



Program

Tuesday, June 4

15h00 – 18h00 An Introduction To Metal Nanoparticles And Nanoalloys

15:00 – 15:40 **Riccardo Ferrando**

Università di Genova, Italy

Tutorial 1: Structures Of Metal Nanoparticles And Nanoalloys

15:40 – 16:20 **Richard E. Palmer**

University of Swansea, UK

Tutorial 2: Nanoparticle Nucleation And Growth

16:30 – 17:10 **Christian Ricolleau**

Université Paris 7 Denis Diderot, France

Tutorial 3: Understanding Nanoalloy Properties Through New Generation Aberration-corrected Electron Microscopy

17:10 – 17:50 **Emmanuel Cottancin**

Université Claude Bernard Lyon, France

Tutorial 4: Plasmonic Properties Of Nanoalloys In Relation With Their Chemical Structure

18h00 – 19h30 Welcome Party and Conference Registration

Wednesday, June 5

Session 1 **Chair: Riccardo Ferrando and Pascal Andreezza**

8h30 – 9h10 *Registration*

9h10 – 9h30 *Opening*

9h30 – 9h50 *IRN activity presentation*

9h50 – 10h10 Atomic Ordering In Large Bimetallic Particles From
O1 DFT+Topological Calculations
Konstantin Neyman, Universitat de Barcelona, Spain

10h10 – 10h30 Site-specific Wetting Of Iron Nanocubes By Gold Atoms In Gas-
O2 phase Synthesis
Junlei Zhao, University of Helsinki, Finland

10h30 – 11h00 *Coffee Break*

Session 2 **Chair: Francesco Bisio**

11h00 – 11h20 Shell Thickness Induced Core Transformation In Core(Fe)-
O3 shell(Au) Magnetic Nanoparticles
Marie-José Casanove, Université de Toulouse, France

11h20 – 11h40 Magnetic Properties Of Ferromagnetic/antiferromagnetic Metallic
O4 Nanocomposites: Influence Of Alloying At The Interface
Davide Peddis, Università di Genova, Italy

11h40 – 12h00 Magnetoplasmonic Nanoalloys
O5 **Alessio Gabbani, Università di Pisa, Italy**

12h00 – 12h20 Fcc-Co Clusters In L₁₀-FePt Matrix As Model Nanocomposite
O6 Magnets
Charles Paleo, Institut Lumière Matière, Lyon, France

12h20 – 14h00 *Lunch*

Session 3**Chair : Caroline Andreazza****14h00 – 14h20
O7**Elucidating Structural Transitions In Nanoalloys
Francesca Baletto, King's College, London, UK**14h20 – 14h40
O8**Core-shell vs Multi-shell Formation In Nanoalloys Evolution From Disordered Configurations
Diana Nelli, Università di Genova, Italy**14h40 – 15h00
O9**Atomic-Resolution Imaging And Ab Initio Modelling Of Surface And Core Melting Of Supported, Size-Selected Au Nanoclusters
Richard Palmer, University of Swansea, UK**15h00 – 15h20
O10**Structure And Chemical Ordering In Nanoalloys From Constrained Monte Carlo Simulations
Magnus Rahm, Chalmers University of Technology, Göteborg, Sweden**15h20 – 15h50***Coffee Break***Session 4****Chair : Ignacio Garzon****15h50 – 16h10
O11**DFTB Parametrization And Global Optimization Of 55-Atom $\text{Cu}_x\text{M}_{55-x}$ (M=Pd, Pt, Au) Nanoclusters
Maxime Van den Bossche, Institut des NanoSciences de Paris, CNRS, France**16h10 – 16h30
O12**Facile Route Towards Mono And Bimetallic Nanocrystals With Size And Shape Control
Christophe Petit, Sorbonne Université, Paris, France**16h30 – 16h50
O13**Modeling Transition Metals And Nanoalloys: Fixing The Misuse Of Cohesive-Energies
Micha Polak, Ben-Gurion University of the Negev, Beer-Sheva, Israel**17h00 – 23h00*****Excursion and Social Dinner***

Thursday, June 6

Session 5 **Chairman : Magali Benoit**

9h10 – 9h30
O14 Application Of Structure Descriptor For Rational Design Of Transition Metal Catalysts
Daojian Cheng, Beijing University of Chemical Technology, People's Republic of China

9h30 – 9h50
O15 Catalytic (And Optical) Properties Of (Supported) Alloy (Ultra)NanoStructures
Alessandro Fortunelli, CNR-ICCOM & IPCF, Pisa, Italy

9h50 – 10h10
O16 Catalysis By Bimetallic Subnanometer Clusters
Stefan Vajda, Academy of Sciences of the Czech Republic, Prague, Czech Republic

10h10– 10h30
O17 Dynamic Structure Of Low Temperature CO Oxidation Catalysts Based On Gas-phase PdNi Nanoclusters Deposited On Alumina Powder Unraveled By Operando XAFS And DRIFTS
Anupam Yadav, KU Leuven, Belgium

10h30 – 11h00 *Coffee Break*

Session 6 **Chair: Veronique Dupuis**

11h00 – 11h20
O18 Atomistic Simulation Of Trimetallic Nanoparticle Growth By Cluster Beam Deposition
Panagiotis Grammatikopoulos, OIST, Okinawa, Japan

11h20 – 11h40
O19 Tailored Multi-element Nanoparticles For Wide Spectrum Antibacterial Coatings
Luca Gavioli, Università Cattolica del Sacro Cuore, Brescia, Italy

11h40 – 12h00
O20 Environmental Plasmonic Spectroscopy Of Silver-Iron Nanoparticles: Chemical Ordering Under Oxidizing And Reducing Conditions
Emmanuel Cottancin, Université de Lyon, France

12h00 – 12h20
O21 Ag-Pt Nanoalloys: An Intriguing Hybrid System Between Chemical Ordering And Phase Separation
Christine Mottet*, CINaM, CNRS, Marseille, France (substituted by Riccardo Ferrando)

12h20 – 14h00 *Lunch*

Session 7

Chair: Panagiotis Grammatikopoulos

**14h00 – 14h20
O22**

Vibrations Of Atomically Defined Metal Clusters And Nanoalloys
**Ignacio Garzón, Universidad Nacional Autónoma de México,
México City, México**

**14h20 – 14h40
O23**

LoDiS: Low Dimensional System Molecular Dynamics. A 0D
Computational Engine For Investigations At The Nanoscale
Raphael Pinto-Miles, King's College, London, UK

**14h40 – 15h00
O24**

A New Basin Hopping Suite For Multi-Component Nanoparticles
Daniele Rapetti, Università di Genova, Italy

15h30 – 16h00

Meeting of the IRN groups

16h00 – 18h30

Poster session with refreshments

Friday, June 7

Session 8 **Chair: Luca Gavioli**

9h10 – 9h30
O25 The Surface Segregation Of Gold In Pd_nPt_{13-n}Au₄₂ Trimetallic Clusters: A DFT Study
Ali Kemal Garip, Zonguldak Bulent Ecevit University, Zonguldak, Turkey

9h30 – 9h50
O26 Nanoparticle-Support Interactions And Catalytic Activities Of Noble-Metal Nanoparticle-Based Catalysts
Theodoros Pavludis, Swansea University, UK

9h50 – 10h10
O27 Physical Synthesis And Characterization Of Plasmonic Ag@CaF₂ Nanoparticles
Sergio D'Addato, Università di Modena e Reggio Emilia, Modena, Italy

10h10 – 10h30
O28 Plasmonics Of Noble Metal Nanoparticles In A Hot Thermodynamic Bath
Michele Magnozzi, Università di Genova, Italy

10h30 – 11h00 *Coffee Break*

Session 9 **Chair: Riccardo Ferrando**

11h00 – 11h20
O29 Capturing Spatial Contributions To Excitations Through Fourier Transform Of Induced Density Obtained In δ -kick RT-TDDFT Calculations
Rajarshi Sinha-Roy, Aix-Marseille University, Marseille, France

11h20 – 11h40
O30 How Metallic Are Tiny Pieces Of Noble Metals? Metallicity And Screening In Gold & Silver Clusters
Hans-Christian Weissker, Aix-Marseille University, Marseille, France

11h40 – 12h00
O31 Origin Of Circular Dichroism In Noble Metal Alloy Clusters: A Combined Experimental And Theoretical Spectroscopic Investigation
Mauro Stener, Università di Trieste, Italy

12h00 – 12h20 Concluding remarks

12h20 – 14h00 *Lunch*

Poster session

- P1** Tuning The Magnetic Moment Of Small Late 3d-transition-metal Oxide Clusters, **R. H. Aguilera-del Toro et al., Universidad de Valladolid, Spain**
- P2** Metallic Nanoparticles: Morphological And Structural Stability Dependence Due To Metal And Support Nature, **F. Ait Hellal et al., ICMN Orléans, France**
- P3** Stability And Bonding Patterns In ZnMg Nanoalloys, From A Combined Empirical Potential/DFT Approach, **P. Alvarez-Zapatero et al., Universidad de Valladolid, Spain**
- P4** Unexpected Composition And Size Dependence Of L1₁ Chemical Order In Ag-Pt Nanoalloys, **C. Andreazza et al., ICMN Orléans, France**
- P5** Ageing Of Ag_cPt_{1-c} Thin Films And Nanoparticles, **F. Berthier et al., CNRS, Orsay Cedex, France**
- P6** Experimental Investigation Of Thermal Properties Of Binary Metal Alloys, **T. Boruvka et al., Masaryk University, Brno, Czech Republic**
- P7** Stern-Gerlach Deflection Of Cr_nO_m Clusters, **K. De Knijf et al., Laboratory of Solid-State Physics and Magnetism, Leuven, Belgium**
- P8** Low Temperature Synthesis Of Nanosized Pd-X (X=Mg, Zn) Metallic Systems, **S. Delsante et al., Università di Genova, Italy**
- P9** From Bulk To Size-Dependent Melting Properties Of Au-Ge Nanoparticles, **R. Novakovic et al., CNR Genova, Italy**
- P10** Ligand-Protected AuNPs In Lipid Raft., **A. L. de Marco et al., Università di Genova, Italy**
- P11** The Role Of Metal Traces In Bottom-up Porous Gold Structures In Oxidative Catalysis, **C. Demirci et al., IIT Genova, Italy**
- P12** Structure And Orientation Effects In The Coalescence Of Au Clusters, **R. Ferrando et al., Università di Genova, Italy**
- P13** Thermo-Optical Response Of Plasmonic Arrays Of Metallic Nanoalloys, **M. Ferrera et al., Università di Genova, Italy**
- P14** Ag-Pt Nanoalloys In A Tight Binding Ising Model: Chemical Ordering On FCC Nanoparticles, **A. Hizi et al. CINaM, Marseille**
- P15** Structural Characterization Of Subnanometer Particles, **J. Jašík et al., J. Czech Academy of Sciences, Prague, Czech Republic**

- P16** Interactions Between Liposomes Induced By Functionalized Au Nanoparticles,
E. Lavagna et al., Università di Genova, Italy
- P17** Deuterium Adsorption On Cobalt-Fullerene Complexes, **G. Libeert et al.,
Laboratory of Solid-State Physics and Magnetism, Leuven, Belgium**
- P18** Shape Transformation Of (Bi-)Metallic Nanocrystals, **A. Moisset et al.,
Sorbonne Université, Paris, France**
- P19** Structural Transformations In AuCo Nanoalloys Studied By Metadynamics,
D. Nelli et al., Università di Genova, Italy
- P20** Probing The Evolution Of PdCu And PtCu Bimetallic Nanocrystal Catalysts
Under Operando Conditions By In-situ X-ray Absorption Spectroscopy,
L. Pasquale et al., IIT Genova, Italy
- P21** CeO₂ (111) Electronic Reducibility Tuned By Ultra-Small Supported Bimetallic
Pt-Cu Clusters, **L. O. Paz-Borbón et al., Universidad Nacional Autónoma
de México, Mexico**
- P22** A Gold-Sulphur Atomistic Potential For Molecular Dynamics, **D. Rapetti et al.,
Università di Genova, Italy**
- P23** (Ni,Co) Alloy Nanoparticles: Synthesis, Characterization And Catalytic
Application, **P. Riani et al., Università di Genova, Italy**
- P24** Thermal Gradients Around Irradiated Au NPs In The Biological Environment,
S. Salassi et al., Università di Genova, Italy
- P25** Surface Assisted Synthesis Of C-based Nanostructures On Ag(110), **L. Savio et
al., Università di Genova, Italy**
- P26** Monitoring Oxidation And Reduction Of FeO₂ Islands On Pt(111) Using HREELS
And XPS, **M. Stojkovska et al., Università di Genova, Italy**
- P27** Improving Accuracy Of The Topological Approach For Nanoalloys: Case Study
Of PtCu Nanoparticles, **L. Vega et al., Universitat de Barcelona, Spain**
- P28** Time Dependent Density Functional Theory Calculation For Nano-Plasmonics,
W. Zhao et al., King's College London, United Kingdom