



# 8<sup>th</sup> North America-Greece-Cyprus Workshop on Paramagnetic Materials

**8<sup>th</sup> NAGC 2018**

**Sparta Greece 18-22 June 2018**



## **International Organizing Committee**

George Christou, Dept. of Chemistry, University of Florida, USA

Georgios Papavassiliou, INN, NCSR Demokritos, Greece

Spyros Perlepes, Dept. of Chemistry, University of Patras, Greece

Anastasios Tasiopoulos, Dept. of Chemistry, University of Cyprus, Cyprus

## **Local Organizing Committee**

Georgios Papavassiliou, INN, NCSR Demokritos, Greece  
Vassilis Psycharis, INN, NCSR Demokritos, Greece  
Yiannis Sanakis, INN, NCSR Demokritos, Greece  
Catherine Raptopoulou, INN, NCSR Demokritos, Greece  
Georgios Mitrikas, INN, NCSR Demokritos, Greece

## **Workshop Secretariat**

Vasso Zatta, INN, NCSR Demokritos, Greece  
Alice Jempson, Department of Chemistry, University of Florida USA

## **Sponsored by:**

- NCSR Demokritos (Greece)
- Elsevier
- ANELIS (Greece)
- Spectrum Labs

## **LOCATION AND TIME**

The workshop will take place from June 18 to June 22, 2018 in a new Hotel, **The Mystras Grand Palace Resort & Spa**, which is situated in the middle of the road which connects the city of Sparta and Mystras and close to the foothills of mountain Taygetus.

## **SOCIAL PROGRAM**

### **Reception**

The welcome reception will take place, on Sunday 17, 2018 at 21:00. All registered persons (participants and accompanying members) are cordially invited.

### **Excursion**

An excursion will be arranged for Wednesday June 20, 2018 afternoon.

### **Official Dinner**

The official dinner of the Workshop will take place on Tuesday June 19, 2018 at 21:00.

*...further information in the upcoming book of abstracts*

# TIMETABLE

**Monday June 18, 2018**

**08:50-09:00** Opening of the workshop

**Chairman: S. Perlepes**

**09:00-9:30 Kilikoglou Vassilis**

Cultural heritage and nanoscience: a new relationship with an old background

**09:30-10:00 Constable Edwin**

Magnetism – Quo vadis

**10:00-10:30 Christou George**

Molecular Nanoscience: Synthesis and Properties of Molecular Ce/Mn Clusters related to the Perovskite Repeating Unit

**10:30-10:45 Dermitzaki Despoina**

Heptanuclear heterometallic  $\text{Cu}_5\text{Ln}_2$  (Ln = Gd, Tb) complexes: Synthesis, crystal structures, and magnetic properties studies

**10:45-11:00 Das Gupta Sayak**

Mn-Ce Clusters from Reductive Aggregation: Unusual Long-range Mn·Mn Exchange-coupling through  $\text{Ce}^{\text{IV}}$

**11:00-11:30** *Coffee break*

**Chairman: S. Hill**

**11:30-12:00 Boudalis K. Athanassios**

Determination of magnetic symmetries and antisymmetric exchange interactions in highly symmetric molecular spin triangles

**12:00-12:30 Comba Peter**

Validation of ab-initio predicted magnetic anisotropies in linear hetero-trinuclear  $\text{Dy}^{\text{III}}\text{-Ni}^{\text{II}}_2$  compounds.

**12:30-13:00 Peralta Juan**

Magnetic Exchange Couplings from Density Functional Theory without Self-Interaction

**13:00-13:15 Mayans Julia**

Enhancement of Single Ion Magnet Properties in Lanthanide Clusters by Improving the Magnetic Dilution with Specific d-Metals. A Comparative Study

**13:15-13:30 Skordi Katerina**

$\text{Mn}^{\text{II}}_2\text{Mn}^{\text{III}}_4$  cross-shaped clusters: Synthesis, Structure and Magnetism Studies

**13:30-15:30 Lunch Break**

**Chairman:** E. Constable

**15:30-16:00 Shatruk Mike**

Expanding the Chemistry and Functions of the Blatter Radical

**16:00-16:30 Preuss Kathryn**

Making/Breaking Pancake Bonds: Reversible Crystal-to-Crystal Switching

**16:30-17:00 Ma Shengqian**

Advanced Porous Organic Polymers: Task-Specific Design and Functionalization

**17:00-17:15 Kampouri Stavroula**

Photocatalytic Hydrogen Generation from a Visible-Light Responsive Metal-Organic Framework System

**17:15-17:30 Nguyen Tu**

Lanthanide-based Near-infrared Emitting Metal-organic Frameworks with Tunable Excitation Wavelengths and High Quantum Yields

**17:30-18:00 Coffee Break**

**Chairman:** A. Tasiopoulos

**18:00-18:30 Bekiari Vlasoula**

Chemical hydrogels as sorbents of positively charged metal ions from aqueous systems

**18:30-19:00 Al Wahedi Fowad Yasser**

Silica Encapsulated Metal Oxides as H<sub>2</sub>S Adsorbents

**19:00-19:30 Stylianou Kyriakos**

Rational design and synthesis of metal-organic frameworks for carbon capture

**19:30-19:45 Anderson L. Samantha**

Nucleobase Pairing and Photodimerization in a Biologically Derived Metal-Organic Framework

**19:45-20:00 Mylonas-Margaritis Ioannis**

1D- Coordination Polymers and metal complexes from the combination of 2-pyridyl oximes with polycarboxylic acids

## Tuesday June 19, 2018

**Chairman:** G. Mitrikas

**09:00-9:30 Libby Eduardo**

Bioinorganic Chemistry in Extreme Volcanic Environments

**09:30-10:00 Shafaat Hanah**

EPR spectroscopic investigations of metal binding specificity and oxygen activation in heterobimetallic Mn/Fe proteins

**10:00-10:30 Lancaster Kyle**

Mechanistic Details Concerning Hydroxylamine Oxidation by Heme P460 Cofactors

**10:30-10:45 Zahariou Georgia**

On the Spin Configuration of the  $\text{Mn}_4\text{O}_5\text{Ca}$  cluster of Photosystem II in the  $\text{S}_3$  oxidation state

**10:45-11:00 Gluz Naama**

A bioinspired water soluble manganese cluster for electrocatalytic water oxidation

**11:00-11:30 Coffee break**

**Chairman:** M. Shatruk

**11:30-12:00 Musfeldt Jan**

Multiferroics in high magnetic field: phase diagrams, magnetoelastic coupling, and spin-charge interactions

**12:00-12:30 Papavassiliou George**

MHz Broadline NMR & HRTEM in the Study of Polaron Dynamics in Mott Insulators

**12:30-13:00 Jang Jae Hyuck**

Real-time observation of oxygen vacancy ordering in  $\text{LaCoO}_3$  system using Cs-corrected STEM

**13:00-13:15 Pissas Michael**

Slow magnetic relaxation in ferrimagnetic  $\text{Y}_3\text{Fe}_5\text{O}_{12}$

**13:15-13:30 Krnel Mitja**

Random-anisotropy ferromagnetic state in the  $\text{Cu}_5\text{Gd}_{0.54}\text{Ca}_{0.42}$  intermetallic compound

**13:30-15:30 Lunch Break**

**Chairman:** H-J. Kim

**15:30-16:00 Pantelides Sokrates**

Impurities and defects in graphene

**16:00-16:30 Christodoulou Sotirios**

From Quantum Dots to Optoelectronic Devices: Properties, Challenges and Perspectives

**16:30-17:00 Aliaga-Alcalde Nuria**

Progress of Curcuminoids in Nanoscience

**17:00-17:15 Boukos Nikolaos**

ZnO based resistive switching memory devices

**17:15-17:30 Russell Webster Brad**

Effects of Cl<sup>-</sup> and NO<sub>3</sub><sup>-</sup> Ions on Cerium Dioxide Nanocluster Structures

**17:30-18:00 Coffee Break**

**Chairman:** G. Christou

**18:00-18:30 Escuer Albert**

Nickel(II) Supramolecular Assemblies: From Mesocates to Helicates

**18:30-19:00 Papatriantafyllopoulou Constantina**

Homo- and Hetero- metallic Metal-Organic Frameworks with Biomedical and Environmental Applications

**19:00-19:30 Psycharis Vassilis**

Structural relations in hybrid organic-inorganic halide perovskites and the role of hydrogen bonds

**19:30-20:00 Tasiopoulos Anastasios**

High Nuclearity Clusters from the Use of Diols in Mn Chemistry

## Wednesday June 20, 2018

Chairman: S. Alhassan

**09:00-9:30 Jurga Stefan**

Ionic Liquids for Nanotechnology

**09:30-10:00 Davies Gemma-Louise**

Exploring the Design of Magnetic Resonance Imaging Contrast Agents for Diagnostics in Healthcare

**10:00-10:15 Sanakis Yiannis**

Variable Temperature Mössbauer and EPR spectroscopic studies of iron based pharmaceuticals

**10:15-10:30 Fardis Michael**

Hyperfine structure effects in Nuclear Magnetic Resonance: some case studies

**10:30-11:00 Zaleski Jeff**

Activated Diradicals: From Small Molecule Bioreagents to Nanomedicine Applications and Nanocatalysis of CO<sub>2</sub> Reduction

**11:00-11:30 Coffee break**

Chairman: S. Jurga

**11:30-12:00 Pedersen Kaspar**

A Non-Innocent Coordination Chemistry Approach to 2D Conductive Magnets

**12:00-12:30 Piligkos Stergios**

Molecular multifunctionality preservation upon surface deposition for a chiral Single-Molecule Magnet

**12:30-13:00 Szczytko Jucek**

Coupling of light and magnetism – from optical spin Hall effect to Bose-Einstein condensates in magnetic microcavities

**13:00-13:30 Eddaoudi Mohamed**

MOF Design to Applications: Impact of Pore System Control on Gas Separations and Storage

## Thursday June 21, 2018

**Chairman:** Y. Sanakis

**09:00-9:30 Hill Steve**

Advanced Magnetic Resonance Investigations of Metal-Metal Bonded Systems:  
Potential New Routes to Single-Molecule Magnets

**09:30-10:00 Mitrikas George**

Hydrogen Atom in the box: what can we learn from Pulse EPR spectroscopy?

**10:00-10:30 Chiesa Mario**

Paramagnetic Materials in Catalysis. EPR Approaches to the Characterization of  
Heterogeneous Catalysts

**10:30-11:00 Kay Chris**

From DNA binding to MASERS: Adventures in the wonderful world of EPR  
Spectroscopy

**11:00-11:30 Coffee break**

**Chairman:** C. Housecroft

**11:30-12:00 Lazarides Theodore**

Towards white light luminescence from Eu- and Tb-doped lanthanum Metal-  
Organic Frameworks

**12:00-12:30 Manos Manolis**

Exceptional  $\text{TcO}_4^-$  sorption capacity and highly efficient  $\text{ReO}_4^-$  luminescence  
sensing by  $\text{Zr}^{4+}$  MOFs

**12:30-12:45 Ebrahim Fatmah Mish**

A selective and sensitive metal-organic framework sensor for fluoride anions with  
fast optical response

**12:45-13:00 Newton Graham**

Hybrid molecular metal oxides as tuneable catalysts, supramolecular building blocks  
and switchable material additives

**13:00-13:30 Layfield Richard**

Organo-Lanthanide SMMs: Life Beyond the Venerable Cyclopentadienyl Ligand

**13:30-15:30 Lunch Break**

**Chairman:** J. Musfeldt

**15:30-16:00 Singleton John**

High-magnetic-field explorations of molecular architecture and fundamental physics  
in organic quantum magnets



**16:00-16:30 Halcrow Malcolm**  
Insight into the  $T_{1/2}$  vs.  $T$  (LIESST) Relationship from an Isostructural Series of Spin-Crossover Solvates

**16:30-17:00 Morgan G. Grace**  
Probing the Magnetic and Photophysical Properties of Manganese(III) and Iron(III) Spin Switches

**17:00-17:30 McCusker Jim**  
Spin and Zero-field Spin Polarization Effects on the Photophysical Properties of Molecular Donor-Acceptor Assemblies

**17:30-18:00 Coffee Break**

**Chairman: M. Halcrow**

**18:00-18:30 Housecroft Catherine**  
Tetrapotic bis(4,2':6',4"-terpyridine) and bis(3,2':6',3"-terpyridine) ligands as 4-connecting nodes in metal-organic networks

**18:30-19:00 Corr A. Serena**  
New Series of Li-rich Double Perovskites as Active Materials for All Solid-State Batteries

**19:00-19:30 Kim Hae Jin**  
Microwave-assisted synthesis of spindle-type mesoporous  $\alpha$ - $\text{Fe}_2\text{O}_3$  for stable cycling of lithium batteries

**19:30-19:45 Papawassiliou Wassilios**  
Combined ssNMR, Moessbauer and DFT study on the 1-D spin antiferromagnetic system  $\beta$ - $\text{FeF}_3 \cdot 3\text{H}_2\text{O}$

**19:45-20:00 Polyzou Christina**  
Spin-Crossover Fe(II)-M(II) (M= Ni, Pd, Pt) Bimetallic Hofmann-type Metal Organic Frameworks: Synthesis, Characterization and Magnetic Study

## **Friday June 22, 2018**

**Chairman: S. Pantelides**

**09:00-09:30 Soler Juama Monica**  
Coordination Chemistry of Curcuminoid Ligands

**09:30-10:00 Kaszynski Piotr**  
Unconventional Magnetostructural Behavior of Nitroxyl-Based Organic Radicals

**10:00-10:30 Alhassan Saeed**

Recent Advances in Sulfur Applications

**10:30-10:45 Karagianni Marina**

NMR investigations of the structural stability of Sulfur Copolymers prepared by the Inverse Vulcanization Technique.

**10:45-11:00 Klontzas Emmanuel**

Organically interconnected graphene flakes: A flexible 3-D material with tunable electronic properties.

**11:00-11:30 *Coffee break***

**Chairman: V. Psycharis**

**11:30-12:00 Perlepes Spyros**

Towards Mixed 3d/4f-Metal Molecular Complexes with Interesting Magnetic and Optical Properties

**12:00-12:15 Hale Ashlyn**

Giant Molecules: Exploring Synthetic Parameters on the Path to New Mn-O Torus-like Clusters

**12:15-12:30 Ghosh Totan**

Copper-Peptoid Complex as a Highly Stable and Efficient Homogeneous Water Oxidation Electro Catalyst

**12:30-12:45 Maniaki Diamadoula**

Unusual Coordination Modes, Luminescence Spectra and Single-Ion Magnet Behaviour in Lanthanide(III)-Anil Complexes

**12:45-13:00 Valizadeh Bardiya**

Porous Metal-organic Framework@Polymer Beads for Iodine Capture and Recovery Using a Gas-sparged Column

**13:00-13:15 Pilichos Evangelos**

Coordination Properties and Lanthanide(III)-Assisted Reactivity of a Polydentate Ligand Containing Hydrazone, Oxime and Picolinoyl Functionalities

**13:15-13:30 Closing remarks**

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## PROGRAM Sparta, Crece

Monday, June 18	Tuesday, June 19	Wednesday, June 20	Thursday, June 21	Friday, June 22
08:50– 09:00 <b>WELCOME</b>				
<b>Chair:</b> Perlepes Spyros	<b>Chair:</b> Mitrikas George	<b>Chair:</b> Alhassan Saeed	<b>Chair:</b> Sanakis Yiannis	<b>Chair:</b> Pantelides Sokrates
09:00 -09:30 Kilikoglou Vassilis 09:30-10:00 Constable Edwin 10:00-10:30 Christou George 10:30-10:45 Dermitzaki Despoina 10:45-11:00 Das Gupta Sayak	09:00-09:30 Libby Eduardo 09:30-10:00 Shafaat Hanah 10:00-10:30 Lancaster Kyle 10:30-10:45 Zahariou Georgia 10:45-11:00 Gluz Naama	09:00-9:30 Jurga Stefan 09:30-10:00 Davies Gemma-Louise 10:00-10:15 Sanakis Yiannis 10:15-10:30 Fardis Michael 10:30-11:30 Zaleski Jeff	09:00-9:30 Hill Steve 09:30-10:00 Mitrikas George 10:00-10:30 Chiesa Mario 10:30-11:00 Kay Chris	09:00-09:30 Soler Juama Monica 09:30-10:00 Kaszynski Piotr 10:00-10:30 Alhassan Saeed 10:30-10:45 Karagianni Marina 10:45-11:00 Klontzas Emmanuel
<b>Coffee break 11:00 – 11:30</b>	<b>Coffee break 11:00 – 11:30</b>	<b>Coffee break 11:00 – 11:30</b>	<b>Coffee break 11:00 – 11:30</b>	<b>Coffee break 11:00 – 11:30</b>
<b>Chair:</b> Hill Steve	<b>Chair:</b> Shatruck Mike	<b>Chair:</b> Jurga Stefan	<b>Chair:</b> Housecroft Catherine	<b>Chair:</b> Psycharis Vassilis
11:30 – 12:00 Boudalis Athanassios 12:00 – 12:30 Comba Peter 12:30 – 13:00 Peralta Juan 13:00 – 13:15 Mayans Julia 13:15 – 13:30 Skordi Katerina	11:30-12:00 Musfeldt Jan 12:00-12:30 Papavassiliou George 12:30-13:00 Jang Jae Hyuck 13:00-13:15 Pissas Michael 13:15-13:30 Krnel Mitja	11:30-12:00 Pedersen Kaspar 12:00-12:30 Piligkos Stergios 12:30-13:00 Szczytko Jucek 13:00-13:30 Layfield Richard	11:30-12:00 Lazarides Theodore 12:30-12:45 Ebrahim Fatmah Mish 12:45-13:00 Newton Graham 13:00-13:30 Eddaoudi Mohamed	11.30-12:00 Perlepes Spyros 12:00-12:15 Hale Ashlyn 12:15-12:30 Ghosh Totan 12:30-12:45 Maniaki Diamadoula 12:45-13:00 Valizadeh Bardiya 13:00-13:15 Pilichos Evangelos 13:15-13:00 Closing remarks
<b>Lunch Break 13:30-15:30</b>	<b>Lunch Break 13:30 – 15:30</b>	<b>Lunch Break 13:30 – 14:30</b>	<b>Lunch Break 13:30 – 15:30</b>	
<b>Chair:</b> Constable Edwin	<b>Chair:</b> Kim Hae Jin	<b>EXCURSION</b>  Departure from hotel at 15:00	<b>Chair:</b> Musfeldt Jan	
15:30 – 16:00 Shatruck Mike 16:00 – 16:30 Preuss Kathryn 16:30 – 17:00 Ma Shengqian 17:00 – 17:15 Kampouri Stavroula 17:15 – 17:30 Nguyen Tu	15:30-16:00 Pantelides Sokrates 16:00-16:30 Christodoulou Sotirios 16:30-17:00 Aliaga-Alcalde Nuria 17:00-17:15 Boukos Nikolaos 17:15-17:30 Russell Webster Brad		15:30-16:00 Singleton John 16:00-16:30 Halcrow Malcolm 16:30-17:00 Morgan G. Grace 17:00-17:30 McCusker Jim	
<b>Coffee break 17:30– 18:00</b>	<b>Coffee break 17:30– 18:0</b>		<b>Coffee break 17:30– 18:00</b>	
<b>Chair:</b> Tasiopoulos Anastasios	<b>Chair:</b> Christou George		<b>Chair:</b> Halcrow Malcolm	
18:00 – 18:30 Bekiari Vlasoula 18:30 – 19:00 Al Wahedi Fowad Yasser 19:00 – 19:30 Stylianos Kyriakos 19:30 – 19:45 Anderson Samantha 19:45 – 20:00 Mylonas-Margaritis Ioannis	18:00-18:30 Escuer Albert 18:30-19:00 Papatriantafyllopoulou Constantina 19:00-19:30 Psycharis Vassilis 19:30-20:00 Tasiopoulos Anastasios		18:00-18:30 Housecroft Catherine 18:30-19:00 Corr A. Serena 19:00-19:30 Kim Hae Jin 19:30-19:45 Papawassiliou Wassilios 19:45-20:00 Polyzou Christina	
	<b>21:00 WORKSHOP BANQUET</b>			