8th North America-Greece-Cyprus Workshop on Paramagnetic Materials

8th 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
08:50-09:00 Opening of the workshop

Chairman: S. Perlepes

09:00-09:30 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 Cu₅Ln₂ (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 Ce⁴⁺

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 Dy³⁺-Ni²⁺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
Mn²⁺Mn³⁺₄ cross-shaped clusters: Synthesis, Structure and Magnetism Studies
13:30-15:30 **Lunch Break**

15:30-16:00 **Shatruk Mike**
Expanding the Chemistry and Functions of the Blatter Radical

**Chairman: E. Constable**

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 H₂S 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 Mn4O5Ca cluster of Photosystem II in the S3 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 LaCoO3 system using Cs-corrected STEM

13:00-13:15 Pissas Michael
Slow magnetic relaxation in ferrimagnetic Y3Fe5O12

13:15-13:30 Krnel Mitja
Random-anisotropy ferromagnetic state in the Cu5Gd0.54Ca0.42 intermetallic compound

13:30-15:30 Lunch Break
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- and NO3- Ions on Cerium Dioxide Nanocluster Structures

17:30-18:00 Coffee Break

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 CO₂ 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 TcO$_4^-$ sorption capacity and highly efficient ReO$_4^-$ luminescence
sensing by 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

13:0-13:30 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
Tetratopic 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 $\alpha$-Fe$_2$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 $\beta$-FeF$_3$*3H$_2$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
<table>
<thead>
<tr>
<th>Time</th>
<th>Monday, June 18</th>
<th>Tuesday, June 19</th>
<th>Wednesday, June 20</th>
<th>Thursday, June 21</th>
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<td><strong>Chair:</strong> Perlepes Spyros</td>
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<td>21:00</td>
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