

23-26 JANUARY 2018  
IBEROSTAR CANCÚN, MEXICO

# ATLANTIC BASIN CONFERENCE ON CHEMISTRY

PROGRAM BOOK



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# ABCChem Welcome Message

Welcome to the Atlantic Basin Conference on Chemistry!

On behalf of the contributing societies, the American Chemical Society, the Brazilian Chemical Society, the Canadian Society for Chemistry, the European Association for Chemical and Molecular Science, the Federation of African Societies of Chemistry, the Latin American Federation of Chemical Associations, the Mexican Chemical Society and the South African Chemical Institute, we, the Sponsoring Committee, with great pleasure, welcome all attendees, speakers and guests to the inaugural Atlantic Basin Conference on Chemistry (ABCChem). We are thrilled that you have chosen to join us in beautiful Cancún, Mexico.

As you know, ABCChem is a new, joint conference that will bring together chemists, students, engineers and scientific colleagues from regions around the Atlantic Basin. It has been created to provide opportunities for attendees to share and exchange diverse perspectives, innovative research and scientific ideas. During this exciting time, international presenters will facilitate discussions around four tracks: Chemistry in Biology, Green Chemistry, Materials and Nano Chemistry and Physical/Analytical. With over 150 oral and poster sessions, you will be fully engaged in dialogue resulting in collaboration and innovation. As well, there will be major opportunity for informal networking.

All of the ABCChem committees and associated staff have worked to prepare this conference in hopes that you find it beneficial. We are looking forward to the outcome, suggestions to improve the program and all further opportunities.

**Warm regards,**

**Elsa Reichmanis, Ph.D., ACS Past President**

**David Cole-Hamilton, Ph.D., EuCheMS President**

**Peter Loock, Ph.D., CSC Awards Director**

**Mary Rosales, Ph.D., SQM President**

**Aldo J. G. Zarbin, Ph.D., SBQ President**



# ABCChem Committees

## Sponsoring Societies Committee

**Elsa Reichmanis**, *Committee Chair*, Past President, ACS - United States

David Cole-Hamilton, President, EuCheMS - United Kingdom

Peter Loock, Awards Director, CSC - Canada

Mary Rosales, President, SQM - Mexico

Aldo J. G. Zarbin, President, SBQ - Brazil

## Technical Programming Committee

**Paul Weiss**, *Committee Chair*, Editor, ACS Nano - United States

Mamia El Rhazi, Vice Chair, FASC - Morocco

Ann English, Conference Director, CSC - Canada

Bice Martincigh, President, SACI - South Africa

Luis Oro, Past President, EuCheMS - Spain

Norberto Peporine Lopes, SBQ - Brazil

Eduardo Pereira, President, FLAQ - Chile

Lena Ruiz Azuara, Past President, SQM - Mexico

## Budget Committee

**Bill Carroll**, *Committee Chair*, Past President, ACS - United States

Francesco De Angelis, Treasurer, EuCheMS - Italy

André Galembeck, Incoming Treasurer, SBQ - Brazil

Jason Pearson, Incoming Treasurer, CSC - Canada

Olivia Sparza, Director, SQM - Mexico



## *Host Society Welcome Message*

The Mexican Chemical Society welcomes you to this first ABCChem, a meeting that brings together chemical professionals from countries around the Atlantic Basin. We are very happy to have you, our colleagues, in Cancún—allowing us to both meet you and get to know more about your chemical research. Some attendees are from locations close by, others are more distributed geographically, but in all cases we are brought together here by both our common ocean and a shared interest in chemistry.

Meetings open opportunities for starting collaboration with colleagues from different institutions which can lead to better results by the nature of our different professional experiences as well as different facilities. Recent cuts in funding for science in different parts of the world makes collaboration an even more important way of carrying out research projects.

We hope that this meeting will be an excellent opportunity to have fruitful scientific discussions and be the beginning of new friendships with our colleagues. We also wish that this first ABCChem serves as the start of a long list of periodic meetings of this type.

We, the Mexican hosts, are very happy to welcome you to this beautiful resort where you can not only enjoy beautiful beaches but also learn something of the very rich Mayan culture.

**Welcome to the ABCChem meeting and enjoy your visit to Cancún!**

**Dr. María del Jesús Rosales Hoz**

**President**

**Mexican Chemical Society**



## General Information

### Registration and Badges

Registration will be located in the Foyer Caribe, and on-site registration will be available. All ABCChem participants and speakers must be registered to attend meeting events. Badges must be displayed at all times during the conference.

### Lost and Found

Items lost or found in meeting rooms should be turned in to the ABCChem Operations Office located in the Convention Office room. Items not claimed from the operations office by the end of the conference will be turned over to hotel security.

### In Case of Emergency

The phone number to report emergencies in Mexico is 911. To reach an ambulance, call 065, fire department, 068, and police department, call 060.

### To Reach a Hospital

There are several hospitals in the area. To reach Hospital Galenia, dial +52 (998) 891-5200, Hospiten Cancún +52 (998) 881-3700, or Amerimed Cancún Hospital +52 (998) 881-3400. For more information on hospitals, ask at your hotel or dial tourist assistance.

### Currency Exchange

Currency may be exchanged at most major airports and some banks; however many banks require an account there for such transactions. ATMs are another option and often offer a better exchange rate, but a commission fee is added to each transaction.

### Transportation Inside Cancún's Hotel Zone

Uber is available as one transportation option in Cancún, as well as taxis. Most hotels have current taxi fares and destinations posted, but ask at the front desk for more information if necessary. Additionally, buses are available along the hotel zone.

### General Tourist Assistance

While visiting Cancún, call 078 from any phone for free information on tourist attractions, airports, car rental companies, embassies and consulates, fairs and exhibitions, hotels, hospitals and financial services. Additionally, the Consular Corps liaison office provides basic visitor information and helps connect international visitors to accredited consular representatives in Mexico. Casa Consular is located in Cancún's hotel zone on Kukulcan Boulevard, km 13.

### Tourist Attractions

While in Cancún, enjoy the city's beaches or visit ancient Mayan architecture in the Tulum Archaeological Zone. Another option is an eco-archaeological park Xcaret where you can swim in a lagoon or visit Mexico's first butterfly sanctuary. Additionally, you can tour the Isla Mujeres, La Tortugranja turtle farm.

### ABCChem Recording Policy

The use of any device to capture images (e.g., cameras and camera phones) or sound (e.g., tape and digital recorders) or stream, upload or rebroadcast speakers or presentations is strictly prohibited at all official ABCChem meetings and events without the express written consent from the ABCChem Sponsoring Societies Committee.



## Schedule-at-a-Glance

### Tuesday, 23 January

12:00 PM – 7:00 PM

5:00 PM – 7:00 PM

#### Registration

*Foyer Caribe*

Welcome Reception

*Pool Deck*

### Wednesday, 24 January

7:30 AM – 6:00 PM

9:00 AM – 10:00 AM

10:00 AM – 10:50 AM

10:50 AM – 11:00 AM

11:00 AM – 12:00 PM

#### Registration

*Foyer Caribe*

Plenary Session: Jorge Peón Peralta

*Grand Caribe 5-6*

Invited Speaker Sessions

*Grand Caribe 7-8, Isla Ballroom 1-6*

Coffee Break

*Grand Caribe 1-4*

Concurrent Oral Abstract Sessions

*Grand Caribe 7-8, Isla Ballroom 1-6*

12:00 PM – 1:30 PM

#### Lunch Break

1:30 PM – 2:25 PM

2:00 PM – 3:20 PM

3:20 PM – 3:30 PM

3:30 PM – 4:10 PM

4:10 PM – 5:30 PM

5:30 PM – 6:25 PM

6:30 PM – 8:00 PM

Plenary Session: Aziz Amine

*Grand Caribe 5-6*

Invited Speaker Sessions

*Grand Caribe 7-8, Isla Ballroom 1-6*

Coffee Break

*Grand Caribe 1-4*

Concurrent Oral Abstract Sessions

*Grand Caribe 7-8, Isla Ballroom 1-6*

Poster Presentations & Expo

*Grand Caribe 1-4*

Plenary Session: Doug Stephan

*Grand Caribe 5-6*

Younger Chemists Networking Session

*Grand Caribe 1-4*





# Schedule-at-a-Glance

## Thursday, 25 January

**7:30 AM – 6:00 PM**

### Registration

*Foyer Caribe*

9:00 AM – 10:00 AM

Plenary Session: Avelino Corma

*Grand Caribe 5-6*

10:00 AM – 10:50 AM

Invited Speaker Sessions

*Grand Caribe 7-8, Isla Ballroom 1-6*

10:00 AM – 12:00 PM

### A Crash Course in Professional Development for Younger Chemists

*Miramar 3*

10:00 AM	Introduction and Welcome – Natalie LaFranzo
10:10 AM	Scientific Presentations- Tips, Tricks and Tools – Alice Soldà
10:30 AM	Innovation and Leadership Styles – Natalie LaFranzo
10:50 AM	Intermission
11:00 AM	A postdoc in Europe? Why and how? – Victor Mougel
11:20 AM	Social Media and Networking – Matthew Grandbois
11:40 AM	Panel Discussion

10:50 AM – 11:00 AM

Coffee Break

*Grand Caribe 1-4*

11:00 AM – 12:00 PM

Concurrent Oral Abstract Sessions

*Grand Caribe 7-8, Isla Ballroom 1-6*

**12:00 PM – 1:30 PM**

### Lunch Break

1:30 PM – 2:25 PM

Plenary Session: Fernando Galembeck

*Grand Caribe 5-6*

2:00 PM – 3:20 PM

Invited Speaker Sessions

*Grand Caribe 7-8, Isla Ballroom 1-6*

3:20 PM – 3:30 PM

Coffee Break

*Grand Caribe 1-4*

3:30 PM – 4:10 PM

Concurrent Oral Abstract Sessions

*Grand Caribe 7-8, Isla Ballroom 1-6*

4:10 PM – 5:30 PM

Poster Presentations & Expo

*Grand Caribe 1-4*

5:30 PM – 6:25 PM

Plenary Session: Timothy Egan

*Grand Caribe 5-6*



## Schedule-at-a-Glance

### Friday, 26 January

#### 7:30 AM - 5:00 PM

9:00 AM - 10:00 AM

10:00 AM - 10:50 AM

10:50 AM - 11:00 AM

11:00 AM - 12:00 PM

#### Registration

*Foyer Caribe*

Plenary Session: Galo Soler Illia

*Grand Caribe 5-6*

Invited Speaker Sessions

*Grand Caribe 7-8, Isla Ballroom 1-6*

Coffee Break

*Grand Caribe 1-4*

Concurrent Oral Abstract Sessions

*Grand Caribe 7-8, Isla Ballroom 1-6*

#### 12:00 PM - 1:30 PM

#### Lunch Break

1:30 PM - 2:25 PM

Plenary Session: Laura Kiessling

*Grand Caribe 5-6*

2:00 PM - 3:20 PM

Invited Speaker Sessions

*Grand Caribe 7-8, Isla Ballroom 1-6*

3:20 PM - 3:30 PM

Coffee Break

*Grand Caribe 1-4*

3:30 PM - 4:10 PM

Concurrent Oral Abstract Sessions

*Grand Caribe 7-8, Isla Ballroom 1-6*

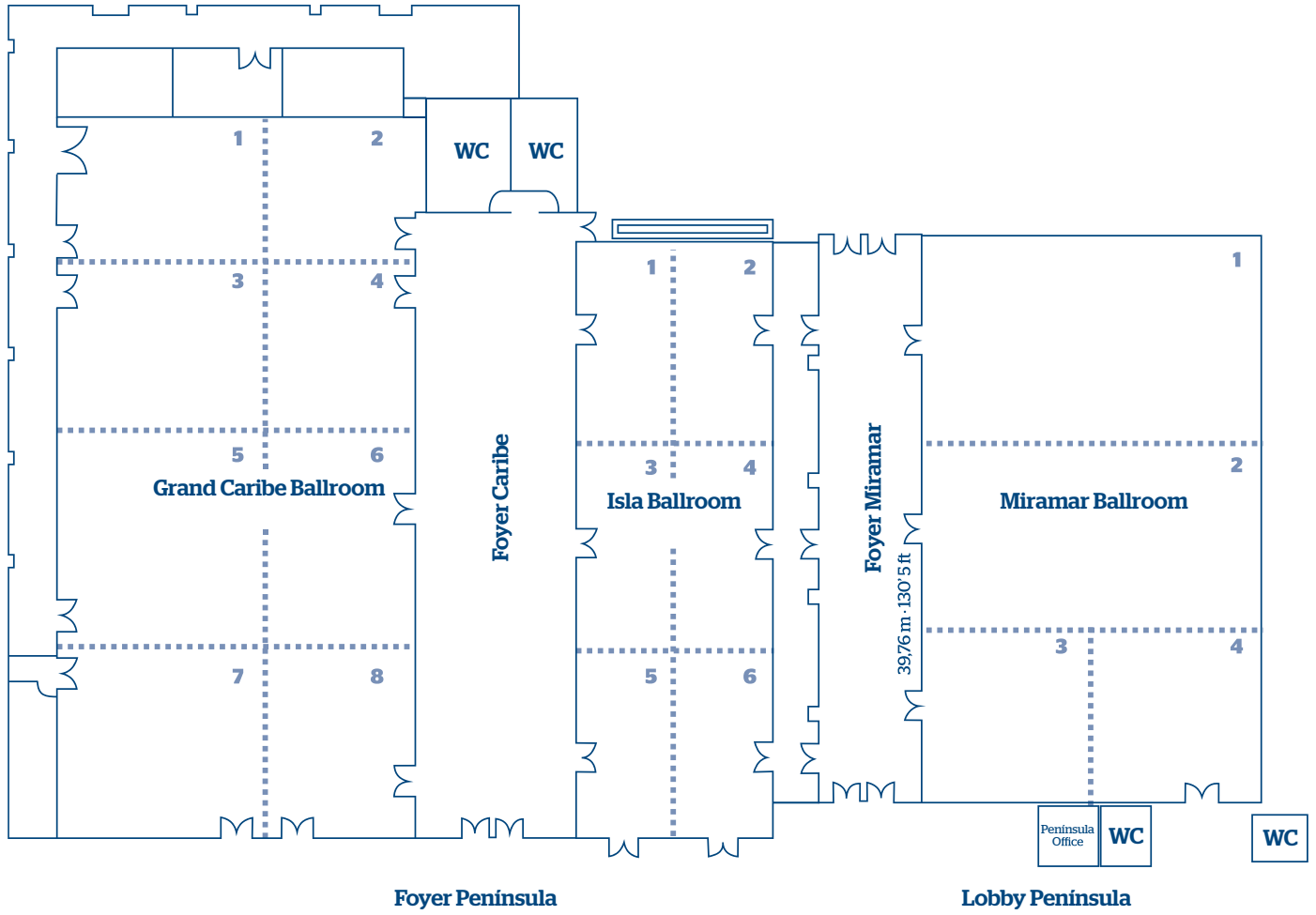
5:30 PM - 8:00 PM

Closing Banquet

*Miramar 1-2*



# Meeting Room Floor Plan



**Plenary Session**

| **Jorge Peón Peralta**  
**M. J. Rosales-Hoz**, *Organizer, Presiding*

**GRAND CARIBE 5/6**

**9:00 AM**

**1.** Bichromophoric systems: Design variables and applications.  
**J. Peón Peralta**

**Chemistry in Biology**

| **A. Amine, N. P. Lopes**, *Organizers*  
**L. Quintanar**, *Presiding*

**ISLA BALLROOM 1/2**

**10:00 AM**

**2.** Discovery and characterisation of novel glycoenzymes for glycoside synthesis and antigen removal using metagenomic screens. **S.G. Withers**

**10:30 AM**

**3.** Carbamoylimidazoles as novel cruzain inhibitors having in vitro and in vivo activity against *Trypanosoma cruzi*. **A.D. Andricopulo**, M. Souza, R. Ferreira, C.O. Rezende Junior, L.G. Ferreira, R. Chavez, B. Slafer, L.G. Magalhaes, R. Krogh, F.C. Cruz, L.C. Dias

**10:50 AM**

Intermission

**11:00 AM**

**4.** Withdrawn

**11:20 AM**

**5.** Exploration of molecular recognition processes. **K.M. Merz**

**11:40 AM**

**6.** Neurotransmitter sensing via aptamer-field-effect transistors. **A. Andrews**

**Green Chemistry****Green Chemical Synthesis & Catalysis**

| **K. Barta, R. Palkovits**, *Organizers*  
**D. Cole-Hamilton**, *Presiding*

**ISLA BALLROOM 5/6**

**10:00 AM**

**7.** One-pot synthesis of pyrrolo[3,4-b]pyridin-5-onas by MCR: Diversity oriented synthesis approach. **E. González-Zamora**

- 10:30 AM**                      **8.** Selective hydrofunctionalization of alkynes promoted by rhodium-N-heterocyclic carbene catalysts. **L.A. Oro**
- 
- 10:50 AM**                      Intermission
- 
- 11:00 AM**                      **9.** Chelating azolyidene and Ru<sup>II</sup> complexes: Effect of pendant arm and co-ligands in catalytic transfer hydrogenation. **J. Olguín**
- 
- 11:20 AM**                      **10.** Recent advances in sustainable methods for fluorination and fluoroalkylation. **S.B. Munoz**, V. Krishnamurti, X. Ispizua Rodriguez, G. Prakash
- 
- 11:40 AM**                      **11.** Eco-friendly route to functionalized amines and suzuki cross-coupling reactions. **H. Kumpaty**, P. Kha

**Materials &  
Nano Chemistry**

| **J. P. Attfield, H. Huppertz, Organizers**  
**L. Ruiz Azuara, Presiding**

**GRAND CARIBE 7/8**

- 10:00 AM**                      **12.** Aerosol-based synthesis of nanosized and nanostructured materials as versatile and sustainable synthetic methodologies. **A. García Márquez**
- 
- 10:30 AM**                      **13.** Catalytic conversion of ethanol to butadiene: Detailed DFT investigation of the complex reaction mechanism. **V. Butera**, Y. Choe, Y. Tanabe, T. Miyazawa, T. Fujitani
- 
- 10:50 AM**                      Intermission
- 
- 11:00 AM**                      **14.** Optical confinement to induce forbidden phosphorescence in BA1q. **L. Gonzalez Urbina**
- 
- 11:20 AM**                      **15.** Toward a thermodynamic profile for Cadmium-based quantum dot surface chemistry using isothermal titration calorimetry. **M.Y. Gee**, A.B. Greyak
- 
- 11:40 AM**                      **16.** Bis and tris-chelate pyridylimidazolyl-2-chalcogenone M<sup>2+</sup> (M = Fe, Co, Ni and Zn) complexes: Structural and magnetic properties. **D. Plaza Lozano**, J. Olguín, N. Ortiz Pastrana



## Wednesday Morning

### Materials & Nano Chemistry

### Materials for Catalysis

| J. P. Attfield, H. Huppertz, *Organizers*  
A. Corma, *Presiding*

ISLA BALLROOM 3/4

**10:00 AM** 17. Unraveling the mystique of mixed halide lead halide perovskites. **P.V. Kamat**

**10:30 AM** 18. Immobilization of Metallo-NHC complexes onto silica surfaces: Preparation, structure elucidation and catalytic performances. **C. Thieuleux**

**10:50 AM** Intermission

**11:00 AM** 19. Synthesis of NHC-stabilized metal nanoparticles and their catalytic application in the selective hydrogenation of alkynes. **C. Claver**, M. Diaz de los Bernardos, S. Perez Rodriguez, C. Godard

**11:20 AM** 20. Electrocatalytic behaviour of cobalt phthalocyanines in the presence of graphene quantum dots. **S.S. Centane**

**11:40 AM** 21. Earth-abundant heterogeneous catalysts for CO<sub>2</sub> reduction and water oxidation. **V. Mougel**, T. Huan, F. Jaouen, M. Fontecave



## Wednesday Afternoon

### Plenary Session

| Aziz Amine  
M. El Rhazi, *Organizer, Presiding*

GRAND CARIBE 5/6

**1:30 PM** 22. Analytical aspects of biosensors based on enzyme inhibition. **A. Amine**

### Chemistry in Biology

| A. Amine, N. P. Lopes, *Organizers*  
A. D. Andricopulo, *Presiding*

ISLA BALLROOM 1/2



# Wednesday Afternoon

- 2:30 PM** 23. Integrative metabolomics analysis of the Brazilian Biodiversity. **N.P. Lopes**
- 
- 3:00 PM** 24. Synthesis of halogenated furanones with bactericidal activity against drug-resistant strains of *Pseudomonas aeruginosa*. **M. Martinez-Vazquez**, V. Castro-Torres, N. Ramirez-Duran, P. Moreno-Pérez, R. García-Contreras
- 
- 3:20 PM** Intermission
- 
- 3:30 PM** 25. Vinylaziridines useful intermediates for synthesising sphingosines. **S. Castillon**, I. Gimenez, M. Escudero-Casao, A. Cardona, M. Corro, Y. Díaz, I. Matheu
- 
- 3:50 PM** 26. Synthesis of solvatochromic probes to label the mycobacterial cell wall and their use in studies of the effect of host microenvironment on anti-tuberculosis drug efficacy in vivo. **S.G. Keyser**, M. Kamariza, A. Utz, A. Pezacki, C.R. Bertozzi

**Green  
Chemistry**

**Nanoscience &  
Green Chemistry**

| **K. Barta, R. Palkovits**, *Organizers*  
**F. Heidari**, *Presiding*

**ISLA BALLROOM 5/6**

- 2:30 PM** 27. Supramolecular approaches to control selectivity in transition metal catalysis via the second coordination sphere. **J. Reek**
- 
- 3:00 PM** 28. Full property recovery after multiple recycling steps of melt-reprocessed polymer networks and cross-linked polymer composites: Novel one-step synthetic approaches for models of fully recyclable, reprocessable rubber tires and non-isocyanate-based polyurethanes. **J. Torkelson**, K. Jin, L. Li, X. Chen
- 
- 3:20 PM** Intermission
- 
- 3:30 PM** 29. Bioplastics and their role in achieving global sustainability. **C.I. Awuzie**
- 
- 3:50 PM** 30. Ethical and societal implications of nanotechnology: Practical information for nanoscientists. **L.M. Gibbs**

**Materials &  
Nano Chemistry****Polymer  
Materials**

| J. P. Attfield, H. Huppertz, *Organizers*  
E. González-Zamora, *Presiding*

ISLA BALLROOM 3/4

**2:30 PM**

**31.** Polymers to patterns: Using self-assembly to produce complex nanopatterns on semiconductors and flexible substrates. **J.M. Buriak**, E.J. Lubber, C. Jin, B.C. Olsen

**3:00 PM**

**32.** Anchored metal polymers derived from metal complexes of the Group 11 with unsaturated N-heterocyclic carbene ligands. **F.J. Zuno Cruz**, D.O. González Ábrego, G. Sánchez Cabrera, H. López Ruiz, N. Andrade López, M. Rosales-Hoz, M.A. Leyva, J.R. Torres Lubián

**3:20 PM**

Intermission

**3:30 PM**

**33.** Preparation of hyperbranched polyethyleneimine(hpei)-cysteamine intergrated thin film composite membranes for heavy metal removal. **B.E. Mosikatsi**

**3:50 PM**

**34.** Effect of temperature in the isomerization of 1-butene using supported  $Al_2Br_6$  catalysts. **S. Kanitkar**, N. Kumar, J. Carter, K. Ding, G. Hutchings, J.J. Spivey

**Physical &  
Analytical  
Chemistry****Analytical  
Chemistry**

| B. S. Martincigh, *Organizer*  
E. M. Flores, *Presiding*

GRAND CARIBE 7/8

**2:30 PM**

**35.** Increasing metabolite coverage and data quality in untargeted LC-MS metabolomics. **D. Vucko**

**3:00 PM**

**36.** Development of monolithic capillary columns and  $\mu$ -chip for separation of intact proteins for nanoscale liquid chromatography. **W.P. Batiston**, E. Carrilho

**3:20 PM**

Intermission





## Wednesday Afternoon

**3:30 PM**

37. Withdrawn

**3:50 PM**

38. Fighting low quality pharmaceuticals through the development and optimization of an affordable paper-medium antibiotic assay. **A. Cooper**, M. Lieberman



## Wednesday Evening

**Green Chemistry**

| **K. Barta, R. Palkovits**, *Organizers*

**GRAND CARIBE 1-4**

**4:10 - 5:30 PM**

39. Production of biodiesel from vegetable oil. **E.K. Ortiz**

40. Direct C(sp<sup>2</sup>)-H trifluoromethylation of enamides using Ruppert-Prakash reagent. **X. Ispizua Rodriguez**, S.B. Munoz, V. Krishnamurti, G. Prakash

41. Green approach for the removal of pollutants from aqueous systems. **J.F. Amaku**, B.S. Martincigh

42. Sustainable approaches to iron-catalyzed cross-coupling of aryl chlorides and tosylates. **E. Bisz**, M. Szostak

**Materials &  
Nano Chemistry**

| **J. P. Attfield, H. Huppertz**, *Organizers*

**GRAND CARIBE 1-4**

**4:10 - 5:30 PM**

43. Withdrawn

44. Maximizing catalysis of nanoparticles via their monolayer assembly on nitrogen-doped graphene. **X. Guo**

**4:10 - 5:30 PM****45.** Withdrawn

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**46.** Synthesis of organosilica nanoparticles using sugarcane waste ash and application as adsorbent material. **D.A. Fungaro**, J. Santos, P. Corio, S. Rovani

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**47.** Cellulose-based nanostructured composites and devices: The case of graphite and metal oxide films. **B.C. Batista**, P. Abreu Filho, J. Santos, R. dos Santos, F. Galembeck

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**48.** Self-cleaning membrane to control fouling by suspended particles. **D. Chen**, C. Pomalaza-Raez, P. Wirges

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**49.** Poly(acrylic acid) grafted ceramic microfiltration membrane to mitigate fouling of natural organic matter. **D. Chen**, Q. Yang

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**50.** Au-Au vs Au-S interactions: Fluorination directing the crystalline supramolecular arrangement in luminescent gold compounds. **L. Moreno Alcántar**, M. Flores-Álamo, H. Torrens Miquel

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**51.** Hydrogels of acrylic acid and chemically modified lignin for the removal of heavy metal ions. **D. Rico García**, E. Orozco, L. Guerrero, S. Hernandez

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**52.** Poly and pseudomorphism of a crystalline carbazole-xylylene-carbazole rotor and their characteristic intramolecular dynamics. **A. Aguilar**, S. Pérez-Estrada, B. Rodríguez-Molina

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**53.** Synthesis, characterization and photophysics properties of carbazole-acceptor-carbazole molecular compasses. **L.A. Rodríguez**, A. Aguilar, B. Rodríguez-Molina

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**54.** Amphidynamic behavior in crystalline rotors with bromo-carbazole stators. **J.A. Colin**, B. Rodríguez-Molina

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**55.** Withdrawn

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**56.** Suzuki-Miyaura reactions and solvent-free oxidation of benzyl alcohol by synthesized nitrogen-doped CNTs/Pd catalyst. **A.H. Labulo**, B. Omondi, V. Nyamori

**4:10 - 5:30 PM**

**57.** Unexpected reactivity of phosphorene in dry DMSO. **M. Serrano Ruiz**, M. Caporali, G. Manca, A. Ienco, M. Peruzzini

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**58.** Magnetic coordination polymers built from oxamate and oxamidate ligands. **H.O. Stumpf**, C.L. Pereira, E.F. Pedroso

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**59.** Carbon-supported PtRu nanoparticles as methanol fuel cell catalysts. **H.S. Abbo**, S. Titinchi

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**60.** Eggshells and membranes for removal of Cr (VI) from aqueous solutions. **J. Badillo Camacho**

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**61.** *In vitro* evaluation of a coordination compound copper (II) mixed chelates (Casiopeina® III-ia) loaded in a niosomal system. **Z. Aguilar Jimenez**, L. Ruiz Azuara

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**62.** Synthesis and reactivity of transition metal clusters containing functionalized alkynes as ligands. **E.J. Aldeco**, A. Carrasco, J.L. Silva, O.R. Reyes, M.J. Rosales-Hoz

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**63.** Isomerization in gold(I) complexes with 1,2-bis(diphenylphosphine) ethylene and fluorinated thiolates ligands. **G. Islas**, L. Moreno Alcántar, M. Flores-Álamo, H. Torrens Miquel

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**64.** Learning about molar ratio curves: The case of several non-quantitative formation reactions. **A. Rojas-Hernandez**, M. Ramírez-Silva, G. Álvarez-Romero, M. Palomar-Pardavé

**Plenary  
Session**

| **Doug Stephan**  
A. M. English, *Organizer, Presiding*

**GRAND CARIBE 5/6****5:30 PM**

**65.** Frustrated Lewis pair chemistry: An avenue to metal-free synthesis and catalysis. **D. Stephan**

**Plenary Session**

| **Avelino Corma**  
L. A. Oro, *Organizer, Presiding*

**GRAND CARIBE 5/6**

**9:00 AM**

**66.** Green chemistry with heterogeneous catalysis. **A. Corma**

**Chemistry in Biology**

| **A. Amine, N. P. Lopes, Organizers**  
L. Ruiz Azuara, *Presiding*

**ISLA BALLROOM 1/2**

**10:00 AM**

**67.** Metal-induced aggregation of human lens crystallins: Uncovering the bioinorganic facet of cataracts disease. **L. Quintanar**

**10:30 AM**

**68.** Bioorthogonal organometallic chemistry: Overview, applications and state-of-the-art. **A. Unciti-Broceta**

**10:50 AM**

Intermission

**11:00 AM**

**69.** Withdrawn

**11:20 AM**

**70.** Exploring the properties of the oxo-centered triruthenium: From fundamental aspects to potential biological applications. **C.F. Silva**, L.C. Ramos, S. Nikolaou

**11:40 AM**

**71.** Development of drug-eluting transplants. **B. Kane**, B. Akinbobuyi, C.A. Chang, J.M. Quintana, B. Naziruddin

**Green Chemistry****Green Chemical Synthesis & Catalysis**

| **K. Barta, R. Palkovits, Organizers**  
L. A. Oro, *Presiding*

**ISLA BALLROOM 5/6**

**10:00 AM**

**72.** Sustainability through chemistry: Conversion of CO<sub>2</sub> into fuels and chemicals. **C.J. Mota**

- 10:30 AM**                      **73.** Catalytic production of chemicals from waste bio-oils.  
**D. Cole-Hamilton**, Y. Shi
- 
- 10:50 AM**                      Intermission
- 
- 11:00 AM**                      **74.** Direct arylation as a greener synthetic tool for the preparation of organic materials. **T.M. Pappenfus**
- 
- 11:20 AM**                      **75.** Novel biofuel synthesis from furfuryl alcohol and butanol over heteropoly acid catalysts. **S.M. Kendell**, J. Sepulveda, C. Castillion, S. Fierros, P. De Hoyos
- 
- 11:40 AM**                      **76.** Greening the organic chemistry laboratory: Comparison of microwave-assisted and classical nucleophilic aromatic substitution reactions. **D.R. Latimer**

**Materials &  
Nano Chemistry****Carbon Materials**

| **J. P. Attfield, H. Huppertz**, *Organizers*  
**M. J. Rosales-Hoz**, *Presiding*

**ISLA BALLROOM 3/4**

- 10:00 AM**                      **77.** Carbon nanostructures-based multifunctional nanocomposites obtained as thin films at liquid/liquid interfaces: from preparation to applications. **A.J.G. Zarbin**
- 
- 10:30 AM**                      **78.** Synthesis and characterization of carbon nanofibers/ Zinc oxide/poly (para-phenylenediamine) ternary nanocomposites. **E. Halim**, K. Lafdi, G. Drochioiu, L. Vacareanu, M. Grigoras, M. El Rhazi
- 
- 10:50 AM**                      Intermission
- 
- 11:00 AM**                      **79.** Carbon nanoreactors: making use of their unique shape.  
**N.J. Coville**
- 
- 11:20 AM**                      **80.** Graphene oxide hybrids and composites: applications in energy devices and structural components. **G.G. Silva**
- 
- 11:40 AM**                      **81.** Capping sulfides from mercaptobenzene and mercaptopyridine carbonyl diphosphine ruthenium clusters with potential application as catalytic materials.  
**G. Sánchez Cabrera**, F.J. Zuno Cruz, A. Cruz Acosta, C. Martínez Macias, M.G. Hernández Cruz, M. Rosales-Hoz, M.A. Leyva



## Thursday Morning

### Physical & Analytical Chemistry

### Physical Chemistry

| B. S. Martincigh, *Organizer*  
S. B. Jonnalagadda, *Presiding*

GRAND CARIBE 7/8

- 10:00 AM**                      **82.** Molecular photodissociation and photoinduced ring opening in the gas and solution phase. **M. Ashfold**
- 
- 10:30 AM**                      **83.** Computational study of the Criegee intermediate through ozonolysis reaction. **M. Almatarneh**, I. Elayan, Z. Ahmad
- 
- 10:50 AM**                      Intermission
- 
- 11:00 AM**                      **84.** Structural effects on the kinetics and mechanism of the oxidation of iron(II) complexes. **R. Khattak**, M. Sayed, I.I. Naqvi
- 
- 11:20 AM**                      **85.** Accurate models for phosphorus organocatalytic design. **M. Fianchini**, F. Maseras
- 
- 11:40 AM**                      **86.** Catalysts to the rescue for destroying and monitoring pesticides: from waste to nanomaterials. **E.S. Orth**, L. Hostert, Y. Santos, L. Nascimento, V. Silva, J. Ferreira, W. Takarada, S. Blaskiewicz, J. Fonsaca, T. Almeida, A.J.G. Zarbin

### A Crash Course in Professional Development for Younger Chemists

MIRAMAR 3

- 10:00 AM**                      Introduction and Welcome **Natalie LaFranzo**
- 10:10 AM**                      Scientific Presentations- Tips, Tricks and Tools **Alice Soldà**
- 10:30 AM**                      Innovation and Leadership Styles **Natalie LaFranzo**
- 10:50 AM**                      Intermission
- 11:00 AM**                      A postdoc in Europe? Why and how? **Victor Mougel**
- 11:20 AM**                      Social Media and Networking **Matthew Grandbois**
- 11:40 AM**                      Panel Discussion



## Thursday Afternoon

### Plenary Session

| Fernando Galembeck  
N. P. Lopes, *Organizer, Presiding*

GRAND CARIBE 5/6

- 1:30 PM**                      **87.** Chemical electrostatics: Chemical mechanisms for electrostatic charging, beyond electrochemistry. **F. Galembeck**, T.A. Burgo, B. Batista

**Chemistry in Biology**| **A. Amine, N. P. Lopes, Organizers**  
**S. G. Withers, Presiding****ISLA BALLROOM 1/2****2:30 PM**

**88.** Topical drug delivery into skin probed by label-free spectromicroscopy. **E. Ruehl**, K. Yamamoto, A. Klossek, R. Schulz, P. Patoka, G. Ulrich, T. Ohigashi, M. Weigand, R. Flesch, H. Pischon, M. Radbruch, S. Ahlberg, F. Rancan, A. Vogt, U. Blume-Peytavi, P. Schrade, S. Bachmann, R. Haag, E. Fleige, M. Giubudagian, M. Calderón, G. Ulm, B. Kästner, L. Munkhenk, A. Gruber, J. Lademann, S. Hedtrich, M. Schäfer-Korting, N. Kosugi, R. Netz

**3:00 PM**

**89.** Investigation of calix[*n*]arene as drug carriers for tyrosine kinases inhibitors by theoretical methods. **M. Athar**, M. Lone, P.C. Jha

**3:20 PM**

Intermission

**3:30 PM**

**90.** Pathogenic bacteria screening and specific detection in one hour. **M.N. Bui**, A. Abbas

**3:50 PM**

**91.** Synthesis and characterization of biogenic selenium nanoparticles with antimicrobial properties made by *Staphylococcus aureus*, methicillin-resistant *Staphylococcus aureus* (MRSA), *Escherichia coli* and *Pseudomonas aeruginosa*. **D. Medina Cruz**, T. Webster, A. Roy

**Green Chemistry**| **K. Barta, R. Palkovits, Organizers**  
**L. M. Gibbs, Presiding****ISLA BALLROOM 5/6****2:30 PM**

**92.** CO<sub>2</sub>-Switchable materials and surfaces. **P. Jessop**

**3:00 PM**

**93.** Global freshwater systems: Sustainability and economic viability. **H. Taft**

**3:20 PM**

Intermission

**3:30 PM**

**94.** Rapid removal and recovery of phosphorus from water using a nanoiron sponge. **F. Heidari**, J. Brockgreitens, A. Abbas

**3:50 PM**

**95.** Lipid extraction of wet algal biomass via osmotic shock: *Chlorella vulgaris*. **A. Ansari**

**Materials &  
Nano Chemistry****Metal Oxides**

| J. P. Attfield, H. Huppertz, *Organizers*  
A. J. G. Zarbin, *Presiding*

ISLA BALLROOM 3/4

**2:30 PM**

**96.** Mixed oxides as novel recyclable catalysts for water treatment by advanced oxidation processes. **S.B. Jonnalagadda**, S. Maddila, V. Dasireddy

**3:00 PM**

**97.** Optimized synthesis of supported tungsten and nickel oxide nanoparticles for catalytic air/steam gasification of asphaltenes for enhanced oil recovery. **K.M. Ceron**, C.A. Franco, F.B. Cortés

**3:20 PM**

Intermission

**3:30 PM**

**98.** Phthalocyanine-cobalt ferrite based nanocomposites as bifunctional photocatalysts in water purification. **S. Mapukata**

**3:50 PM**

**99.** Amine-functionalized magnetite nanoparticles as a reusable nano-adsorbent for the removal of heavy metal ions. **S. Titinchi**, V. Paulsen, H.S. Abbo, G. Gerhard

**Physical &  
Analytical  
Chemistry****Analytical  
Chemistry**

| B. S. Martincigh, *Organizer*

GRAND CARIBE 7/8

**2:30 PM**

**100.** Chemical potential and chemical hardness in charge transfer processes. **J. Gázquez**

**3:00 PM**

**101.** Simultaneously determination of traces  $\text{Cd}^{2+}$  and  $\text{Pb}^{2+}$  using a new hybrid nanocomposite of bismuth nanoparticles-carbon nanofibers/ionic liquid. **M. El Rhazi**, L. Oularbi, M. Turmine

**3:20 PM**

Intermission





## Thursday Afternoon

**3:30 PM**

**102.** Nano biosensors for dengue virus detection. **A. Mulchandani**, D. Wasik, M. Yates

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**3:50 PM**

**103.** New paper/polymer hybrid microfluidic microplate for rapid quantitative detection of multiple disease biomarkers. **X. Li**, S. Sanjay



## Thursday Evening

**Chemistry in  
Biology**

| **A. Amine, N. P. Lopes**, *Organizers*

**GRAND CARIBE 1-4**

**4:10 - 5:30 PM**

**104.** Emphasis on the circularly polarized luminescence studies for chemical biology applications. **G. Muller**

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**105.** Probing the scope of fatty acid biosynthesis using a novel fluorescent screen: Applications in biofuel and pharmaceutical production. **K. Charov**, M. Burkart

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**106.** Study of the substituent variation and hydrogenation of 5-X-H<sub>2</sub>salbu ligand in Cu(II) coordination compounds and their effect on biological activity. **C.S. Novoa Ramirez**, V. Gomez Vidales, M. Flores-Álamo, R. Robles Zepeda, J. Delgado Dominguez, I. Becker Fauser, L. Ruiz Azuara

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**107.** Structure-based design and SAR studies of ATP citrate lyase inhibitors as anticancer agents. **L. Sun**

---

**108.** Synthesis and characterization of mixed copper (II) compounds with N<sub>2</sub>O tridentate Schiff base ligands with possible biological activity. **A.S. Becerril**, J. Gracia Mora, L. Ruiz Azuara

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**109.** Partially acetylated polyethyleneimine for topology preserving G-quadruplex binding. **M.R. Elshaer**, J. Mizvesky

---

**110.** Synthesis of quinazoline-2,4,6-triamine derivatives and evaluation of their antiproliferative activity on cancer cell lines. **F. Hernández-Luis**, C. Mouret-Hernández, C. Mendoza-Martínez, F. Sánchez-Bartez, I. Gracia-Mora

**4:10 - 5:30 PM**

**111.** Study of mixed chelate coordination compounds (Casiopeínas®) with DNA one of several targets of these type of compounds. **Y. Figueroa**, L. Ruiz Azuara

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**112.** Withdrawn

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**113.** Tracking heme loading of a protein in live cells by Fluorescence-Lifetime Imaging Microscopy (FLIM). **A.M. English**, S. Dastpeyman

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**114.** Authentic/ alternative assessment, V: Performance of science majors/non-majors on the categorizing grid. **M. Camacho**

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**115.** Authentic/ alternative assessment, V: Classification of organic compounds, reactions/mechanisms by science majors. **M. Camacho**

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**116.** Authentic/ alternative assessment in chemistry/ science education V: Effect of the auto quiz on the achievement of science college students. **M. Camacho**

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**117.** Cancer Profile™, key to prevent cancer before it attains visually detectable size. **E.K. Schandl**

**Physical &  
Analytical  
Chemistry****| B. S. Martincigh, Organizer****GRAND CARIBE 1-4****4:10 - 5:30 PM**

**118.** Kinetics, mechanism and simulation of the reaction of nitrobenzenethiol with benzoquinone derivatives. **V.T. Adeleke**, R.H. Simoyi, S.B. Jonnalagadda, B.S. Martincigh

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**119.** Optimization of disulfide bond reduction for use in point-of-care microfluidic based devices with applications in early cancer diagnosis.  
**S.R. Cook**

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**120.** Prediction of skin penetration of peptides with antimicrobial activity.  
**S.N. Jaramillo**

---

**121.** Self-organization phenomena in surface chemistry and precipitation reactions. **B.C. Batista**

**4:10 - 5:30 PM**

**122.** Analysis of the adsorption isotherm in optical sensing of ammonia in polyaniline. **J. Elizalde-Torres**, M. González-Cardel

---

**123.** Determination of pKa value and study of the decomposition of O-ethylthiocarbonate. **A. Rojas-Hernandez**, K. Sanpedro-Montoya, M. Páez-Hernández, J. Flores-Aguilar, M. Palomar-Pardavé

---

**124.** Method development for the determination of total mercury and mercury thermospecies in coal. **M. Mathebula**, K. Mandiwana, N. Panichev

---

**125.** Proximate analysis, translocation and elemental distribution of celosia trigyna L from the western geographical region in Nigeria. **A.E. Ofusori**

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**126.** DNA detection by PCR-free nanoaggregation-enhanced chemiluminescence. **O. Saiapina**, R. Singh, A. Feltmeyer, J. Juzwik, B. Arenz, A. Abbas

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**127.** Electrochemical sensor based on modified carbon paste electrode for carbaryl determination. **F. Salih**, B. Achiou, A. Ouarzane, M. Ouammou, S. Alami Younssi, M. El Rhazi

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**128.** Withdrawn

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**129.** Withdrawn

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**130.** Extraction and identification of bioactive compounds from the leaves and stem bark of *Clerodendrum glabrum*. **Z.W. Teclegeorgish**

**Plenary  
Session**

| **Timothy Egan**  
**B. S. Martincigh**, *Organizer, Presiding*

**GRAND CARIBE 5/6**

**5:30 PM**

**131.** Exploration of the haem detoxification pathway in the malaria parasite *Plasmodium falciparum* in the search for new antimalarials. **T.J. Egan**

**Plenary  
Session**

| Galo Soler Illia  
E. Pereira, *Organizer, Presiding*

GRAND CARIBE 5/6

**9:00 AM**

**132.** Nanosystems built through self-assembled nanobuilding blocks: Towards responsive and programmable materials. **G. Soler Illia**

**Green Chemistry  
Accident Prevention  
& Risk Perception  
in Laboratory  
Practice**

| K. Barta, R. Palkovits, *Organizers*  
N. Langerman, *Organizer, Presiding*  
H.J. Elston, *Presiding*

ISLA BALLROOM 5/6

**10:00 AM**

**133.** ACS safety initiatives: Impact on the global chemistry enterprise. **N. Langerman**

**10:30 AM**

**134.** Risk perception in academic laboratories. **I. Schroeder**

**10:50 AM**

Intermission

**11:00 AM**

**135.** US safety initiatives as influences on global laboratory safety. **R. Phifer**

**11:20 AM**

**136.** Analyzing academic laboratory accidents to prevent accidents. **C. Merlic**

**11:40 AM**

**137.** Approaching research and scale-up safety through process-oriented solutions. **H.J. Elston**

**Materials & Nano  
Chemistry**

| J. P. Attfield, H. Huppertz, *Organizers*  
B. S. Martincigh, *Presiding*

**Applied Materials  
& Nano Chemistry**

ISLA BALLROOM 3/4

**10:00 AM**

**138.** The role of nanostructured materials in enhancing the photophysical behaviour of phthalocyanines. **T.T. Nyokong**

- 10:30 AM**                      **139.** Selective recovery of thorium by wrinkled mesoporous carbon.  
**K.J. Balkus**, Z. Wang
- 
- 10:50 AM**                      Intermission
- 
- 11:00 AM**                      **140.** Holmium based metal-organic frameworks for gas separations and cancer therapy. **J.P. Vizuet**, K. Balkus
- 
- 11:20 AM**                      **141.** Facile fabrication of crack-free large-area 2D and 3D inverse opal films of transition metal oxides. **Y. Djaoued**, H. Li
- 
- 11:40 AM**                      **142.** Physicochemical properties of metallophthalocyanines when conjugated to magnetic nanoparticles.. **G.G. Matlou**, N. Kobayashi, M. Kimura, T.T. Nyokong

**Materials &  
Nano Chemistry**

| **J. P. Attfield, H. Huppertz**, *Organizers*  
**A. Andrews**, *Presiding*

**Biomaterials**

**GRAND CARIBE 7/8**

- 10:00 AM**                      **143.** Hybrid materials and their medical applications. **L. de Cola**
- 
- 10:30 AM**                      **144.** Advancing functional materials for biomedical applications using laser metal deposition. **H. Kumpaty**, S. Kumpaty
- 
- 10:50 AM**                      Intermission
- 
- 11:00 AM**                      **145.** Extraction and characterization of chitin and chitosan from pupae and adult black soldier fly (*Hermetia illucens*). **C. Uche**, M. Zimri, L. Petrik, T. Onwordi, O. Fatoba
- 
- 11:20 AM**                      **146.** Crystalline carbazole-based rotors as promising organic materials.  
**B. Rodriguez-Molina**
- 
- 11:40 AM**                      **147.** Towards heterobimetallic supported catalysts through a surface organometallic chemistry approach. **C. Camp**

**Plenary Session**

| Laura Kiessling  
P. Weiss, *Organizer, Presiding*

GRAND CARIBE 5/6

1:30 PM

148. Imaging mycobacteria. **L.L. Kiessling**

**Green Chemistry**

| K. Barta, R. Palkovits, *Organizers*  
R. Phifer, *Presiding*

ISLA BALLROOM 5/6

2:30 PM

149. Green Chemistry: A tool to sustainable development in Africa.  
**A. Adewuyi**, F. Vargas Pereira, B. Rao

3:00 PM

150. 25 years of green chemistry and policy. **A. Noce**

3:20 PM

Intermission

3:30 PM

151. Green chemistry through external partnership. **L. Tan**

3:50 PM

152. Life Cycle Inventory (LCI) as an excellent tool for teaching fundamentals of sustainability to chemistry and chemical engineering students. **M. Sabahi**

**Materials & Nano Chemistry**

| J. P. Attfield, H. Huppertz, *Organizers*  
A. Amine, *Presiding*

**Nano & Molecular Materials**

ISLA BALLROOM 3/4

2:30 PM

153. Super-structured nanomaterials. **T. Odom**

3:00 PM

154. Surfactant-assistant hydrothermal synthesis of nanocrystalline hydroxyapatite from phosphogypsum waste. **H. Bensalah**, M. Bekheet, S. A. Younssi



# Friday Afternoon

**3:20 PM**

Intermission

**3:30 PM**

**155.** Relocation of a small molecule in a biocompatible supramolecular gel. **C. Bohne**

**3:50 PM**

**156.** Phosphorene as a hosting platform for metal nanoparticles. **M. Caporali**, M. Serrano Ruiz, F. Telesio, S. Heun, G. Nicotra, C. Spinella, M. Peruzzini

**Physical &  
Analytical  
Chemistry**

**Analytical  
Chemistry**

| **B. S. Martincigh**, *Organizer*  
**M. El Rhazi**, *Presiding*

**GRAND CARIBE 7/8**

**2:30 PM**

**157.** Green sample preparation methods for challenging matrices and trace element determination. **E.M. Flores**

**3:00 PM**

**158.** Hadamard-transform fluorescence EEM spectroscopy. **H. Loock**

**3:20 PM**

Intermission

**3:30 PM**

**159.** Withdrawn

**3:50 PM**

**160.** Novel LC-UV method for estimation of drug release from carvacrol loaded nanobeads: Design of experiment approach. **F. Tandel**

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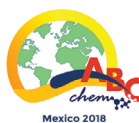
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