion University, USA

Coffee Break

Track 2: Materials Science & Engineering

Session Introduction

Title: Accelerated material design
Alex V. Vasenkov, CFD Research Corporation, USA
Title: Simple models for plastic deformation and slip avalanches: From crystals to bulk metallic glasses to granular materials
K. A. Dahmen, University of Illinois, USA
Title: Plasticity improvement of Zr-based Bulk Metallic Glasses (BMGs) by laser treatment
P. K. Liaw, The University of Tennessee, USA
Title: Electronic and phonon ransport in bulk quantum dot engineered semiconductors
Pierre F. P. Poudeu, University of Michigan, USA
Title: High throughput tribometer for friction, wear, and adhesion measurements
Vivek Kalihari, The Dow Chemical Company, USA

Lunch Break

Title: Energy of slip nucleation and transmission at grain boundaries
Michael D. Sangid, Purdue University, USA
Title: The materials science of powder sorbents for CO_2 capture at high temperatures
Steven J Milne, University of Leeds, UK
Title: Homogeneity measures in functionally graded materials
Jerzy Ratajski, Koszalin University of Technology, Poland
Title: Structural and dielectric characterization of Nickel-Cobalt oxide nanocomposite
Raveendran R, Nanoscience Research Laboratory, India
Title: Determination of the mechanical properties of carbide composites by spherical instrumented indentation
Fjodor Sergejev, Tallinn University of Technology, Estonia

Coffee Break

Title: Thermo-Mechanical large deformation responses of an aluminum alloy processed by Equal Channel Angular Pressing (ECAP)
Muneer Baig, King Saud University, Kingdom of Saudi Arabia
Title: Entrapment of fungus *Rhizomucor tauricus*, removal of Zn (II) from aqueous solution and spectroscopic characterization
A.V.N Swamy, JNTUniversity, India
Title: Potential use of leaf biomass, *Araucaria heterophylla* for removal of Pb^{+2}
Ch. V.R. Murthy, Andhra University, India
Title: Effect of bio field treatment on the physical and thermal characteristics of Vanadium pentoxide powders
Shrikant Patil, Trivedi Foundation, USA

Title: Evolution of Nickel Silicide contacts in Silicon nanowires during thermal cycling
Alex Katsman, Israel Institute of Technology, Israel
Title: Fixed-free single walled Boron Nitride nanotube based mass sensor
S. P. Harsha, Indian Institute of Technology Roorkee, India

Track 4: Biophysics & Systems Biology
Track 5: Engineering Physics

Title: Mechanical and electrical interactions between cardiomyocytes and cardiac myofibroblasts in a model of fibrotic remodeling
Guy M. Genin, Washington University, USA
Title: Biophysics models and applications in the study of polysaccharides
Antonio Peramo, University of Michigan, USA
Title: Aerosols hand book
Lev Ruzer, Lawrence Berkeley National Laboratory, USA
Title: Modulation of the mechanical response of biomolecular complexes by the dynamics of applied tension
Ruxandra I. Dima, University of Cincinnati, USA
Title: Ultrashort laser modification of transparent materials: Synergy of excitation/relaxation kinetics, thermodynamics, and mechanics
Nadezhda M. Bulgakova, University of Southampton, UK
Title: Pulse power ablation of melanoma and hepatocellular carcinoma with nanosecond pulsed electric fields
Stephen J Beebe, Old Dominion University, USA
Title: Management of heavy metals in ground water- A case study
Sampath kumar M. C, B.M.S College of Engineering, India

Cocktail: Sponsored by Journal of Material Sciences & Engineering

Day 2 October 23, 2012

Registrations

Versailles B

Track 1: Nanotechnology & Nanoscience

Session Introduction

Title: Atomistic simulations of peptide unfolding and translocation by AAA$^+$ biological nanomachines
George Stan, University of Cincinnati, USA
Title: Application of cellulose nanobiocomposite coating in fruits
Kelen Cristina dos Reis, Universidade Federal de Lavras, Brazil
Title: Green-Nanotechnology based smart composite for structural integrity monitoring
Mohamed Saafi, University of Strathclyde, UK
Title: Shape-dependent oriented scaffolding of plasmonic nanoparticles by topological defects for colloidal dimer self-assembly in liquid crystals
Ivan I. Smalyukh, University of Colorado at Boulder, USA
Title: Electric tweezers
Donglei (Emma) Fan, University of Texas at Austin, USA

Coffee Break

Title: Thermosensitive magnetic nanostructured media for hyperthermia and bioimaging
Karen S. Martirosyan, University of Texas at Brownsville, USA
Title: Fabrication and characterization of well-defined organic nanopillar arrays on surfaces
Hai-Feng Frank JI, Drexel University, USA
Title: Fibronectin adsorption on electronically nanostructured biomaterial surfaces
Andreas Kortge, University of Rostock, Germany
Title: Structural complexity at nanoscale: From single nanoparticle to membrane
Xiao-Min Lin, Center for Nanoscale Materials, USA
Title: Prospects for engineering semiconductor nanowire materials for optoelectronics
Harry E. Ruda, University of Toronto, Canada
Title: Lateral energy transfer in thin film quantum dot induced via plasmonic effects
Seyed M. Sadeghi, University of Alabama, USA

Lunch Break

Title: p-Type conduction in ZnO nanowires from Sb-Decorated Head-to-Head basal plane inversion domain boundaries
Andrew B. Yankovich, University of Wisconsin Madison, USA
Title: Real-Time probing of nanophase evolution in solutions
Yugang sun, Center for Nanoscale Materials, USA
Title: The ionic liquid effect on the preparation of epoxy-silica nanocomposites
Henri S. Schrekker, UFRGS, Brazil
Title: Influence of quality factor on the dynamics of single walled carbon nanotube based mass sensor
Anand Y Joshi, G.H.Patel College of Engineering & Technology, India

Title: High temperature nanophotonics: Controlling the flow of thermal radiation
V. Rinnerbauer, Massachusetts Institute of Technology, USA
Title: Controlled GeSi nanoislands: Fabrication and properties
Zhenyang Zhong, Fudan University, China

Coffee Break

Title: Nanocomposite alternatives to rare-earth permanent magnets
Everett E. Carpenter, Virginia Commonwealth University, USA
Title: Engineered nanopores for protein detection
Liviu Movileanu, Syracuse University, USA
Title: Synthesis and characterization of anti-microbial Ag-TiO_2 nano composite particles and their coatings onto 3-D filters
Cansu Noberi, Yildiz Technical University, Turkey
Title: Natural rubber with gold nanoparticles: Estimation of the amount of nanoparticles in a sample using wavelet transforms
Alexandre Siqueira, Unesp, Brazil

Panel Discussion

Breakout

Track 3: Biomaterials & Biomedical Materials
Track 8: Nonlinear Dynamics and Chaos

Title: Biopolymer-Cell implants and injectable gels for CNS Repair
Eugene P. Goldberg, University of Florida, USA
Title: Use of biomaterials for delivery of chemotrophic proteins in the central nervous system
Elisa Tamariz, Universidad Veracruzana, Mexico
Title: Understanding role of length scale and temperature in indentation induced creep and thermal behavior of Si based materials
VikasTomar, Purdue University, USA
Title: Polyoxometalate (POM) nanocluster- Induced phase transition in phospholipid biomembranes
Y. Elaine Zhu, University of Notre Dame, USA
Title: Next generation polymer nanocomposite electrolytes for lithium ion batteries
Haleh Ardebili, University of Houston, USA

Coffee Break

Title: Radiopaque polymeric microspheres for clinical applications
Ketie Saralidze, Maastricht University, Netherlands
Title: Modal damping as index of structural quality
Sofia Panteliou, University of Patras, Greece
Title: The next generation of controlled drug delivery devices based on Micro-Electro-Mechanical-Systems (MEMS) and novel integration of biomaterials
Noel M. Elman, Massachusetts Institute of Technology, USA
Title: Mora tree *(Maclura tintorea)* leaves as a component in polymer
Svetlana Nikolaeva,Costa Rica's National University, Costa Rica
Title: Sulfonated poly (indene) and PVDF hybrid polyelectrolyte polymer membranes for use in fuel cells
Deyse Elisabeth Ortiz Suman Carpenter, University of Blumenau, Brazil

Panel Discussion

Lunch Break

Poster Presentations

B2B meetings

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Day 3 October 24, 2012

Versailles B

Registrations

Track 6 : Atomic and Nuclear Physics
Track 7 : Optics
Track 9 : Advances in Instrumentation and Techniques
Track 10: Materials Chemistry

Session Introduction

Title: Enhancement and recovery in atomic force microscopy images
Alex Chen, University of North Carolina, USA
Title: Smart materials design in non-linear optics for telecommunications
Jacqueline M. Cole, University of Cambridge, UK

Title: Hollow sphere of copper oxide microparticle prepared by free template and low temperature hydrothermal method

Kanda Wongwailikhit, Rangsit University, Thailand

Coffee Break

Title: Spin polarized current in Graphene pumped by a THz-Signal

Aziz N. Mina, Beni-Suef University, Egypt

Title: Enhancement of washfastness of the Lemongrass oil treated mosquito repellent Nylon nets by air plasma pretreatment

Hasabo A Muhammad Ahamed, Africa City of Technology, Sudan

Title: Structural, optical, photoconductivity and humidity sensing properties of biocomposite doped Cobalt oxide

Udaya Aruldoss, Anna University, India

Panel Discussion

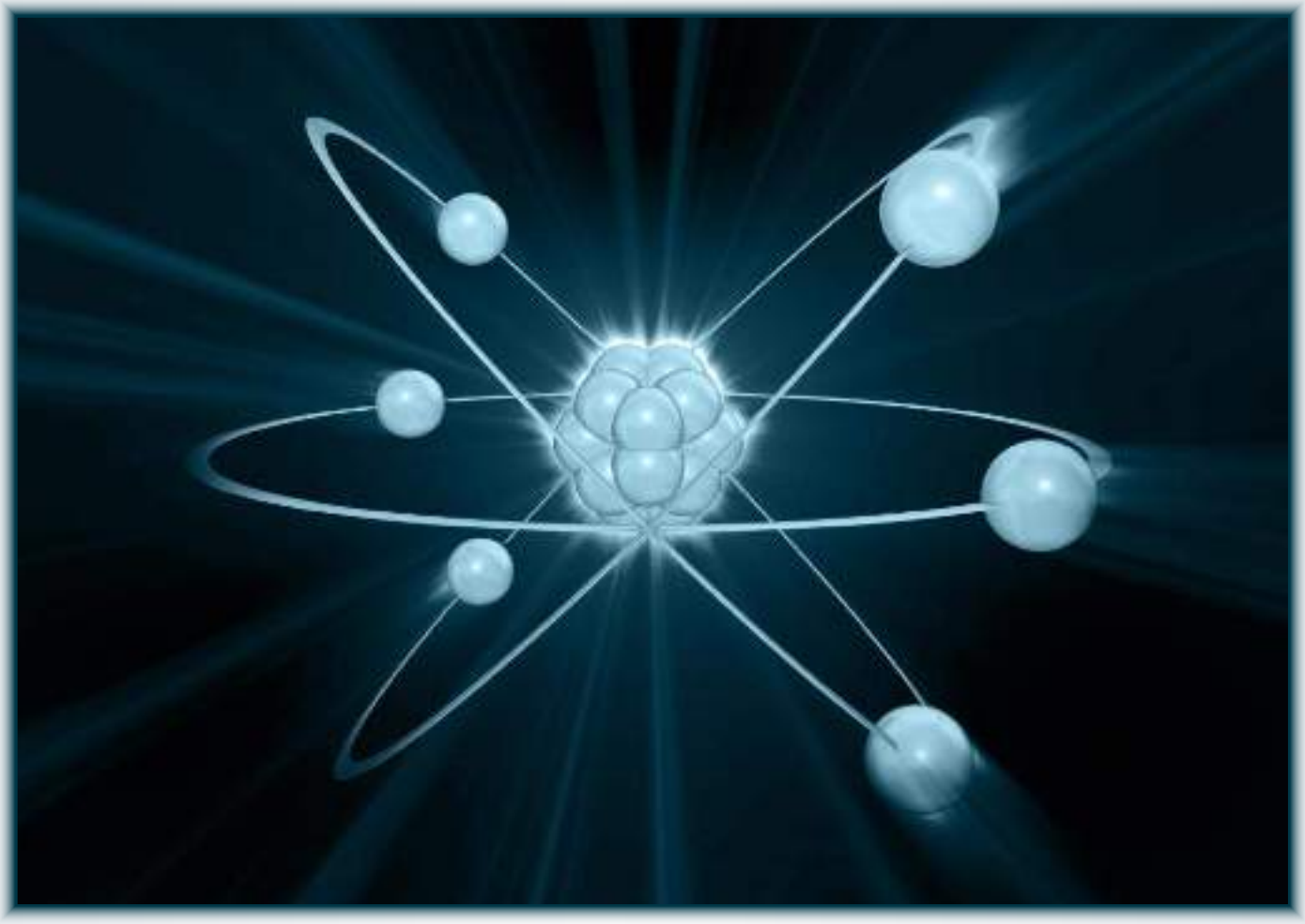
Lunch Break

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