NANOMATERIALS

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Advances in nanoparticles: synthesis, characterization, theoretical modelling, and applications

Recent advances in the synthesis of nanoparticles (NPs) and in atomic-scale characterization, coupled with insights from theoretical modelling, have opened exciting possibilities to tailor knowledge-based NPs for many applications, such as catalysis, plasmonics, sensors, magnetism, nanomedicine.

Scope

The number of scientific papers with “nanoparticle” as keyword has increased almost linearly in the last ten years from ~13000 in 2006 to ~46000 in 2016. This impressive worldwide interest stems from the striking scientific appeal of nanoparticles (NPs), which constitute a bridge over the troubled waters between the atomic and bulk worlds, as well as from their actual or potential applications in fields as diverse as catalysis, optics, magnetism, drug delivery. The preparation of NPs is a crossroad of materials science where chemists, physicists, and engineers frequently meet, leading to a continuous improvement of existing techniques and to the invention of new methods. This symposium will bring together leading experts on advanced techniques for nanoparticle synthesis, in order to promote cross fertilization and to inspire progresses in the control of nanoparticle size, shape, composition and functionalization as well as in the fabrication of NPs with complex morphologies. Characterization techniques with high spatial resolution, spectroscopic capability and chemical sensitivity are an essential tool not only to investigate the output of the synthesis procedures but also to elucidate the structure-property relationships of the NPs. For this reason, this symposium will also attract leading experts in state-of-the-art (or beyond) characterization techniques for NPs structural/chemical analysis. This interdisciplinary forum will be completed by the participation of renowned experts in theoretical modelling and simulation of NPs structure and properties, which is of paramount importance both for understanding atomic and electronic structure and to predict non- trivial unexpected behaviors and new phenomena. The symposium will pay particular attention to new directions in technological applications. Given the “hot topic” nature of the symposium and the unique interdisciplinary discussion opportunities it will provide, we expect a numerous and high quality attendance.

Hot topics to be covered by the symposium:

1. Recent development in nanoparticle synthesis techniques

- Chemical
- Lithographic
- Bottom-up
- Combinatorial

2. Structural / chemical analysis of nanoparticles

- Spectroscopic techniques
- High resolution microscopy/chemical mapping
- Advanced scattering techniques

3. Theoretical modelling of nanoparticles

- Atomic ordering and electronic structure
- Dynamical processes, excitations, reactions
- New algorithms and calculation strategies

4. Technological applications of nanoparticles

- Structure-property relationships
- Theoretical predictions vs experiment

Confirmed invited speakers:

- Patricia Abellan, Uni. Leeds (UK)
- Petra De Jongh, Uni. Utrecht (NL)
- Graeme Henkelman, Uni. Texas (US)
- Björgvin Hjorvarsson, Uni. Uppsala (SE)
- Torben R. Jensen, Uni. Aarhus (DK)
- Christoph Langhammer, Uni. Chalmers (SE)
- Yong Lei, Uni. Ilmenau (DE)
- Antonio Miotello, Uni. Trento (IT)
- Richard Palmer, Uni. Swansea (UK)
- Luca Prodi, Uni. Bologna (IT)
- Abhishek Sarkar, KIT (DE)
- Mukhles Sowwan, OIST Okinawa (JP)
- Petra Szilagyi, Queen Uni. London (UK)
- Narayanan Theyencheri, ESRF Grenoble (FR)

- Tejs Vegge, DTU (DK)

International scientific committee

- Rajeev Ahuja (SE)
- Jaakko Akola (NO)
- Lucia Amidani (FR)
- José-Ramón Ares (ES)
- Tomasz Ciach (PL)
- Asunción Fernández (ES)
- Cesare Franchini (AT)
- Horst Hahn (DE)
- Joseph Kioseoglou (GR)
- Giovanni Mattei (IT)
- Amelia Montone (IT)
- Alberto Naldoni (CZ)
- Claudia Zlotea (FR)

Special issues

Dear participants interested in the following Special Issue

Works presented in this Symposia L can be chosen for publication in the following special issues of ***Nanomaterials***:

Advances in Nanoparticles: Synthesis, Characterization, Theoretical Modelling, and Applications (This can be linked to the following link http://www.mdpi.com/journal/nanomaterials/special_issues/advance_nanopar...)

Please, note that the papers will follow the usual peer review process and guidelines for authors.

START AT	SUBJECT View All	NUM.	ADD
09:00	*Welcome to participants*		
09:15	High-Throughput Virtual Screening to Rationally Design and Prepare Protein - Carbon Nanoparticle Hybrids	**L.1.5**	☆
09:30	The Making and Breaking of Lead-Free Double Perovskite Nanocrystals of Cesium Silver-Bismuth Halide Compositions	**L.1.2**	☆
09:45	Controlling the morphology of silver nanoparticles deposited by plasma-enhanced atomic layer deposition (PEALD) for plasmonic applications	**L.1.3**	☆
10:00	Synthesis and Surface Functionalization of Ge Quantum Dots	**L.1.4**	☆
10:15	*Coffee break*		
	Magnetism : Bjørn C. Hauback		
11:00	Magnetic metamaterials	**L.2.1**	☆
11:30	Investigating the Structure and Magnetic Properties of Amorphous Ni60Nb40 Alloy	**L.2.2**	☆
11:45	Room temperature antiferromagnetism in FeN and Fe2N nanocrystals on GaN	**L.2.3**	☆

START AT	SUBJECT View All	NUM.	ADD
12:00	Rational Design of Organometallic Precursors to the Synthesis Iron Germanide Nanocrystals	**L.2.4**	☆
12:15	Surfactant concentration dependence on magnetite nanoparticles growth and properties	**L.2.5**	☆
12:30	*Lunch*		
	Nanocatalysts : Giovanni Mattei		
14:00	Pulsed laser irradiation inducing superheating and phase explosion to produce nanocatalysts	**L.3.1**	☆
14:30	Various Morphologies/Phases of Hybrid Particles Produced by Pulsed Laser Irradiation in Liquid Media	**L.3.2**	☆
14:45	Photocatalytic degradation of 2,4-D in aqueous solution using Mn doped Graphene/Zinc Oxide nanoparticle under LED radiation	**L.3.3**	☆
15:00	Preparation and photocatalysis property of uniform MoS2 nanosheets in-situ grown on the surface of graphene thin film	**L.3.4**	☆
15:15	Development of Gas Phase Condensation for the growth of Metal/MetalOxide nanocomposites with application in CO2 reduction catalysis	**L.3.5**	☆
15:30	*Coffee break*		
	Electronic and Optical Properties : Antonio Miotello		
16:00	Alloy Nanoparticles as Plasmonic Hydrogen Sensors	**L.4.1**	☆
16:30	Si Quantum Dots for Single Electron Transistor: Synthesis, Characterization and Theoretical Comparison	**L.4.2**	☆
16:45	Overview of Optical Characteristics on the Surface Defects in InP Colloidal Quantum Dot	**L.4.3**	☆
17:00	Photoionization cross section of a donor impurity in GaN/InGaN core/shell quantum dot under hydrostatic pressure	**L.4.4**	☆
17:15	Selective excitation of chiral response in clusters of nanoparticles with vector complex source vortex beams	**L.4.5**	☆

START AT	SUBJECT View All	NUM.	ADD
	High resolution characterization : Petra Szilagyi		

START AT	SUBJECT View All	NUM.	ADD
09:00	REVEALING THE ATOMIC STRUCTURE AND DYNAMICS OF SIZE-SELECTED NANOCLUSTERS WITH VARIABLE-TEMPERATURE, ABERRATION-CORRECTED STEM	**L.5.1**	☆
09:30	Prospects of Using Molecular Electron Energy Loss Spectroscopy on individual functionalized metallic nanoparticles	**L.5.2**	☆
10:00	In-Situ Atomic-Scale Observation of Intermediate Pathways of Melting and Crystallization of Supported Bi-Nanoparticles in the TEM	**L.5.3**	☆
10:15	Heat-induced 3D morphological changes of a single Au nanostar using a fast in-situ tomography approach	**L.5.4**	☆
10:30	*Coffee break*		
	Theory and Modelling : Hannes Jónsson		
11:00	Computational Design of Nano-structured Catalysts from DFT, Genetic Algorithms and Machine Learning	**L.6.1**	☆
11:30	Ammonia Decomposition over Alumina-supported Ru Catalyst: Theoretical and Experimental Studies	**L.6.2**	☆
11:45	Unbiased potential energy surface exploration for metal atom decorated C60 with and without electric field	**L.6.3**	☆
12:00	First principles investigation of Ti nanoparticle oxidation	**L.6.4**	☆
12:15	Structural Diversity of Quasi 1D Zinc Oxide: A Global Optimisation Approach	**L.6.5**	☆
12:30	*Lunch*		
	Nanomedicine and Imaging : Yong Lei (tbc)		
14:00	Dye-Doped Silica Luminescent Silica Nanoparticles for Nanomedicine	**L.7.1**	☆
14:30	Carbon Dots Doped with Dysprosium: A Bimodal Nanoprobe for MRI and Fluorescence Imaging	**L.7.2**	☆
14:45	CTAB-FREE SELECTIVE PRECIPITATION OF GOLD NANOPRISMS IN THE PRESENCE OF GOLD NANOSPHERES	**L.7.3**	☆
15:00	Improving the optical tunability of metal phosphide quantum dots: Lessons learned from metal phosphide surface chemistry and interfaces	**L.7.4**	☆

START AT	SUBJECT View All	NUM.	ADD
15:15	Surface engineered fluorescent silica nanoparticles as probe for the investigation of the biofilm EPS matrix	**L.7.5**	☆
15:30	Investigation of the interaction between fluorescently labelled silica nanoparticles and the EPS of Pseudomonas biofilms	**L.12.4**	☆
15:45	*Coffee break*		
	Energy Conversion and Storage : Torben R. Jensen (tbc)		
16:00	Template-based techniques for preparing nanoparticles for energy conversion and storage applications	**L.8.1**	☆
16:30	Shape-Tunable SrTiO3 Nanocrystals for Facet-Dependent Optical Property and Photocatalytic Activity Characterization	**L.8.2**	☆
16:45	Characterization of the photoelectric properties of hematite nanoparticles synthesized with controlled morphologies	**L.8.3**	☆
17:00	Photocatalytic degradation of phenol using Cd-doped ZnO nanorod photocatalyst under sunlight illumination	**L.8.4**	☆
17:15	Facile Synthetic Routes to Cadmium-Free Metal Phosphide (InP, Zn3P2) Quantum Dots	**L.8.5**	☆
	Poster Session : Luca Pasquini, Bjørn C. Hauback, Hannes Jónsson		
17:30	Influence of dopant concentration on the properties of the yttrium aluminum garnet	**L.P.1**	☆
17:30	Resistive Random Access Memories as Next Generation High Performance Computing Systems	**L.P.2**	☆
17:30	Synthesis and characterization of WO3-doped ZnO Nanoparticles fixed on glass surface for photocatalytic degradation of dye	**L.P.3**	☆
17:30	Microwave vaporization and ionization of the metal wires with high boiling point	**L.P.4**	☆
17:30	Structure and surface plasmon resonance of gold nanoparticles fabricated by ion coater	**L.P.5**	☆
17:30	Structural Insight into Glassy PdSi Alloys from Spectroscopy and Mass Spectrometry	**L.P.6**	☆

START AT	SUBJECT View All	NUM.	ADD
17:30	Invertert circuits in complementary technology using inorganic nanoparticle-based TFTs	**L.P.7**	☆
17:30	Characterization of artificial and aerosol nanoparticles with reference-free grazing incidence X-ray fluorescence analysis	**L.P.8**	☆
17:30	DFT study of CO and oxygen adsorption on Pt nanoparticles: adsorption site and cluster size effects	**L.P.9**	☆
17:30	Surface Functionalization of Germanium Nanosheets	**L.P.10**	☆
17:30	Recyclable peroxidase-mimicking FePd nanocatalysts	**L.P.11**	☆
17:30	Investigation of Au nanoparticles supported on ZnO for CO oxidation using density functional theory	**L.P.12**	☆
17:30	Hybrid TiO2-SiO2 structure derived from rice straw and enhanced photocatalytic properties	**L.P.13**	☆
17:30	Density functional study of hydrogen adsorption on 55-atom Pt-Ni nanoclusters	**L.P.14**	☆
17:30	Preparation and characterization of Cu2ZnTiS4 and Cu2ZnTiSe4 nanopowders	**L.P.15**	☆
17:30	Outcomes of Na+ substitution with Li+ or K+ ions in NaGdF4 upconverting nanoparticles	**L.P.16**	☆
17:30	Shrinking of CH3NH3PbBr3 perovskite nanocrystals via Ostwald ripening	**L.P.17**	☆
17:30	Time-resolved study of calcium carbonate precipitation	**L.P.18**	☆
17:30	Linear and non-linear optical spectroscopy of CdSe:Er tetrapod-shaped nanoparticles	**L.P.19**	☆
17:30	Synthesis of binary Ga/Al nitride nanopowders via transamination/deamination of mixed gallium and aluminium tris(dimethyl)amides	**L.P.20**	☆

START AT	SUBJECT View All	NUM.	ADD
17:30	Modelling the Tunelling Conductivity of Nanotube Composites Authors : Ivan Karbovnyk (1), Dmytro Lykashevych (2), Dmytro Chalyy (2), Andriy Stelmashchuk (1), Halyna Klym (3) Affiliations : (1) Ivan Franko National University of Lviv, 107 Tarnavskogo Str., Lviv, 79017, Ukraine (2) Lviv State University of Life Safety, 35 Kleparivska Str., Lviv, 79000, Ukraine (3) Lviv Polytechnic National University, 12 Bandera Str., Lviv, 79013 Ukraine Resume : An approach to calculating integral conductivity of a model nanotube/dielectric composite system is discussed. Conductivity of random nanotube network formed in the dielectric medium is simulated considering tunneling conductivity between individual nanotubes being in close proximity and taking into account intrinsic conductivity of nanotubes. 3D model of a dielectric volume filled randomly with conductive nanotubes (nanotube/dielectric composite) is presented. Computer simulations performed in the frame of this model allowed us to calculate the total conductivity of such composite. The influence of tunneling distance parameter of the system conductivity was investigated. The results of the simulations coincide with experimental data obtained by other researchers and also indicate the difference for the cases of overlapping nanotubes (“soft core” model) and non-overlapping nanotubes (“hard core” model). The comparison with measured results shows that "hard core" model can be effectively used for predicting the parameters of fabricated composite being an important step towards the creation of the material with desired properties.	**L.P.21**	☆
17:30	Selective control of chiral response in clustered nanoparticles via material selection	**L.P.22**	☆
17:30	Comparsion between graphene oxide obtained by "top-down" and "bottom-up" methods.	**L.P.23**	☆
17:30	Optical, photocatalitic and antibacterial properties of GPTMS- functionalized ZnO QDs	**L.P.24**	☆

START AT	SUBJECT View All	NUM.	ADD
09:00	*Plenary Session (Main Hall)*		
12:30	*Lunch*		
	Nanoalloys and catalysis : Patricia Abellan		
14:00	In situ observation of atomic redistribution in gold-silver nanorods	**L.9.1**	☆
14:30	Unlocking the Potential of Nanoparticles Comprising Immiscible Elements for Direct H2O2 Synthesis	**L.9.2**	☆

START AT	SUBJECT View All	NUM.	ADD
14:45	Internal phase structure and thermal transformation of laser generated Au-Fe nanoparticles characterized by in situ STEM	**L.9.3**	☆
15:00	Alloying effects in plasma-created nanoparticles: Combining metals with differing physical-chemical properties	**L.9.4**	☆
15:15	Synthesis And Characterization Of Magnetic Fe3O4/MnO2 Nanocomposite And Its Application In Dye Degradation.	**L.9.5**	☆
15:30	*Coffee break*		
16:30	Investigating the reduction process of doped and undoped Ceria nanoparticles using EELS with in-situ TEM	**L.10.2**	☆
16:45	Use of graphene oxide to prepare enhanced catalytic ceria nanoparticles arranged in two dimensions	**L.10.3**	☆
17:00	Water-dispersible copper sulfide nanocrystals via ligand exchange	**L.10.4**	☆
17:15	Nanoparticle Shape Identifiers: Towards Identification and Classification of Complex Nano Shapes	**L.10.5**	☆
18:00	*Graduate Student Award & Reception 18:00-21:00 (Main Hall)*		

START AT	SUBJECT View All	NUM.	ADD
	New materials and methods : Salvador Eslava		
09:00	High entropy oxides with tailorable properties: Fundamental aspects and prospects	**L.11.1**	☆
09:30	Using a graphene substrate to influence structure and properties of alkali earth oxide nanoclusters	**L.11.2**	☆
09:45	Dynamic nuclear polarization enhanced solid-state NMR as a powerful tool for surface investigation with sub-Ångstrom resolution	**L.11.3**	☆
10:00	Correlation between chemical microstructure and fracture in creep tested 14%Cr ODS steel	**L.11.4**	☆
10:15	CLAY FOR CARBON CAPTURE AND STORAGE	**L.11.5**	☆
10:30	*Coffee break*		

START AT	SUBJECT	View All	NUM.	ADD
	Hybrid and composite nanomaterials : Petra E. de Jongh			
11:00	Metal-organic frameworks: an approach to simultaneously control guest particle structure and surface chemistry		**L.12.1**	☆
11:30	Zeolite supported platinum nanoparticles for small organic molecule oxidation and reduction in fuel cell		**L.12.2**	☆
11:45	Proteins as supramolecular hosts for fullerenes		**L.12.3**	☆

START AT	SUBJECT	View All	NUM.	ADD
12:00	Microfluidic synthesis and investigation of spatially resolved kinetic pathways for complex gold nanostructures		**L.12.5**	☆

Authors : Luca Boselli, Qi Cai, Valentina Castagnola, Kenneth A. Dawson
Affiliations : Centre for BioNano Interactions, School of Chemistry, University College Dublin, Belfield, Dublin, Ireland.

Resume : An incredible variety of synthetic strategies have been developed in the last 10 years in the production of shaped gold nanoparticles (GNPs).[1-3] In particular, branched GNPs have shown to be of interest for their physicochemical properties (SERS, NIR-SPR) and potential in the biological/biomedical field.[4-5] However, from the synthetic point of view there is a lack of understanding on how these branched features are generated and the synthesis still suffer of high in-batch and batch-to-batch variability both in terms of size and shape distribution therefore limiting the translation of these materials to biomedical applications. The use of microfluidic reactors has been proposed as a way to ensure higher control of the thermal and chemical environment, leading to an improved control in the nanoparticles uniformity.[6-9] In this work, we propose the use of microfluidic synthesis in continuous flow to generate high quality and reproducible branched gold NPs with minimum human interference and we analyse the mechanism behind the formation of a NP, especially in relation to the chosen reducing agent. Commonly the mechanism behind NPs formation is regulated by thermodynamic processes (known as nucleation and growth) but also by kinetic processes, which limit the level of control on the NPs properties. The microfluidic approach allows us to isolate kinetic intermediates in order to investigate the shape evolution over time. We demonstrated how, in some case, the growth pathway of gold nanostructures might involve unexpected differently shaped reaction intermediates. The evolution study of GNPs allowed not only to elucidate reaction mechanisms, but also to develop synthetic strategies for the production of a number of new and diverse complex gold nanostructures. We believe that the approach adopted in this work represents a key step toward the development of a more regulated and controllable synthesis of NPs necessary for their application in the field of nanomedicine. References 1. Grzelczak, M.; Pérez-Juste, J.; Mulvaney, P.; Liz-Marzán, L. M., Shape control in gold nanoparticle synthesis. Chemical Society Reviews 2008, 37 (9), 1783-1791. 2. Hao, E.; Schatz, G. C.; Hupp, J. T., Synthesis and optical properties of anisotropic metal nanoparticles. Journal of Fluorescence 2004, 14 (4), 331-341. 3. Bakr, O. M.; Wunsch, B. H.; Stellacci, F., High-yield synthesis of multi-branched urchin-like gold nanoparticles. Chemistry of materials 2006, 18 (14), 3297-3301. 4. Talamini, L.; Violatto, M. B.; Cai, Q.; Monopoli, M. P.; Kantner, K.; Krpetic, Z.; Perez-Potti, A.; Cookman, J.; Garry, D.; P. Silveira, C., Influence of size and shape on the anatomical distribution of endotoxin-free gold nanoparticles. ACS nano 2017. 5. Chithrani, B. D.; Ghazani, A. A.; Chan, W. C., Determining the size and shape dependence of gold nanoparticle uptake into mammalian cells. Nano letters 2006, 6 (4), 662-668. 6. Zhao, C.-X.; He, L.; Qiao, S. Z.; Middelberg, A. P., Nanoparticle synthesis in microreactors. Chemical Engineering Science 2011, 66 (7), 1463-1479. 7. Song, Y.; Hormes, J.; Kumar, C. S., Microfluidic synthesis of nanomaterials. Small 2008, 4 (6), 698-711. 8. Wagner, J.; Köhler, J., Continuous synthesis of gold nanoparticles in a microreactor. Nano letters 2005, 5 (4), 685-691. 9. Nightingale, A. M.; Phillips, T. W.; Bannock, J. H.; de Mello, J. C., Controlled multistep synthesis in a three-phase droplet reactor. Nature communications 2014, 5.

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12:15	*Closing remarks*			

Symposium organizers

Bjørn C. HAUBACK
Institute for Energy Technology

Instituttveien 18, NO-2007 Kjeller, Norway

Mail : bjorn.hauback@ife.no

Hannes JÓNSSON
University of Iceland

VR-III, Hjardarhagi 2-6, Iceland

Luca PASQUINI
Department of Physics and Astronomy, University of Bologna

Viale C. Berti-Pichat 6/2 I-40127 Bologna Italy

Phone : +39 051 2095149
Mail : luca.pasquini@unibo.it

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