Egyptian National Committee of Crystallography (ENCC)

and

The Egyptian Society of Crystallography and Its Applications (ESCA)

Celebrate

The International Year of Crystallography (IYCr2014)

By organizing

The 12th International Workshop

On

Synchrotron Radiation in Nanomaterials Research

15-18 November, 2014

El-Gouna, Hurghada, Red Sea, Egypt

THE WORKSHOP
IS HELD UNDER THE AUSPICES OF

Prof. Dr. Mahmoud Sakr

President of
Academy of Scientific Research and Technology

Honorary Chairmanship

Prof. Dr. Tarek Hussein

Vice President of SESAME Council

Chairman

Prof. Dr. Karimat El-Sayed

President of ENCC and ESCA, Ain Shams University

Co-Chairman

Prof. Dr. Ibrahim Farag

Vice-President of ESCA, National Research Center

Sponsored by:

- ✓ **Academy of Scientific Research and Technology (ASRT), Egypt.**
- ✓ **International Center of Diffraction Data (ICDD).**
- ✓ **Panalytical:**

PANalytical is the world's leading supplier of analytical instrumentation and software for X-ray and related techniques. The company offers solutions for X-ray diffraction (XRD), X-ray fluorescence (XRF), near-infrared (NIR) spectrometry, optical emission spectroscopy (OES) and pulsed fast and thermal neutron activation (PFTNA). The product portfolio includes a broad range of XRD, XRF, NIR, OES and PFTNA systems and software for scientific research and development, for industrial process control applications and for semiconductor metrology.

PANalytical instrumentation is widely used for the analysis and materials characterization of products such as cement, metals and steel, nanomaterials, plastics, polymers and petrochemicals, industrial minerals, glass, catalysts, semiconductors, thin films and advanced materials, pharmaceutical solids, recycled materials and environmental samples.

Founded in 1948, as part of Philips, PANalytical currently employs a staff of over 1,000 people worldwide. Its headquarters are in the Netherlands as are two supply and competence centres and its own X-ray tube. Fully equipped application laboratories are located in Japan, China, USA, and the Netherlands. Research activities are based in the Netherlands and the UK. A sales and service network in more than 60 countries ensures unrivalled levels of customer support to a growing customer base. In 2002, Panalytical was incorporated into Spectris as one of their autonomous operating businesses.

PANalytical

Contents

Page

Page

Organizer Profile

The Egyptian National Committee of Crystallography (ENCC):

In 1976, the crystallographers were able to inaugurate the Egyptian National Committee of Crystallography (ENCC) and in 1978 Egypt became a member of the International Union of Crystallography. It was the first National Committee of Crystallography to join the IUCr in the Arab World. It is one of a number of Egyptian National Committees (ENCs) belonging to the Academy of Scientific Research and Technology (ASRT). The ENCs functions are to represent as well as engage Egypt internationally within relevant multidisciplinary scientific communities. ENCC also serves a unique role in bringing together crystallographers with a wide range of perspectives. This role is increasingly important for maintaining a high level of professionalism in a community that spans several disciplines and professional societies and that needs communication and coordination internationally. ENCC enriches different scientific related area representing a particular discipline within the field of crystallography and covering a wide range of crystallographic techniques and applications (Single crystal, Powder Diffraction, Materials Science, Neutron Scattering, Small Angle Scattering, Small Molecules, Biological Macromolecules, Synchrotron Radiation).

Primary functions of ENCC are:

- To inform crystallographers in Egypt concerning the activities of the IUCr.
- To advise the President of the National Academy of Sciences on matters pertaining to Egypt participation in the IUCr.
- To nominate to the National Research Council persons to represent the crystallographers in the Egypt as delegates to the General Assemblies of the IUCr and other meetings sponsored by the Union.
- To provide information and guidance for such delegates.
- To plan and sponsor scientific meetings in Egypt in consonance with the objectives of the IUCr.
- To perform duties as are required of National Committees of adhering countries under the statutes of the IUCr.
- To take any action directed toward the benefit and advancement of the science of crystallography throughout the world.

The Egyptian Society of Crystallography and Its Applications (ESCA):

It is founded in 1995 as a leading scientific society of crystallography in Africa and Arab countries. ESCA is active in providing awareness of the latest developments in various scientific topics in X-ray crystallography and its applications. They are done through the organization of general lectures, National and International Schools and Workshops in cooparation with different scientific institutions and industry.

Organizing and Programme Committee

• ***Yehia Abbas***	Suez Canal University
• ***Ahmed Ramadan***	Helwan University
• ***Aida Elshabiny***	National Research Center
• ***Aisha Moustafa***	National Research Center
• ***Alaa Akl***	Minia University
• ***Gihan Kamel***	Helwan University
• ***Sameh Ibrahim***	Ain Shams University
• ***Ahmed Farghly***	National Research Center
• ***Mohamed Bakr***	Ain Shams University
• ***El-Sayed Shalaby***	National Research Center

Scientific Committee

- ***Karimat El-Sayed*** Ain Shams University
- ***Ibrahim Farag*** National Research Center
- ***Salah Arafa*** American University in Cairo (AUC)
- ***Mostafa Radwan*** Fayoum University
- ***Amer El-Korashy*** British University in Egypt

Objectives

The Workshop in celebrating the International Year of Crystallography (IYCr2014), aims to provide a forum for exchange of knowledge in order to get the latest developments in structure determination and characterization of nanomaterials. The main objective is to highlight the powerful capabilities of Synchrotron radiation (SR) in nanomaterials research aspects. During this occasion, Nanomaterials fabrication methods will be demonstrated and combined with the advanced SR applications covering different techniques such as X-ray Diffraction (XRD), Small Angle Scattering (SAXS) and Extended X-ray Absorption Fine Structure (EXAFS). Hands-on computer training on some programs in the field will be also arranged.

Topics

- Synchrotron Radiation Concepts and Application.
- Synthesis of nanomaterials.
- Nanomaterials ab-initio Structure Determination.
- Synchrotron applications in Nanomagnetic Materials and X-Rays Magnetic Microscopy.
- Synchrotron Radiation for Advanced Bio-imaging and Nano-FTIR.
- EXAF: From Spectroscopy to Structural Investigation of Nanomaterials.
- Microstructure Determination.
- PDF Applications in Amorphous and Nanocrystalline Materials.
- Energy and Synchrotron Radiation.

Basic Policy

The Organizing Committee will observe the basic policy of nondiscrimination and affirm the rights and freedom of scientists throughout the world to adhere or to associate in international scientific activity without regards to such factors as citizenship, relegion, creed, political stance, ethnic origin, race, colour, language age or sex in accordance with the statutes of the International Council for Science.

Program and Time Table

First Day (15 November, 2014) Chairman: Prof. Yehia Abbas		
07.00	***Departure from Cairo***	
11.00	***Visit to Wind Station (Zaafrana)***	
13.00 – 14.00	***Registration and Accommodation***	
14.00	***Lunch***	
17.00 – 17.30	***Opening Ceremony***	
17.30 – 18.30	Celebrating the International Year of Crystallography	**Prof. Karimat El-Sayed**
18.30 – 19.30	Introduction to Synchrotron Radiation and Applications	**Prof. Yehia Abbas**
20.00	***Dinner***	
Second Day (16 November, 2014) Chairman: Prof. Mostafa Radwan		
07.00–08.30	***Breakfast***	
09.00–10.00	Synthetic Methods Of Nanomaterials: Shape & Size Control Via Chemical Methods	**Dr. Mona Bakr**
10.00–11.00	Quantitative structure determination of Nano-structured materials using PDF analysis	**Dr. Ahmed Masadeh**
11.00–12.00	Nanomagnetism in the Light of Circular Polarized X-Rays	**Prof. Eberhard Goering**
12.00–12.30	***Coffee Break***	
12.30–13.30	Global Energy Challenge and Synchrotron Radiation	**Prof. Llewellyn Smith**
14.00	***Lunch***	
17.00–19.30	Program's Training: "Pair Distribution Function Analysis of Nanomaterials (PDF)"	**Dr. Ahmed Masadeh**
20.00	***Dinner***	

Third Day (17, November 2014) Chairman: Prof. Amer El-Korashy		
07.00 – 08.30	***Breakfast***	
09.00–10.00	Application of EXAF: Spectroscopy to Structural Investigation of Nanomaterials	**Prof. Giuseppe Dalba**
10.00–11.00	Synchroland: All-in-one facility: (Advanced Bioimaging of Microspectroscopy & Nano-FTIR)	**Dr. Gihan Kamel**
11.00–12.00	Microstructure determination using X-ray diffraction	**Dr. Matteo Leoni**
12.00–12.30	***Coffee Break***	
12.30–14.30	Program's Training: "Whole Powder Pattern Modeling: PM2K [WPPM]"	**Dr. Matteo Leoni** **Dr. Mahmoud Abd Ellatif**
14.30	***Lunch***	
15.30 – 20.00	**Free/Excursion**	
20.00	***Dinner***	
Fourth Day (18 November, 2014) Chairman: Prof. Salah Arafa		
07.00–08.30	***Breakfast***	
09.00–10.00	Time and Spatially Resolved X-Rays Magnetic Microscopy at Maxymus**	**Prof. Eberhard Goering**
10.00–11.00	***Closing Ceremony: Recommendations***	
11.00–13.00	***Check Out***	
13.00	***Departure to Cairo***	

- **Posters' Session (Presentation):**

Second and Third Days (16 and 17 November 2014): 12.00 – 20.00.

** Maxymus = MAgnetic X-raY Microscope with UHV Spectroscopy

Opening Ceremony

- **Prof. Dr. Mahmoud Sakr,**
  President for Acadmy of
  Scientific Research & Technology, Egypt

- **Prof. Dr. Tarek Hussain,**
  Vice-President for SESAME Council
  Scientific Research & Technology, Egypt.

- **Prof. Dr. Karimat El-Sayed**,
  Chairman of ESCA

- **Prof. Dr. Ibrahim Farag**,
  Co-Chairman of ESCA

- **Prof. Dr. Giuseppe Dalba**
  Department of Physics, Faculty of Sciences,
  University of Trento

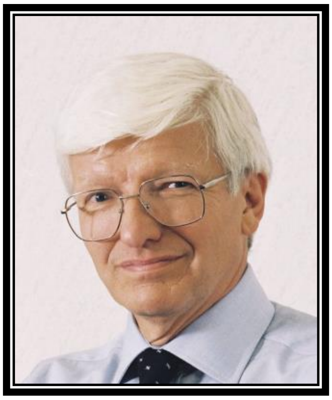
LECTURERS BIOGRAPHY

• Professor Sir Chris Llewellyn Smith FRS

Director of Energy Research,

Oxford University

www.energy.ox.ac.uk



Biography:

Chris Llewellyn Smith is Director of Energy Research, Oxford University (see www.energy.ox.ac.uk), and President of the Council of SESAME (Synchrotron-light for Experimental Science and Applications in the Middle East). He has chaired the Council of ITER, the global fusion energy project, directed the UK's fusion programme, and served as Provost and President of University College London, Director General of CERN (1994-1998, when the Large Hadron Collider was approved and construction started), and Chairman of Oxford Physics. His theoretical contributions to the 'standard model' of particle physics were recognised by his election to the Royal Society in 1984. He has written and spoken widely on science funding, international scientific collaboration and energy issues, and served on many advisory bodies nationally and internationally, including the UK Prime Minister's Advisory Council on Science and Technology (1989-92). His scientific contributions and leadership have been recognised by awards and honours in seven countries on three continents.

- **Prof. Dr. Karimat El-Sayed**

  Professor of Material Science

  Physics Department, Faculty of Science,

  Ain-ShamsUniversity, Abbassia, 11371,

  Cairo, Egypt.

  P.O. Box 8014 Masaken Nassr City, 11371,

  Cairo, Egypt

Qualification:

- Ph.D. in Crystallography (London University, 1965)
- B.Sc., in Physics with an honor degree (Ain Shams University, 1957).

Academic Position:

- Professor of material Science.
- Head of the Physics Department, AinShamsUniversity (1992-1994).
- Visiting Professor at KingAbdul-AzizUniversity, Jedda, Saudi-Arabia (1975-1980). During this period I was the head of the Physics Department and I was able to start and establish the courses and the student Laboratory of the four years for the Physics Department (The Girl Sector)

Scientific Activities:

- Published over 65 papers in crystallography and material science. Some of these papers were presented in International Congresses. The research papers were chosen to be in applied science.
- Supervised 28 Ph.D. and M.Sc. Thesis.

- Organized 11 workshops in cooperation with the Egyptian of Society and the International Union of Crystallography and many one day Seminars in different topics of crystallography and material science
- Attending over 50 international and national congress, conferences and Workshops

International and National Honoring:

- Marshak Lectureship from the American Physical Society (APS)
- Invited to give lectures in the following Places: Stanford University, Berkley University, National Science foundation, Daleware University, Danish Society of Crystallography, Nehru Center for Aluminum in India
- Recipient of the International Award of (L'Oreal-UNESCO) in the field of Material Science (Africa and Middle East Region)(2003).
- Fellow of World Innovation
- Holder of the Supreme Medal of Science and Art from the first degree (given by the President of the Country (1970)).
- Chair Person of the International Union of Crystallography Teaching Commission (1999/2002).
- Member of the High Supreme Council of Higher Education (President of the Country) ((1992/ -----).
- Member of the National Committee of Applied and Pure Physics (1982/-)
- Member of the National Committee of Crystallography (1981/——).
- Member of the American Crystallographic Association (1965--2008-).
- Member of the Third World Women-Scientists Organization.
- President of the Egyptian Society of Crystallography and Application (ESCA) (by Election) (1995----).
- Vice-President of the Egyptian Society of Solid state for Six years (by election) from (1984-1990).
- Chair Person of the Permanent Committee of promoting associate professors (by election from 1982-1986).
- Listed in the Who’s Who Bibliography as one of the selective scientist all over the world.

Editor of the following Proceedings:

- X-Ray Powder Diffraction and Application (1990).
- Mathematical Crystallography (1993).
- Fourth Arab Conference on Physics Teaching.
- Computational Methods in X-ray Powder Diffraction Analysis.
- Thin Film Technology and Application.
- Crystallography Teaching and Application.
- Translating a book about teaching Crystallography for School Children to Arabic with major new addition, it is now in Arabic at the IUCr Web. Site.
- Computer based Crystallographic Teaching.
- Recent Advances in Powder Diffraction.

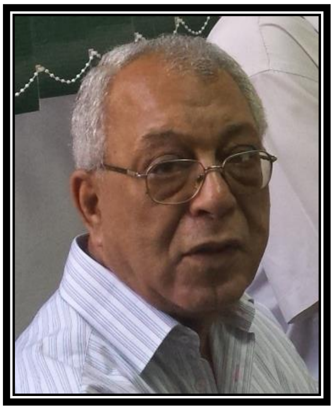
- **Prof. Dr. Yahia Abbas**

  Professor of Material Science

  Physics Department, Faculty of Science,

  Suez Canal University,

  Ismailia – Egypt.



Emplyment:

1963 - 1984: Neutron & Reactor Physics Department, Atomic Energy Authority, Cairo, Egypt.

1984 - 1989: Assistant Professor, Physics Department, Faculty of Science, Suez Canal University, Ismailia, Egypt.

1989 - 1997: Professor of Physics, Head of Physics Department, Faculty of Science, Suez Canal University, Ismailia, Egypt.

1997 - 2003: Vice – Dean for Higher Studies and Scientific Research, Faculty of Science, Suez Canal University, Ismailia, Egypt.

Present Employment: Professor, Physics Department, Faculty of Science, Suez Canal University Ismailia, Egypt.

Education:

1963: B. Sc. (Physics), Ain-Shams University, Cairo, Egypt.

1968: M. Sc. (Nuclear Physics), Cairo University, Cairo, Egypt.

1976: Doctor of Science (Physics) Grenoble University, Grenoble, France.

Thesis Entitled: Neutron Diffraction Studies of Crystal and Magnetic Structures of Rare Earths Oxychalcogenides

Research Field & Experience:

- X- Rays and neutron diffraction studies of magnetic Materials and take the responsibility for the development of the tow neutron Diffraction spectrometers at Egyptian nuclear reactor (ET-RR-1).
- Crystal and magnetic structures determination.
- The diffraction methodologies.
- Nanostructured materials.
- Advanced ceramics.
- Intermetallics.
- Qualitative and Quantitative phase analysis.
- Advanced magnetic materials and spintronics.

Scientific Activities:

Fellow – Founder of most of the Egyptian Scientific Societies:

- Egyptian Society of Nuclear Sciences.
- Egyptian Society of Solid State Science.
- Egyptian Society of Crystallography (General Secretary).
- Egyptian Physical Society.
- National Committee of Crystallography (Academy of Scientific Research and Technology).
- National Committee of New Materials (Academy of Scientific Research and Technology).
- National Committee of Scientific Instruments (Academy of Scientific Research and Technology).
- National Committee of Synchrotron Radiation (Academy of Scientific Research and Technology).
- National Committee for Radiation Protection (Atomic Energy Authority and Technology).

Scientific Missions:

Invited visiting professor at the universities of most of the European Countries, United States, Japan, Russia and India.

Scientific Researchs & Papers:

- Supervisor of more than 40 M. Sc and Ph.D. Thesis.
- Author of more than 80 published in International and Egyptian Scientific Journals.

• Dr. Mona Bakr

Director of Nanotech Egypt Co. Inc.
Assistant Professor of Nanotechnology
& Ultrafast Spectroscopy National
Institute of Laser Enhanced Sciences
Cairo University Giza - Egypt.
Tel: +202 38581 440
Fax: +20 238 58 1441
Email: monabmohamed@gmail.com

Education:

Dr. Mohamed gained her B.Sc. 1991 and her MSc, in Chemistry in 1994. She received her PhD in 2002 from Georgia Tech, Atlanta, USA under supervision of Prof. Mostafa El-Sayed, then post-doctoral at University of Lausanne and senior research scientist in EPFL Switzerland. Dr. Mona Bakr Mohamed is Currently Associate Prof. at National Institute of Laser Enhanced Science, Cairo University.

Research Focus:

Her research interest is focused on synthesis and characterization of metallic, magnetic and semiconductor nanocrystals of different shape and size, as well as their optical properties and ultrafast dynamics using different laser techniques. Her research group 22 graduate students are working on constructing novel nanomaterials for solar cell applications, photoelectronic devices, biomedical imaging, cancer therapy, nanocatalysis, and water treatment.

Publications & Awards:

She has 45 publications published in international journals such as Small, ACS Nano, Advanced Functional Mater., J. Phys. Chem, Physical Rev., Nano letters, Chemical phys. Letters, she supervised many students and formed the scientific school of more than 35 MSc and PhD students in various universities all over Egypt Dr. Mohamed receives three national grants from STDF and IMC to support her work on nanomaterials for solar cell applications and for biomedical imaging. Finally; for her work in the area of nanomaterials, Dr. Mohamed was elected by the academy of scientific research (ASRT) to State Encouragement Award in Advanced Technological Science "Basic Science" in 2010.

• Dr. Ahmad S. Masadeh

Department of Physics

The University of Jordan

Amman 11942, Jordan

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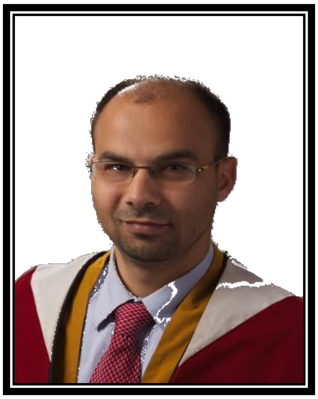

Education :

2004 – 2008: **Ph.D.** in Experimental Condensed Matter Phys., Michigan State Univ., MI, USA
- *Dissertation Title: Quantitative Structure Determination of Nanostructured Materials Using the Atomic Pair Distribution Function (PDF) Analysis.*
- *Supervisor: Prof. Simon J.L. Billinge.*

2002 – 2004 **M.S.** in Physics, Michigan State Univ., East Lansing MI, USA
1994 – 1998 **B.S.** in Physics, Yarmouk University, Irbid, Jordan.

Research fields:

- Investigation of atomic **arrangements** in **nanostructured** materials (such nanoparticles) using the atomic pair distribution function (PDF) technique.
- Studying the atomic structure of pharmaceutical materials at different atomic length scales using the pair distribution function methods.
- Characterization of the local atomic distortions in crystaline materails at different length using three dimensions direct real space probe, the pair distribution function (PDF) technique.

Skills and Experience:

- Experience in conducting x-ray powder diffraction experiment using synchrotron or in-house X-ray machine.
- Experience in conducting total scattering experiment using synchrotron or in-house X-ray machine.
- Experience in analyzing total scattering data, using local structure PDF methods, resulting in quantitative structural information at different atomic length scales.
- Experience in atomic structure analysis (Rietveld).
- Very familiar with Linux, Matlab, SPEC and LATEX.

Professional Experience:

2014 – Present:	Chair of Physics Department at the University of Jordan
May12-now:	Member of the interim user's executive committee of SESAME synchrotron.
2008:	PDF-Workshop speaker, 4th American Conference on Neutron Scattering, Santa Fe, NM, hosted by the Lujan Neutron Scattering Center at Los Alamos National.
2005:	Lecturer of PDF structural studies-Workshop, MSU, East Lansing, MI
2005:	Workshop Co-organizer, “PDF structural studies-Workshop”, MSU, East Lansing, MI
2005-2006:	NIRT (Nanoscale Interdisciplinary Research Team) seminar organizer, MSU, East Lansing, MI.

Professional Memberships:

- American Physical Society (APS)
- American Chemical Society (ACS)
- American Crystallographic Association (ACA)
- Materials Research Society (MRS)
- Neutron Scattering Society of America (NSSA)

• Prof. Dr. Eberhard Goering

Modern Magnetic Systems Departement,
Magnetic X-Ray Spectroscopy Group,
Max-Planck-Institute for Intelligent Systems,
Heisenbergstr. 3, 70569 Stuttgart,
Germany.

Studies:

WS 1983/84 - SS 1990 Technical-High-School Darmstadt, Germany
Studies in physics with final degree: Diploma

11.07.1990 Final exam (Diploma)
Final grade: very good (sehr gut)

Diploma thesis: "Development of a low field SQUID – magnetometer and investigation of new ternary Uranium and Cerium compounds"; 'Institute of Technical Physics';
Working Group: Prof. Dr. F. Steglich, Technical-High-School Darmstadt, Germany

06.03.1996 PhD in physics
Final grade: with honours (summa cum laude)
Total final grade: very good (magna cum laude)

PhD thesis: "Photoemission studies at well-defined single crystal surfaces of V_2O_3 and VO_2";
Working Group: Prof. Dr. S. Horn, University of Augsburg, Germany

Professional career:

January 1991 - March 1996:
Scientific Assistant to Prof. Dr. S. Horn, "Experimental Physics II", University of Augsburg".

April 1996 – June 200:
Scientific Assistant to Prof. Dr. Gisela Schütz (University of Augsburg and University of Würzburg).

Since Juli 2001:

Senior Scientist in a permanent position at Max-Planck-Institute for Metals Research in Stuttgart, Department of Prof. Dr. Gisela Schütz "Modern Nano-structured Magnetic Materials".

18.06.2003:

Qualified as University Lecturer (Habilitation) at the Faculty of Physics at the University of Würzburg.

Subject of the „Habilitation": „Investigations on the microscopic origin of the magneto-crystalline-anisotropy using X-ray magnetic circular dichroism and resonant magnetic X-ray reflectometry"

02.02.2005:

Continued as University Lecturer at the Faculty for Physics and Mathematics at the University of Stuttgart (Umhabilitation).

Group leader at the MPI-IS department Schütz:

- Leader of the MPI-IS UHV compatible x-ray Microscopy group MAXYMUS at the HZB/BESSY 2.
- Leader of the MPI-IS XMCD project at the ANKA/WERA Synchrotron at the KIT/Karlsruhe.
- Leader of the MPI-IS magnetic reflectometry ErNST project. Main Topics: XMCD methodical developments, magnetic oxides and nanostructures, magnetic thin film and interface phenomena

- # Prof. Dr. Giuseppe Dalba

Department of Physics
Faculty of Sciences
University of Trento
Via Sommarive 14, I-38100 Povo (Trento), Italy
fax: +39-0461-881696
tel : +39-0461-881570
e-mail: giuseppe.dalba@unitn.it
http://alpha.science.unitn.it/~rx/raggi_x/index.html

Research topics:

- Local structure and dynamics in crystalline and non-crystalline solids, studied by correlation-sensitive probes, such as EXAFS.
- Local behaviour of negative thermal expansion in solids.
- Characterization of the local structure of luminescent materials (Porous Silicon, Si based nanosystems, rare-earth doped compounds) and its influence on photo and electro-luminescence.
- Characterization of thermal and static disorder in amorphous systems.
- Research on the relationship between local structure and ionic conduction properties of supersonic glasses.
- Study of the local environment of highly diluted doping elements, belonging to III and V group, in thin films of hydrogenated amorphous germanium.
- Refining the knowledge of the effects of thermal disorder on EXAFS spectroscopy.
- Study of luminescent nanostructures excited by synchrotron radiation carried outby SNOM microscopy.

• Dr. Gihan Kamel

Lecturer

Physics Department, Faculty of Science,

Helwan University, 11792,

Cairo, Egypt

Current position:

- SINBAD Beamline Researcher at DAΦNE-LIGHT, INFN-Laboratori Nazionali di Frascati, Rome, Italy, 2014-2015.

Educational profile:

- Ph.D. in Physics, University of Rome, La Sapienza, Rome, Italy.
- M.Sc. in Physics, Helwan University, Cairo, Egypt.

Scientific Activities:

- Member of the Egyptian National Committee of Crystallography, ENCC, Academy of Scientific Research and Technology, 2013-now.

- Member of the Technology Transfer Office Advisory Board, TTO, Helwan University, Egypt, 2013-now.

- Member of the SESAME (Synchrotron-Light for Experimental Science and Applications in the Middle East) Users' Committee, 2012-now.

- Attended over 30 international and National scientific events, participating with posters and/or oral presentations.

- Scientific skills comprise the structure-to-function relationship of biomolecules using X-ray Crystallography, FTIR microspectroscopy, Langmuir-monolayers, Brewster angle microscopy, Small-Angle X-ray Scattering, X-ray Fluorescence, and Atomic Force Microscopy.

Awards:

- ***ParOwn*** Governmental Grant with the Proposal: "Theoretical and Practical Training on Macromolecular Crystallography Using New Programs for Protein Structure Solution", accomplished in the Institute of Crystallography (IC), National Research Council (CNR), Italy. During the period of February-July 2007.

- Prof. Dr. Matteo Leoni

Rovereto (TN, Italy), 30/12/1970
Matteo.Leoni@unitn.it
http://diffraction.guru
☏ +39 0461 882416
🖷 +39 0461 882672

Career:

- Graduated in Materials Engineering with full votes (110/110 cum laude) at the University of Trento (TN, Italy), with a thesis on Experimental determination of residual stresses in ceramic coatings in 1995.
- Research contractor in the Microstructure/XRD lab at the University of Trento (1995).
- PhD in Materials Engineering, University of Roma “Tor Vergata” with a curriculum in surface engineering, 1999.
- Post-doc c/o Prof. E.J.Mittemeijer’s Department at the Max-Planck Institut für Metallforschung, Stuttgart (D).
- Post-doc and assistant professor c/o University of Trento, Department of Materials Engineering and Industrial Technologies (I).
- Associate professor c/o University of Trento, Department of Civil, Environmental and Mechanical Engineering (I), current.

Publications:

- Author of ca. 130 scientific papers in international journals and almost the same number of contributions (several oral) to international conferences.

Main scientific interests:

- Correlation between structure, microstructure and properties of nanostructured, modular and faulted materials.
- Development of novel algorithms and mathematical description for the analysis and classification of nanostructured and layered materials with and without defects (mainly based on traditional and advanced diffraction methods)

- Development of the PM2K code for Whole Powder Pattern Modeling (WPPM) and of the DIFFaX+/MODULAR code for the refinement of faulted, modular and intermediate periodicity structures from (X-rays, neutron and/or electron) diffraction data;
- X-ray diffraction and multiphysics modeling of relevant 2D materials and layered systems showing faults (e.g. LDHs, clays, phosphonates, perovskites, titanates, hydroxides, zeolites etc.) and correlation between defects and activity (e.g. catalytic, optical, thermoelectrical, sequestration, drug delivery, solubilisation)
- Development of fast algorithms (running on GPU) for crystallography and imaging
- Microstructure analysis of nano catalysts, and self-assembled nanosized powders
- Novel materials based on poly-substituted titania and tailored microstructure for electro and photocatalysis;
- Matching between computational Materials Science and X-ray diffraction;
- Perovskites for catalysis and solar energy conversion;
- Development and in situ (on leaf) evaluation of the performance of nanostructured agrochemicals;
- Production and characterization of nanostructured and interlayered pharmaceuticals, agropharmaceuticals and pesticides: structure and microstructure
- Shape memory alloys: crystallography, defects and microstructure understanding via fast synchrotron-based diffraction.

LECTURES

L01

Impact Of Crystallography On Our Life In Handred Years

Prof. Karimat El-Sayed

President of ENCC and ESCA, Ain Shams University, Egypt.

The discovery of Bragg's Law, which has been used later for the structure analysis of different kind of materials, made large Contribution to all field of natural sciences. Scientists discovered that there were good correlation between properties and structures, that governs; Chemical, physical, mechanical and biological properties of different kind of materials .In this presentation I will talk about the development of structure analysis over hundred years and I will discuss the impact of this discovery on biology, material science and pharmacy and all natural science and the reflection of all these discoveries on our life. Moreover as I consider myself as a part of this history, I will talk also about the crystallography in the 60th and also about the famous crystallographers that I met and how they did their research at that times.

L02

Introduction to Synchrotron Radiation and Applications

Prof. Yahia Abbas

Physics Department, Faculty of Science, Suez Canal University, Ismailia, Egypt

A synchrotron is a machine that accelerates charged particles such as electrons to extremely high energies - creating an electron beam that travels at almost the speed of light. However, when high-energy electrons are forced to travel in a circular orbit, they release extremely intense radiation – or ‘synchrotron light’ ranging from infrared to hard x-rays supplied at the end-stations of beamlines. The unique properties of synchrotron light mean that experimental results are far superior in accuracy, clarity, specificity and timeliness to those obtained using conventional laboratory equipmen. Current (third generation) synchrotron light sources optimise the intensity of the light by incorporating long straight sections into the storage ring for ‘insertion devices’ such as undulator and wiggler magnets. Laboratories around the world are now working to overcome the technical challenges associated with the development of fourthgeneration light sources, which are likely to utilise hard x-ray free-electron lasers (FEL). Their research fields include structural and chemical information from diverse sample types ranging from biological to industrial materials.

L03

Synthetic Methods Of Nanomaterials: Shape & Size Control Via Chemical Methods

Mona Bakr

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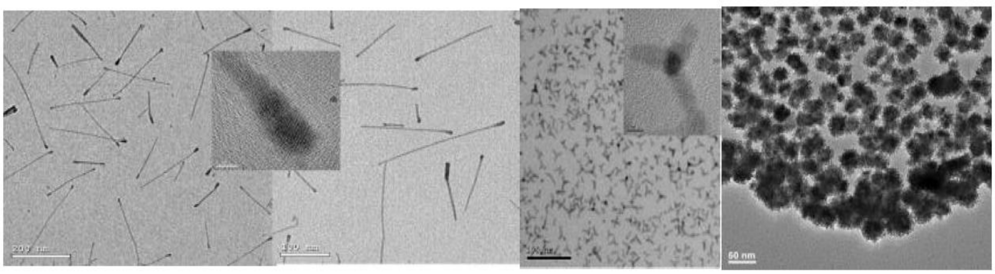
This talk will summarize the different methods to prepare different types of nanomaterials (i.e. metallic, semiconductor, magnetic, carbon nanomaterials). The advantage and limitation of every method will be stated. More emphasis on the chemical synthesis and how to control the particle size and shape will be discussed in details. Chemical synthesis allows us to design nanomaterails and control their morphology and chemical structure. Methods to obtain hybrid nanostructure such as plasmonic-semicondcutor, or plasmonic graphene nanocomposites have been developed in our laboratory and their combined optical and electric properties have been studied. These materials show enhanced photoelectric response which made them good candidate for photovoltaic applications.



TEM images of plasmonic-semicondcutor and graphene plasmonic Hybrid nanostructure

L04 & T01

Quantitative structure determination of Nano-structured materials using PDF analysis.

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The atomic pair distribution function (PDF) is a total scattering based technique, which includes both Bragg and diffuse scattering, and can provide quantitative information about the local structure of the materials at different length scales.

The PDF method is powerful tool to study complex and nanostructured materials at different length scales. The nanoscale order has been observed in Na3BiO4. [1] The size and structure have been addressed in series of CdSe nanoparticles (NPs), with diameter sizes ranging from 2 to 4 nm, prepared by the methods of Peng et al.[2]. The PDF data were collected at the APS, using high energy x-rays.

I will discuss how the PDF yields precise structural information about the NPs such as local bonding, atomic structure size of the core, and so on, as a function of NP diameter. For example, the core structure of the measured CdSe NPs was found to possess a well-defined Wurtzite structure. The diameter of CdSe NPs extracted from the PDF data is in good agreement with the one obtained form standard methods [3]. Recently, the PDF methods have been reported as a key tool for nanomaterials ab-initio structure determination [4].

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L05

Nanomagnetism in the Light of Circular Polarized X-Rays

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Nowadays polarized x-rays are used as a standard tool to investigate complex magnetic materials. This is based on the x-ray magnetic circular dichroism (XMCD) effect, which provides unique possibilities to study magnetic systems in an element specific way. Due to so called sum rules spin and orbital magnetic moments could be quantitatively separated. Strong and effective cross sections are present to access the 3d transition metals and the 4f rare earth elements, where even smallest amounts of magnetic materials could be studied. The XMCD method itself will be introduced and especially nano-magnetic, diluted magnetic materials, and also paramagnetic systems will be discussed, demonstrating the unique possibilities provided by XMCD. On the other hand via the XMCD effect magnetism strongly modifies x-ray optical properties, which allows to turn merely every x-ray based technique into its magnetic counterpart.

L06

Global Energy Challenge and Synchrotron Radiation

Llewellyn Smith

Director of Energy Research, Oxford University

Providing adequate energy for the world's rising population in an equitable manner, in the face of looming climate change and the prospect (in the long-term) of declining fossil fuels, is the one of the greatest challenges of the 21st century. I will review the challenge and the steps that need to be taken to meet it. I will then give examples of some of the possible contributions of experiments that use synchrotron radiation (which include improving photovoltaics, developing artificial photosynthesis, improving batteries and fuel cells, and developing better engines and catalysts).

L07

Application of EXAF: Spectroscopy to Structural Investigation of Nanomaterials

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Synchrotron radiation beams, thanks to their very high intensity, enhanced brightness and wide energy spectra, have contributed to strengthen the potentialities of well-established techniques as well as to stimulate the emergence of new other investigation techniques for the characterization of new materials. Highly collimated beams can irradiate micrometric areas of the samples so allowing to scan the whole surface of a thin film or to investigate samples constituted by extremely low amount of matter. For these reasons the resort to synchrotron facilities has become a prerequisite for obtaining high quality measurements especially in the x-ray regime for the study of low dimensional systems.

Synchrotron facilities provide a wide range of opportunities for studying nanomaterials, among them X-ray absorption fine-structure (XAFS) spectroscopy constitutes the principal method for characterizing structure and composition of nanomaterials.

The growing interest toward nanomaterials, both from the fundamental and technological viewpoints, is due to their unique physical and chemical properties and their technological applications. XAFS is a powerful tool for studying the local structural and dynamical properties of these systems owing to its selectivity to the atomic species constituting the sample, the sensitivity to the short range order and its independence on the long-range ordering typical of nanomaterials. The sensitivity of XAFS to the electronic and local structural properties allows to relate the atomic structure to the peculiar physical and functional properties of nanomaterials.

In this presentation, after a brief review of the basic theory of XAFS, its potentialities and limitations, the detection modes and experimental setups, a selection of significant applications of XAFS to nanomaterials will be reported. The selected systems will include nanoparticles of different nature and different physical properties. Since a detailed description of the structural and dynamical properties of nanomaterials needs the contribution of various techniques, the XAFS results will be discussed together with complementary results coming from several other experimental and theoretical investigations.

L08

Synchroland: All-in-one facility: Advanced Bioimaging of Microspectroscopy & Nano-FTIR

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Importance of synchrotron radiation, SR, in science and technology cannot be overestimated as its diverse applications are rapidly expanding. Meanwhile you are reading this abstract, variant storage rings all over the world are in action producing the most brilliantly intense radiation. With a set of unique properties, synchrotron radiation exerts a significant impact across a wide range of scientific disciplines having its fingerprint in Physics, chemistry, biology, archeology, art, medicine and space. The first part of the presentation will highlight some of the recent Synchrotron-based studies on nanomaterials investigated in world-wide facilities.

More details will be devoted in the second part to the role of synchrotron radiation in bioimaging of cells and tissues utilizing SR- Fourier transform infrared microspectroscopy, underlining the latest evolving nano-FTIR imaging technique. FTIR imaging has been successfully proved to benefit from synchrotron radiation sources for fast acquisition purposes on single cells with micron-level resolution[1]; this in turn allows analyzing the dynamics of molecular contents and their changes over time in an attempt to fight diseases. These approaches are expected to enhance the current knowledge towards the development of highly required drugs as well as for effective diagnoses and treatments.

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Keywords: Synchrotron radiation, Nanomaterials, Bioimaging, micro-FTIR, nano-FTIR

L09 & T02

Microstructure determination using X-ray diffraction

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The properties of a material are conditioned by its crystalline structure but also by its microstructure. Among the available techniques able to provide microstructure information, X-ray diffraction is one of the most versatile, as it is non-destructive and it simultaneously supplies structure information. Using state-of-the-art analysis techniques such as the Whole Powder Pattern Method, structural modifications, shape and domain size distribution, defect type and concentration can be obtained in static conditions or in situ during the material evolution. Patterns from the most diverse sources, like laboratory diffractometers, synchrotrons, neutron sources or electron microscopes can be analyzed in a fast and straightforward way. Basics and the application to real case of study will be presented. The challenges given by specimens containing small and extreme quantities of defects will be illustrated

L10

Time and spatially resolved soft X-rays magnetic microscopy at MAXYMUS

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The MPI-IS operates a new and versatile state of the art soft X-ray scanning microscope (SXM), called MAXYMUS, which is open for user application and located at the undulator beamline UE46 at the HZB/BESSY in Berlin. One unique possibility of MAXYMUS is the UHV capability providing simultaneous measurements of surface sensitive investigations, using total electron yield detection scheme (TEY), which is usually simultaneously performed with high performance transmission experiments being sensitive to the sample volume utilizing special resolutions below 10nm. This microscope is optimized for XMCD based magnetic investigations, providing strong, variable, and rotatable magnetic fields, a temperature range from about 80-400 K, rotatable sample holders etc. In additional, special scanning modes like zone plate scanning and ultra-fast measuring modes are available, allowing time dependent measurements with better than 40ps time resolution and excitation frequencies up to 16 GHz. A detailed introduction to x-ray microscopy and especially SXMs will be provided, including many magnetic and nonmagnetic examples performed at MAXYMUS. In addition, new features and extensions will be presented.

POSTERS

P01

Preparation and Structure Characterization of LATP Electrolyte for Solid State Battery

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Lithium titanium phosphate, $LiTi_2(PO_4)_3$ (LTP), which is based on the Na-Super-Ionic-Conductor (NASICON) framework with the space group $R\bar{3}c$, was studied as a lithium ion-conductive solid electrolyte. NASICON structure can be described as a covalent skeleton $[A_2(PO_4)_3]^-$ consist of PO_4 tetrahedra and AO_6 octahedra, which form many 3D interconnected channels and two types of interstitial sites (M_1 and M_2) where the conducting Li ions are distributed. LTP conductivity is not high enough for practical application. It was reported that Al doping was effective for the enhancement of Li^+ ion conduction. Thus, this work aims at the preparation and structure characterization of $Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$ (LATP) for lithium ion battery applications. Sol-gel method was used and the pellets were sintered at temperature from 700 to 1050 °C for 2 hr. Structural characterization of the LATP sintered pellets were conducted by X-ray diffraction analysis. It was found that the temperature of 950°C is the optimum one for the preparation of LATP single phase. Thus, these conditions can be used to fabricate all-solid-state Lithium battery.

P02

Thermosalient Effect – A Study Of *N′*-2-propylidene-4-hydroxybenzohydrazide

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Thermosalient materials, or colloquially commonly called "jumping crystals", are promising materials for conversion of thermal (or light) energy to mechanical work on nanoscale [1]. These materials, when heated/cooled undergo a sudden and sharp polymorphic single crystal to single crystal phase transition. During this transition the crystals experience a change in their shape, as well as in the size of the unit-cell, and this change is so large that it causes them to jump up to height that is several times their size. This behaviour usually takes place in the time frame of several microseconds. Jumping crystals show high discontinuity in the change of the crystal lattice; the change can be up to 12% [2].

It was reported [3] that *N′*-2-propylidene-4-hydroxybenzohydrazide shows behaviour somewhat similar to that of jumping crystal. This system was found in three polymorphic modifications (I, II and III), all having the same polar space group $Pna2_1$, with the phase transitions I to II, and III to II reported as topotactic (single crystal to single crystal). It was also reported that during irreversible phase transition from I to II, the polar axis undergoes a strong compression (approximately 15%) and single crystals of phase I are violently shuttered into single crystal fragments of the phase II (without jumping), while in the reversible phase transition III to II the polar axis expands (approximately 14%) and the integrity of the single crystals is preserved – and no movement of crystals is observed.

Our measurements showed somewhat different behaviour – during the irreversible phase transition from I to II some of the crystals did indeed shutter into smaller fragments, but a large number remained intact and showed a typical jumping crystals behaviour – jumping all around over the large distances (several cm). This is typical of other thermosalient materials [1]. Also, during the reversible phase transition II <-> III (both ways) crystals exhibited jumping behaviour, alas somewhat weaker than during the phase transition I to II. This is in contrast to previously reported behaviour and the new model for jumping crystals phenomenon in this system has to be proposed.

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P03

Superparamagnetic Behaviour in the Two Polymorphic Modification of Lithium Stannoferrites LiFeSnO4

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The stannoferrite LiFeSnO4,fine particles has been successfully prepared by solid-state processing technique at pre-sintering temperature of 500 oC for 3 h and the pre-sintered powder was crushed and sintered finally in air at 1000 oC. The structural and microstructural evolutions of the nanophase have been studied using X-ray powder diffraction and the Rietveld method. The refinement results showed that the nanocrystalline ferrite has a two different crystal structure of orthorhombic and double hexagonal close packed LiFeSnO4. The particle size of as obtained samples were found to be ~70 nm through TEM that increases up to ~ 100 nm on calcinations at 1000 oC. (TEM) analysis confirmed the X-ray results. The particle size of the stannoferrite fine particles obtained from the XRD using Scherrer equation. Magnetic measurements obtained from lake shore’s vibrating sample magnetometer (VSM).

P04

Mechanical Strength of Consolidated Nanometer-sized Aluminum Single Crystals: Molecular Dynamics Study

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Nano-scale metal single crystals usually exhibit superior mechanical strength compared to their polycrystalline counterparts. Here we present an advanced large-scale molecular dynamics study on metallic aluminum in both the single crystal and polycrystalline forms. For the single crystals case we studied samples in the size range from 4.1 nm to 40.5 nm. We show that the ultimate mechanical strength deteriorates exponentially as the single crystal size increases. The small crystals superiority is explained by their ability to continuously form vacancies and to recover them. For the polycrystalline form, three aluminum samples with average grain sizes of 6.3 nm, 8.5 nm, and 10.7 nm were consolidated at a pressure of 1 GPa and temperatures ranging from 300 K to 900 K. The consolidated samples exhibit

average grain sizes up to 14.0 nm. The consolidated material developed an average grain size that grew exponentially with the consolidation temperature, with a growth rate dependent on the starting average grain size and the consolidation pressure. The evolution of the microstructure was accompanied by a significant reduction in the concentration of defects. It is found that the ultimate tensile strength increases with increasing the average grain size, reflecting an inverse Hall-Petch effect in the size-range studied. Furthermore, consolidating powder with larger average grain sizes makes the consolidation process less efficient from strength point of view. The deformation process is dislocations-driven up to a critical strain value that extends beyond the elastic region. Beyond this point the deformation process becomes dominated by grains-reorganization mechanism, and recovery of less-defective crystalline structure in grains' interior.

P05

Negative thermal expansion of ScF3: an EXAFS study at the Scandium K-edge from 10 K up to 1100 K

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Thermal expansion is a critical property of materials in many technological applications. The discovery of materials characterized by negative thermal expansion (NTE) in wide temperature intervals not only has opened new perspectives for realizing composites with specifically tailored expansion coefficients, but has also renewed the interest for a deeper understanding of the atomic-scale mechanism of NTE. A significant enhancement in the investigations on the local origin of NTE in crystals has been recently obtained by a careful use of EXAFS spectroscopy, as complementary to diffraction. Diffraction experiments measure the expansion of the distances between average atomic positions, as well as the absolute anisotropic thermal parameters of each atom. EXAFS instead directly measures the expansion of average inter-atomic distances between selected atomic pairs, as well as the Mean Square Relative Displacements (MSRD) parallel to the bond direction. By comparing the expansions measured by EXAFS and by diffraction, one can get the perpendicular MSRD, which measures the intensity of relative vibrations perpendicular to the bond, and can be connected to the tension effect.

In the present work, we present experimental EXAFS studies in a very large temperature range (from 10 K up to 1100 K) on ScF3, a trivalent metal fluoride belonging to the family of perovskite-type compounds with the general formula ABX3, in which A-cation site is vacant. Such crystal structure is often cited as ReO3 -type. At low temperatures ScF3 has been recently shown to have a strong negative thermal expansion (NTE) (60−110 K, αl ≈ −14 ppm K−1). On heating, its coefficient of thermal expansion (CTE) smoothly increases, leading to a room temperature CTE that is similar to that of ZrW2O8 and positive thermal expansion above ≈1100 K. The cubic ReO3 structure type is often used as a simple illustration of how negative thermal expansion can arise from the thermally induced rocking of rigid structural units (the so-called rigid unit mode (RUM)). ScF3 is the first material with this structure to provide a clear experimental illustration of this mechanism for NTE. We present a quantitative analysis of the thermal behavior of distances and MSRDs up to the 5th coordination shell of Scandium. The first shell Sc-F is composed of 6 F in octahedral configuration around Sc. EXAFS monitors a continuous expansion from r = 2.02771 Å at 10 K to r = 2.06178 Å at 1100 K. This result was confirmed by three different methods of analysis. For second (2nd and 3rd shells) and third (4th and 5th shells) peaks, EXAFS monitors a contraction, as in published diffraction data. These results are in good agreement with the Rigid Unit Model. The bending modes, in which fluorine (oxygen) vibrates perpendicular to Sc-F-Sc line, are responsible for the negative thermal expansion in the rigid unit model (RUM). Therefore, cubic ScF3 is an ideal candidate for accurate XAFS study of negative thermal expansion effect with sub-picometer accuracy. The peculiarity of ScF3 is that it is the only trifluoride having an undistorted cubic structure at room temperature and normal pressure, while other metal trifluorides adopt a rhombohedrally distorted (MF3, M=Al, Ga, In, Ti, V, Cr, Fe, Co, Ir, Rh, Ru) or Jahn-Teller distorted monoclinic (MnF3) structure.

P06

Time resolved and in situ XRD for structurally defected nanocrystalline LiF for thermoluminescence investigation

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Fluorites (e.g. LiF and CaF2) are highly sensitive phosphor used in several applications such as integrated optics, colour centre laser and as thermoluminescent material TL. The TL materials are very important in terms of applications (e.g. thermosensors [1] and for radiation dosimetry [2]). TL materials (e.g. fluorites) are characterized as insulators with wide band gap containing intermediate energy levels located between the valance and conduction bands and such energy levels are called trapped levels. Such trapped levels are introduced between valance and conduction bands either by adding some chemical impurities or by causing structural defects in the lattice.

There are many methods to create structural defects in materials and of course it depends on which kind of defects is intended to be created, however ball milling is a very powerful technique that can simply introduce structural defects in materials. As a matter of fact, Fluorites have face centred cubic unit cell and consequently many slip systems so plastic deformation by means dislocations is the most common and probable defect kind for ground fluorides due to the energetic impacts between powder, vial and balls.

X-ray diffraction XRD technique was used to investigate the microstructure details of the ground LiF in order to investigate the correlation between thermoluminance and the microstructure. High resolution diffractometer at MCX beamline in ELETTRA synchrotron was used to perform the XRD experiments at room temperature. On the other side, the furnace at MCX beamline was installed to collect temperature dependence In-situ XRD in order to follow the samples' kinetics in fast time resolution. Although are many methods that can be used to analyse the XRD patterns, Whole Powder Pattern Modeling WPPM [3, 4] approach was found the most appropriate to be chosen mainly because it is based on physical models for the size and the anisotropic strain due to the presence of dislocations.

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P07

Mixed Phase SnO_2 Nanorods Assembled with SnO_2 Nanocrystals for Enhancing Gas-Sensing Performance towards Isopropanol Gas

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The synthesis and the gas sensing properties of a novel mixed phase (i.e., tetragonal and orthorhombic phase) coexistence SnO_2 nanorods is presented. The mixed phases SnO_2 nanorods were obtained by calcinations of SnC_2O_4 synthesized with a chemical precipitation method using $SnCl_2{\cdot}2H_2O$ and PEG 400 as precursors. The resulting nanorods appear as polycrystalline composed of spherical mixed phases SnO_2 nanocrystals and have a high surface area. It was observed that the calcination temperature was the key parameter determining the content of the orthorhombic phase. The as-synthesized compounds were used as sensing materials of the sensors of indirect heating structure and tested for their ability to detect volatile organic compounds (VOCs), such as isopropanol, acetone, alcohol, and formaldehyde. Gas sensing tests showed that these mixed phases SnO_2 nanorods are highly promising for gas sensor applications, as the gas response for isopropanol was significantly enhanced by the presence of orthorhombic phase (S=61.5 to 1000 ppm isopropanol and response time and recovery time of 4 and 10 s). The as-prepared two phases SnO_2 nanorods with the highest content of the orthorhombic phase exhibit excellent gas response, selectivity, and stability toward isopropanol gas at the optimized operating temperature of 255 °C. The enhancement in sensitivity is attributed to the presence of small orthorhombic SnO_2 crystals with average radius shorter than the Debye screening length of 7 nm for SnO_2.

P08

Ion charge state production after K, L and M shell ionization in Pb atom

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A computer technique has been used to simulate the atomic reorganization vacancy cascades in single ionized and state ions of lead (Pbq+ where q=l, 2...70 ionization fold). The highly charged ions and average charge state distributions are carried out after inner-shell ionization. The computer program is made on base of tracing successive x-ray; Auger and Coster-Kronig transitions to filling the holes that exist in atomic subshells. For systematic investigations the problem occurs that for the most elements consistent sets of atomic data (radiative and non-radiative transitions) are not available. Therefore, we calculate radiative transitions probabilities (x- ray transitions) with program using Multiconfiguration Dirac Fock (MCDF) wave functions and non-radiative transitions probabilities with code using Dirac Fock Slater (DFS) wave functions. The shake-off processes and the closing of energetically Forbidden Coater-Kronig channels during the cascade development are considered. It is found that the heavier atom such that lead atom (Pb) and the lower shell or subshell in which an initial vacancy is produced, the higher will be the average ion charge and the more complex will be the charge spectrum.

P09

Broadening Microstructure Analysis Program (BMAP) : Isotropic and Anisotropic Crystallite Size and Strain Calculator

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BMAP calculator is a simplified tool (software) to obtain the microstructure characteristics and investigate the isotropic (uniform) and anisotropic nature characteristics using some common broadening methods. The Scherrer and Stokes-Wilson methods as well as Williamson-Hall plot (microstructure isotropy) and modified Williamson-Hall plot (microstrain anisotropy) are performed in the calculations. The BMAP input data are XRD peak parameters (the full width at half-maximum or integral breadth and peak position) of measured line profile and of those of reference ones for corrections. The linear least squares fit was using to calculate the size-strain values while the correlation coefficient to accept the results. The proposed BMAP program was applying for an XRD of prepared NiO nanoparticles by a sol-gel method for testing. The results of BMAP calculator and MAUD program were compared. The uniform stress model based on the Cauchy-Cauchy approximation, MWHSCC, was the most suitable one in cubic nanostructure Nickel Oxide with average crystallite size of 24 nm and anisotropic stains of $1.54 x 10^{-3}$, $0.61 x 1^{-3}$, $1.77 \ x 10^{-3}$ and $1.49 \ x 10^{-3}$ for (111), (200), (220) and (311) reflections, respectively.

P10

Structural Correlation of High-T_c Superconductors $Bi_2Sr_2Ca_2Cu_3O_{10+x}$

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$Bi_2Sr_2Ca_2Cu_3O_{10+x}$ considered as one of the highest superconducting transition temperature T_c = 110 K in the family of Cuperates. The aim of this work is to investigate the effect of sintering temperatures and in-situ annealing time on the phase quality and superconducting transition temperature T_c. The magnetic properties measured by Superconducting Quantum Interference Device (**SQUID**) have been correlated with the structure properties investigated by X-Ray Diffraction (**XRD**) using the Whole Powder Pattern Fitting method of Rietveld using **MAUD** program. The magnetization measurements shows a double-transitions temperatures at 110 and 85 K, which related to the coexistence of the two phases $Bi_2Sr_2Ca_2Cu_3O_{10+x}$ (Bi-2223) and $Bi_2Sr_2Ca_1Cu_2O_{8+x}$ (Bi-2212), respectively. The presence of the two phases that expected from magnetic characteristics was confirmed by X-ray analysis qualitatively (phase identification) and quantitatively (volume %). However, the quantitative analysis of the two phases was difficult due to the peak overlapping. For intensive structural investigation considering the formation of super-lattice, the 4D-space group has to be applied instead of the 3D-space group in the future work as mentioned by different authors.

P11

Spectroscopic Characterization of the Effect of Gamma Irradiation on the Biosynthesis of Silver Nano-Particles via Green Rout using Local Fungal Isolates from Egyptian Soil and their Antimicrobial Effect

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Development of reliable and eco-friendly process for synthesis of metallic nanoparticles is an important step in the field of application of nanoparticles. One approach that shows immense potential is based on the biosynthesis of nanoparticles using biological microorganisms such as bacteria and fungi. In this study, the production of silver nanoparticles (AgNPs) using local fungal isolates is investigated. after optimizing the preparation condition, gamma irradiation facility from Atomic Energy Authority has been used to improve the structure parameters of the formed nanoparticles. The SPR of silver nanoparticles were analyzed by UV-visible spectroscopy at wave lengths ranging from 200-1000 nm. Characterization of the active group by Fourier transformer infrared (FTIR) that is responsible for the reduction and capping of Ag nanoparticles was carried out and the shape and size were determined via the High Resolution Electron microscope and the Dynamic Light Scattering technique.

Keywords: Fungus, soil, biosynthesis, silver nanoparticles, gamma irradiation, UV/Vis, FTIR, and HRTEM

P12

Controlling Polymorphic Structures and Investigating Dielectric Properties of Ca-doped Zirconia Using Ceramic Solid State Method

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Structural study of $Zr_{1-x}Ca_xO_{2-x}$ samples with x = 0.01-0.15 were prepared using solid state ceramic method. X-ray diffraction analysis revealed that the high temperature zirconia phase can be stabilized by Ca-doping within the concentration range of x = 0.06 – 0.10. Rietveld refinement of the single phase data clearly revealed, that substitution of zirconium by calcium increases both the lattice parameters as well as the tetrahedral bond length. The dielectric constant shows strong temperature dependence at lower frequencies. The dielectric loss factor increases rapidly with the increase in temperature at lower frequencies, and decreases with an increase in frequency at higher temperatures. Thus, the ionic conduction is considered as the dominant process at higher temperatures.

P13

Supramolecular Building Blocks in Construction of Zeolite-Like Metal-Organic Frameworks (ZMOFs): The Metal-Organic Cubes (MOCs)

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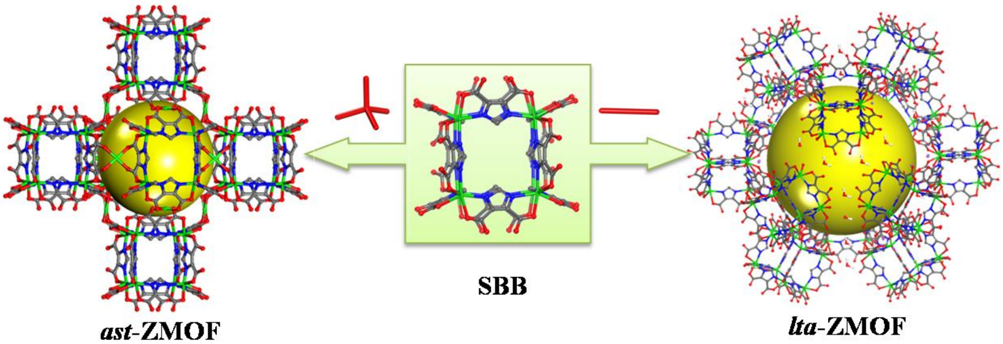
Two zeolite-like metal-organic frameworks (ZMOFs) having the LTA (**1**) and faceted AST (**2**) topologies were synthesized. Based on the finite metal-organic cube (MOC)[1] as supermolecular building block (SBB), such ZMOFs were rationally designed and further targeted in supramolecular assembly processes.

Directed assembly of finite supramolecular polyhedra constructed through assembly of molecular building blocks (MMBs) is an interesting approach toward rational design and synthesis of nanostructures.[2a-e] The ability to control coordination number, and thus geometry, around metal ions through metal-ligand directed assembly afforded the synthesis of pre-designed finite and rigid supramolecular structures with various peripheral functionalities, which could be further employed in super-supramolecular assembly of extended frameworks.[3a-g] Controlling the manner in which such supermolecular building blocks could assemble into extended frameworks is an ongoing challenge. Herein, we report the synthesis and assembly of molecular metal-organic cubes (MOCs) into zeolite-like frameworks having LTA and AST topologies.

A particular set of zeolites share a common building unit composed of eight tetrahedra bridged through oxide ions in a cube-like arrangement. Such building units are commonly known as double four-member rings, d4r. Review of the zeolite database reveals that d4r (cube-like) can assemble into numerous zeolitic frameworks, of which, ACO, AST, ASV and LTA are important to crystal chemistry (Figure 1).[4] The resulting zeolite structure depends on the type of apex-to-apex bridging of the d4r. In the simplest case, linear linkers produce ACO and LTA zeolites while tetrahedral linkers result in AST and ASV zeolites (Scheme 1).



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