proceedings

The 37th International Symposium on Dynamical Properties of Solids

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DyProSo 2019

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Organizers

Università degli Studi di Ferrara

INFN

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AIMagn Associazione Italiana di Magnetismo

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Welcome Message

Dear Participant,

We are pleased to welcome you to the 37th International Symposium on Dynamical Properties of Solids, DyProSo 2019. DyProSo is an international biannual research meeting, first held in Albé (France) in 1967, focused on the functional properties of condensed matter, resulting from elementary excitations, light-matter interactions, molecular motions, transport processes, and other dynamic phenomena occurring in many-body systems. Experimental evidence and investigations, as well as theoretical models and predictions, are particularly pursued, as well as interdisciplinary issues.

This year the event is being held in Ferrara, from 8th to 12th September 2019, and is organized by the Department of Physics and Earth Sciences of the University of Ferrara, a prestigious University dating back to 1391, and by the National Institute of Nuclear Physics (INFN), together with the patronages of the European Magnetism Association (EMa), and the Italian Society of Magnetism (AIMagn). Ferrara is itself a historical city in northern-east Italy; it was founded as a Bizantine castrum in the VI century and underwent a time of splendor and international attractiveness during the dukedom ruled by the Estense family in the XV-XVI centuries. It is dominated by a magnificent castle in the city center and surrounded by a 13 km long track on the walls all around the ancient town, still walkable, which were addressed by poet Lord Byron:

"*…while stranger wonder o'er thy unpeopled wall…*".

We thank Professor Dr. Markus Münzenberg from the University of Greifswald (Germany) for accepting to introduce the Symposium with a Lecture entitled "*Breaking the attosecond limit - From spin metamaterials to novel THz applications*" at the Opening Ceremony set in the impressive Embarcadero Room of the Ancient Castle. Then the Symposium works will continue at the *Aula Magna* of *Palazzo Bevilacqua-Costabili*, another celebrated palace in the city center, dating back to 1430, which currently hosts the Economy and Mangement Department, along the historical Avenue *Via Voltapaletto*. Besides these monuments, a dedicated tour of the city center will be offered to our participants to enjoy the other beauties and the unique history of Ferrara, and then the Social Dinner will complete the visit with the impressive scenario of the *Palazzo Borsa*.

On the scientific level, we are proud to propose to our participants a guided visit to the Legnaro Accelerator at the National Laboratory of Legnaro, one of the four national laboratories of INFN, and a milestone for the experimental physics, as well as for the applied and technological research.

As established DyProSo tradition, to enable promising young researchers to gain experience in speaking in front of an international public, we have set short scientific communications. Indeed, a special purpose of the Symposium is to foster a scientific dialog between young and experienced researchers. In addition, the Symposium Organization will confer awards for the Best Student Presentation, the Best Poster Presentation, and the Best Original Idea among all the scientific contributions.

We thank all the invited speakers for accepting our invitation and all the participants, coming from several countries, for their interest in the event. We wish you all fruitful and stimulating discussions, and a nice stay in Ferrara.

The DyProSo 2019 Chairmen
Federico Montoncello
Vincenzo Guidi

Previous Conferences

- 1967 Albe, France
- 1968 Oberwolfach, Germany
- 1969 Mont Saint-Odile Nancy, France
- 1970 Oberwolfach, Germany
- 1971 Edinburgh, UK
- 1972 Montpellier (Mont Aigoual), France
- 1973 Leoni (Starnberger See), Germany
- 1974 Giswil, Switzerland
- 1975 Pelvous, France
- 1976 Pelvous, France
- 1977 Phonon Conference in Paris, France
- 1978 Stresa, Italy
- 1979 Ferroelectricity Conference in Edinburgh, UK
- 1980 Le Houches, France
- 1981 Überlingen, Germany
- 1982 San Miniato, Italy
- 1983 Leuven, Belgium
- 1984 Mürren, Switzerland
- 1985 Phonon Conference in Budapest, Hungary
- 1986 Überlingen, Germany
- 1987 Ventron, France
- 1988 Sestri, Cinque Terre, Italy
- 1989 Phonon Conference in Heidelberg, Germany
- 1990 Chexbres, Switzerland
- 1991 Autrans, France
- 1992 Schellerau (Dresden), Germany
- 1993 Lunteren, The Netherlands
- 1994 Il Ciocco, Italy
- 1995 Haro (Bilbao), Spain
- 1996 (Crete, Greece—cancelled)
- 1997 Davos, Switzerland
- 1999 Tours, France
- 2001 Kerkrade, The Netherlands
- 2003 Trieste, Italy
- 2005 Ceský Krumlov, Czech Republic
- 2007 Porto, Portugal
- 2009 Antwerp, Belgium
- 2011 Aussois, France
- 2013 Vienna, Austria
- 2015 Freising, Germany
- 2017 Cracow, Poland

General Information

CONFERENCE LANGUAGE
The official conference language is English.

BADGES & VOUCHERS
Badges must always be visibly worn during the scientific sessions, the coffee and lunch breaks as well as the poster session at the conference site.
Please make sure to bring the voucher for the congress dinner and deliver it at the conference staff.
The voucher is valid for one person only and is not transferable.
Attendees who declared restrictions for food (such as vegetarian menu or others) will find a special voucher in their badge to exhibit at their place during the social dinner, in order to support the catering staff.

COFFEE AND LUNCH BREAKS
The conference fee includes admission to the scientific programme, poster sessions and exhibitions, the congress documentation, refreshments and snacks during the coffee and lunch breaks, the participation to the social dinner.

INTERNET AND WLAN
A WLAN code will be provided on site to each attendee and it will be valid during the whole conference. Moreover, the conference area is covered by Eduroam service.

CERTIFICATE OF ATTENDANCE
The certificate of attendance will be provided during registration.

PERSONS WITH SPECIAL NEEDS
Should you require any specific assistance, please let us know how to assist in making your stay at the conference pleasant and comfortable.

EMERGENCY NUMBER:
Emergency telephone number: 112

Conference Chairs

Federico Montoncello, University of Ferrara, Italy
Vincenzo Guidi, University of Ferrara, Italy

Program Committee

Federico Montoncello, University of Ferrara, Ferrara (Italy)
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Ehsan Noroozinejad, University of Advanced Technology, Kerman (Iran)
Winfried Petry, Technische Universität München (Germany)
Kulda Jiri, Institut Laue-Langevin, Grenoble (France)

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Giacomo Gadda, INFN, Ferrara (Italy)
Matteo Valt, University of Ferrara, Ferrara (Italy)
Melissa Tamisari, University of Ferrara, Ferrara (Italy)

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Renato Torre, LENS, Florence, Italy
Piotr Zieliński, Institute of Nuclear Physics PAN, Cracow University of Technology, Poland

Opening Ceremony

The **Opening Ceremony** of the 37th DyProSo Symposium will be held in the **Castle of Ferrara** on 8 September starting from 5 p.m. with the Plenary Talk and closing with a welcome aperitive.

The Registration desk will be placed in **Imbarcadero 1**, whereas, the Opening Conference will be held in **Imbarcadero 2**.

The Welcome aperitive will be held in the Castel's arcade.

The 37th of DyProSo will be opened by the plenary speaker **Prof. Dr. Markus Münzenberg**, University of Greifswald Germany, with a talk entitled

"**Breaking the attosecond limit—From spin metamaterials to novel THz applications**"

Biography

Markus Münzenberg leads a research group at the University of Greifswald and is Professor of Interface and Surface Physics. He completed his PhD thesis in the field of X-Ray Dichroism with experiments at the European Synchrotron Facilities in 2000. After a postdoc at the Massachusetts Institute of Technology (MIT) Cambridge, USA, in the field of spin transport under Jagadeesh S. Moodera, he has established a group in the field of femtosecond dynamics, magnonics and spintronics as a junior professor from 2002 to 2008 at the Georg-August University Göttingen, where was then employed as extraordinary professor until 2013. Since 2014 he is Professor at the University of Greifswald. In the last years he has opened new research fields in ultrafast magnetism, THz spintronics and novel THz emitters, and contributed to the emerging fields of magnonics and spin caloritronics. Recently he joined work on topological spin-textures (skyrmions) and bio-nanomechanics 3D laserlithography for medical applications.

He is a member of the German Physical Society (DPG) and the AG Magnetism of the Association Magnetism, American Physical Society (APS), Institute for Electrical Engineering and Electronics (IEEE) and the Technical Committee of the Intermag (IEEE). He is also active as a member of the board for application review of the Helmholtz Center Berlin (BESSY) and member of the editorial board of the journal Scientific Reports. He is liaison officer for the University for the German Science foundation (DFG) for the University of Greifswald.

Web: https://physik.uni-greifswald.de/ag-muenzenberg/

About—Venue

The 37th of DyProSo will be held in Ferrara, a historical city in northern-east Italy, founded as a Bizantine castrum in the VI century and undergoing a time of splendor and international attractiveness during the dukedom ruled by the Estense family in the XV–XVI centuries.

Ferrara, with a population of 130,000, is a cyclist and pedestrian-friendly city with a high quality of life. It is also a lively cultural centre.

The Estense Duchy acted as a patron to some of the most important scholars and artists of that time.

In 1995, UNESCO granted the city World Heritage status as an example of a city planned in the Renaissance still keeping its historical centre intact, surrounded by more than 9 km of ancient walls.

Reminiscences of the Middle Ages and the Renaissance live on in palaces, churches and museums.

Yearly events include:

- The Palio: celebrations, parades, flag-throwing competitions and a spectacular horse race in the city center;
- Buskers Festival: the world biggest event dedicated to street performance;
- 'Internazionale' Festival: lectures and meetings regarding international politics and economy involving journalists and authors from all over the world;
- 1000 Miglia: a vintage car race throughout Italy

The University of Ferrara, founded in 1391, is one of the oldest universities in Italy. Prominent figures such as Copernicus and Paracelsus studied here.

Today, its twelve Departments offer some fifty-degree programmes, ranging from Architecture to Design, from Medicine to Engineering, from Physics to Biotechnologies and Literature.

The quality of education and research, and the facilities available to students and guests, make Ferrara a top-ranking University in Italy.

The whole city is a dynamic campus, fostering interaction among national and international students.

Source: https://commons.wikimedia.org

The conference will be organized by the University of Ferrara and the National Institute of Nuclear Physics (INFN, Ferrara), over all days—from 8 to 12 September 2019.

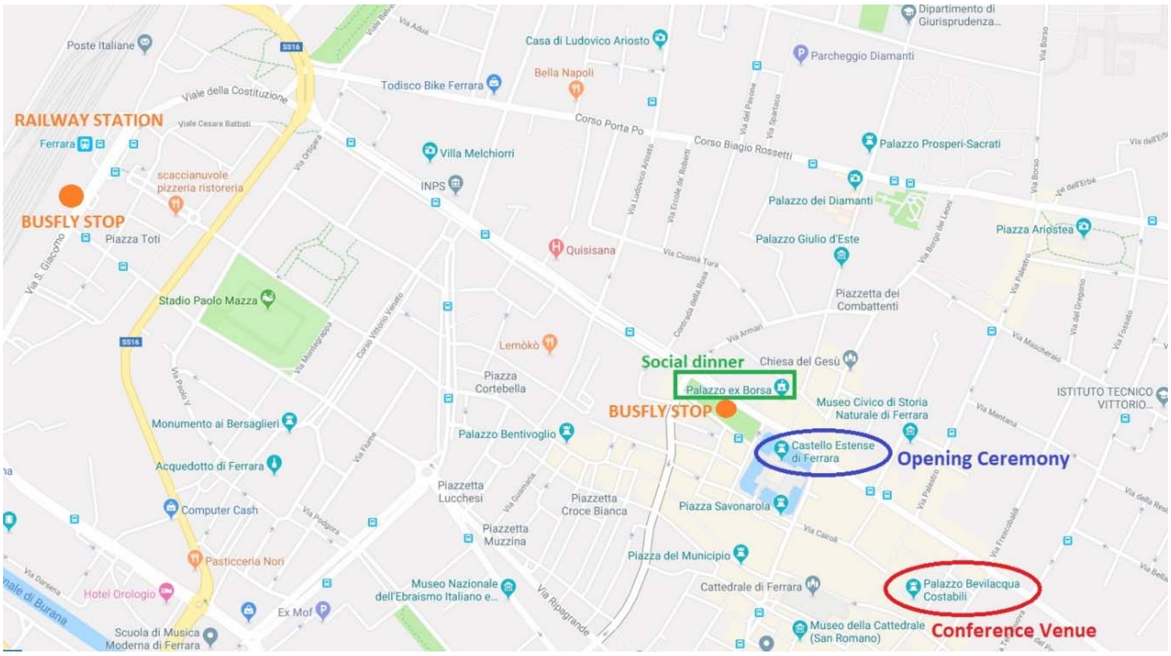
http://www.unife.it

Department of Physics and Earth Sciences:
http://fst.unife.it/en?set_language=en

Institute of Nuclear Physics in Ferrara:
http://www.fe.infn.it/

All **oral contributions** will be held in the "**Aula Magna" of Palazzo Bevilacqua-Costabili** (Economy and Mangement Department), along the historical Avenue Via Voltapaletto n. 11—44121, Ferrara.

Posters, lunches and coffee breaks will be held in the **"Atrium" Palazzo Bevilacqua-Costabili** (Economy and Mangement Department), along the historical Avenue Via Voltapaletto n. 11—44121, Ferrara.


RAILWAY STATION
BUSFLY STOP
Social dinner
Palazzo ex Borsa
BUSFLY STOP
Castello Estense di Ferrara
Opening Ceremony
Palazzo Bevilacqua Costabili
Conference Venue

About—Social Events

- **GUIDED TOUR OF THE LEGNARO ACCELERATOR—September 10th**

  12:00—Departure by bus from Corso della Giovecca 114 (bus stop close to Carabinieri station)

  13:00—Arrival at Legnaro National Laboratory (LNL)

  13:15—14:30 Lunch at LNL canteen

  14:30—17:30 Guided Tour of LNL

  17:45—Departure to Ferrara

  For information about the linear accelerator in Legnaro, please, visit the following links:

  http://www.lnl.infn.it/index.php/en/accelerators-3/accintro
  http://www.lnl.infn.it/index.php/en/visiting-lnl

- **GUIDED WALK TOUR OF THE FERRARA CITY CENTRE—September 11th at 17:00**

  DyProSo2019 offers a guided tour in English language, two hour long, around the Ferrara city centre.

  The tour will start at 17:00 from Palazzo Bevilacqua-Costabili (Economy and Mangement Department), along the historical Avenue Via Voltapaletto n. 11—44121, Ferrara.

- **SOCIAL DINNER—11th September at 19:30**

  The DyProSo 2019 Social dinner will be held in **"Palazzo ex Borsa"**, Corso Ercole I d'Este, 44121 Ferrara FE.

Guidelines for Authors

Oral Presentation Guidelines:

Please, note that speakers will have to bring their presentation on USB flash drives. Own laptops can be used only in exceptional cases. Speakers must show up in the room of their session during the break latest 20 minutes before the start of their session to upload their files and check compatibility. Assistants are in the session room for technical support if required. Speakers are advised to embed all fonts in their PowerPoint file and to bring a backup PDF-version of their presentation.

Duration of presentation (questions/answers included) :

- KEYNOTE, 30 minutes
- INVITED TALK, 20 minutes
- REGULAR TALK, 20 minutes
- STUDENT COMMUNICATION, 10 minutes

Poster Presentation Guidelines:

The Author can attach posters starting from 8:00 a.m. on 9th September. The posters must remain attached during the entire conference. The poster format is A0 (84.1 cm × 118.9 cm), portrait orientation (height > width); suitable tape will be provided for attaching the posters.
The assigned placement of each poster is marked on the panel with the ID poster number corresponding to the abstract ID number assigned during the submission process.
Posters will be held in the "Atrium" Palazzo Bevilacqua-Costabili (Economy and Mangement Department), along the historical Avenue Via Voltapaletto n. 11—44121, Ferrara.

Awards

The Symposium Organization will award the **Best Student Presentation**, the **Best Poster Presentation**, and the **Best Original Idea** among all the scientific contributions.

The Awards Ceremony will be held during the Symposium Closing.

Contact: dyproso2019@fe.infn.it

Scientific Programme

The scientific programme provides:

- **5 keynote talks** (each with 25 min and 5 min discussion):

  Gianluca Gubbiotti, Istituto Officina dei Materiali del Consiglio Nazionale delle Ricerche, Perugia, Italy—*Exploring the Third Dimension in Magnonic Crystals*
  Sandro Szabó, Heinz Maier-Leibnitz Center (MLZ) and Physics Department, Technical University of Munich, Germany—*The Short-Range Order in Zr-Ti Melts*
  Lukas M. Eng, Institute of Applied Physics, School of Science, TU Dresden, Germany—*Near-Field THz Nanoscopy with Novel Accelerator-Based Photon Sources*
  Ion Errea, University of the Basque Country, Spain—*Structural Phase Transitions from First-Principles Calculations*
  Elisabetta Comini, SENSOR Laboratory, University of Brescia, Italy—*Metal Oxide Heterostructures and Hybrid Nano Composite for Chemical Sensors*

- 12 **invited talks** (each with 18 min and 2 min discussion)

  Monica Jimenez-Ruiz, Institut Laue-Langevin, Grenoble (France)
  Michael Leitner, Technical University Munich (Germany)
  Stefano Bonetti, Ca' Foscari University, Venice (Italy)
  Mario Santoro, LENS, Firenze (Italy)
  Paolo Vavassori, CIC nanoGUNE Basque Country (Spain)
  Andrea Piovano, Institut Laue-Langevin, Grenoble (France)
  Andrei V. Korol, MBN Research Center at FiZ—Frankfurt am Main (Germany)
  Boris Gorshunov, Moscow Institute of Physics and Technology (Russia) **Laura Chaix**, Institut NEEL—CNRS, Grenoble, (France)
  Nicolò Maccaferri, University of Luxembourg, Luxembourg (Luxembourg)
  Silvia Corezzi, University of Perugia, Perugia (Italy)
  Sultan B. Dabagov, INFN Laboratori Nazionali di Frascati, Frascati (Italy)

- 37 **regular oral** contributions (each with 18 min and 2 min discussion)
- 10 **oral student communications** (each with 8 min and 2 min discussion)
- 10 **poster** presentations.

XXXVII International Symposium on Dynamical Properties of Solids

Registration (16:00-17:00)

Opening Cerimony (17:00-18:30)

17:00	Welcome and Introduction by the conference chair Dr. Federico Montoncello and Prof. Vincenzo Guidi	
17:30	Breaking the attosecond limit - From spin metamaterials to novel THz applications	MÜNZENBERG, Markus

Welcome Buffet (18:30-20:00)

Registration (08:00-08:30)

Morning Session 1 - Chair: Paolo Vavassori (CIC nanoGUNE, Donostia, Basque Country (Spain)) (08:30-10:40)

Keynote talk (08:30-09:00)

08:30	Exploring the third dimension in Magnonic Crystals	GUBBIOTTI, Gianluca

09:00	Direct detection of multiple backward volume modes in yttrium iron garnet at micron scale wavelengths	KETTERSON, John B.
09:20	Dimensionality effects and phase transition dynamics in spintronics materials as seen by X-ray electron spectroscopies	PANACCIONE, Giancarlo
09:40	Spin wave modes in a cylindrical nanowire in crossover dipolar-exchange regime	KLOS, Jaroslaw
10:00	Edge modes in the switching mechanism of finite chains of macrospins	KUŹMA, Dominika
10:20	Domain structure and magnetization reversal mechanism in Co/Pd nanopatterned multilayer	SOBIESZCZYK, Paweł

Coffee Break (10:40-11:10)

Morning Session 2 - Chair: Gianluca Gubbiotti (CNR-IOM - Istituto Officina dei Materiali, Perugia (Italy)) (11:10-12:30)

Invited Talk (11:10-11:30)

11:10	Magneto-plasmonic nanostructures and crystals	VAVASSORI, Paolo

11:30	Measuring interfacial Dzyaloshinskii-Moriya interaction: a review	KUEPFERLING, Michaela
11:50	Reciprocal relation between spin Peltier and spin Seebeck effects	SOLA, Alessandro

Invited Talk (12:10-12:30)

12:10	Time-resolved investigations and biotechnological applications of plasmonic nanostructures	MACCAFERRI, Nicolò

Lunch (12:30-13:45)

Afternoon Session 1 - Chair: Jiri Kulda (Institut Laue-Langevin, Grenoble (France)) (13:45-14:45)

Invited Talk (13:45-14:05)

13:45	Terahertz-Driven Phonon Upconversion in $SrTiO_3$ *	BONETTI, Stefano

14:05	Energy Scale of the Charge Density Wave in Cuprate Superconductors	SACUTO, Alain
14:25	Spin-lattice coupling in the quantum spin ice candidate $Tb_2Ti_2O_7$ revealed by THz spectroscopy	DE BRION, Sophie

Afternoon Session 2 - Chair: Jiri Kulda (Institut Laue-Langevin, Grenoble (France)) (14:45-16:05)

Invited Talk (14:45-15:05)

14:45	Resonant Inelastic X-ray Scattering Study of Excitations in Cuprate Superconductors	CHAIX, Laura

15:05	Spin dynamics and phonons, insights into potential molecular qubits	BENCI, Stefano
15:25	Investigation of phonons and magnons in $[Ni_{80}Fe_{20}/Au/Co/Au]_{10}$ multilayers *	ZDUNEK, Miłosz
15:35	Ab-initio study of the electron-phonon interaction of a single Fe adatom on the MgO/Ag(100) surface	GARAI-MARIN, Haritz
15:45	Proton momentum distributions in strong hydrogen bonds in the solid state	KRZYSTYNIAK, Matthew

Coffee Break (16:05-16:35)

Poster Session - Chair: Giacomo Gadda (INFN), Italy (16:35-17:30)

Morning Session 1 - Chair: Piotr Zieliński (Institute of Nuclear Physics Polish Academy of Sciences, Cracow (Poland)) (08:30-10:40)

Keynote talk (08:30-09:00)

08:30	The short-range order in Zr-Ti melts *	SZABÓ, Sandro

Invited Talk (09:00-09:20)

09:00	Inelastic Neutron Scattering study of Brønsted acidity and water confinement in zeolites	JIMENEZ-RUIZ, Monica

09:20	Advanced Diffusion Strategies for Junction Formation in Germanium	DE SALVADOR, Davide
09:40	The causality-composition law in the non-Debye relaxations models	GORSKA, Katarzyna
10:00	On some enigmatic properties of relaxation functions	HORZELA, Andrzej

Invited Talk (10:20-10:40)

10:20	The influence of non-stoichiometry on the order and dynamics of oxides studied by inelastic neutron scattering	PIOVANO, Andrea

Coffee Break (10:40-11:10)

Morning Session 2 - Chair: Winfried Petry (Technische Universität Muenchen (Germany)) (11:10-12:00)

Keynote talk (11:10-11:40)

11:10	Near-field THz nanoscopy with novel accelerator-based photon sources	ENG, Lukas M.

11:40	A new beamline for advanced photoelectron spectroscopy with narrowband extreme ultraviolet high harmonics at variable high repetition rate	CUCINI, Riccardo

Tour to Legnaro (INFN Laboratory) (12:00-13:15)

Lunch in Legnaro (13:15-14:30)

Legnaro INFN Laboratory visit: Legnaro INFN Laboratory visit (14:30-17:30)

Morning Session 1 - Chair: Andrzej Horzela (Institute of Nuclear Physics, Polish Academy of Sciences, Cracow (Poland)) (08:30-10:40)

Keynote talk (08:30-09:00)

08:30	Structural phase transitions from first-principles calculations *	ERREA, Ion

09:00	Vibrational properties of closo – borane anions in superionic conductors	ŁODZIANA, Zbigniew
09:20	Adsorption of oxygen species on the SnO_2 (110) defective surface: a OFT investigation *	KRIK, Soufiane
09:40	Non-Debye vs. Debye Dielectric Relaxation: How does memory effect arise?	LATTANZI, Ambra
09:50	Efficient calculation of anisotropic Fermi surface problems through Helmholtz Fermi Surface Harmonics (HFSH)	LAFUENTE-BARTOLOME, Jon
10:00	Ensamble sampling for lattice dynamics	JOCHYM, Paweł

Invited Talk (10:20-10:40)

10:20	Polycrystalline time-of-flight inelastic neutron scattering beyond the density of states	LEITNER, Michael

Coffee Break (10:40-11:10)

Morning Session 2 - Chair: Renato Torre (European Lab. for Non-Linear Spectroscopy (LENS) and University of Firenze, Firenze (Italy)) (11:10-12:30)

Invited Talk (11:10-11:30)

11:10	Rubidium at Extreme Conditions	SANTORO, Mario

11:30	Impact of high-pressure evolution of elementary distortions on the phase-transition of $RFeO_3$ *	VILARINHO, Rui
11:50	Investigation of high pressure phase transition by means of infrared spectroscopy in the Cairo frustrated pentagonal magnet $Bi_2Fe_4O_9$	VERSEILS, Marine
12:10	Advances on the modelling of blood flows and pressures in humans through a new multiscale mathematical model	GADDA, Giacomo

Lunch (12:30-13:45)

Afternoon Session 1 - Chair: Alain Sacuto (Université Paris Diderot, Paris, (France)) (13:45-15:25)

13:45	Sub-THz Raman response and critical dynamics in $BaTiO_3$	FONTANA, Marc
14:05	Narrow Optical Gap Ferroelectric Bi_2ZnTiO_6 Thin Films Deposited by RF Sputtering *	FIGUEIRAS, Fábio
14:25	Electron localizations in alloy exhibiting nanotwinning	ZELENÝ, Martin
14:45	Molecular dynamics simulations of ferroelectric perovskites ($BaTiO_3$, $BiFeO_3$) based on the effective Hamiltonian approach *	KLÍČ, Antonín
15:05	Tetragonal Ferroelectric Phase of $GdMnO_3$ Epitaxial Thin Film Grown onto $SrTiO_3$ (001) *	MACHADO, Pedro
15:15	Unravelling the Magnetoelectric Coupling Mechanisms in $TbMnO_3$ through Fe^{3+} substitution *	MAIA, André

Coffee Break (15:25-15:55)

Afternoon Session 2 - Chair: Iñigo Etxebarria (Universidad del País Vasco UPV/EHU, Bilbao (Spain)) (15:55-17:00)

15:55	Piezoelectric response of $K_{0.5}Na_{0.5}NbO_3$ designed by sintering engineering *	GOMES, Mariana
16:05	Archetypal Soft-Mode Driven Antipolar Phase Transition in Francisite $Cu_3Bi(SeO_3)_2O_2Cl$ *	MILESI-BRAULT, Cosme
16:15	Lattice dynamics and Raman spectrum of $BaZrO_3$ single crystals *	TOULOUSE, Constance
16:35	2D transition metal carbides as flexible anode materials *	LEGUT, Dominik

Visit to the city (17:00-19:00)

Social Dinner (19:30-22:30)

Morning Session 1 - Chair: Cesare Malagù (University of Ferrara (Italy)) **(08:30-09:50)**

Keynote talk **(08:30-09:00)**

08:30	Metal oxide heterostructures and hybrid nano composite for chemical sensors *	COMINI, Elisabetta

09:00	Bi_2O_3 and ZnO nanowires growth using Vapor–Liquid–Solid (VLS) process for chemical sensors applications *	MOUMEN, Abderrahim
09:10	Low-dimensional composite material based on modified graphene and metal oxide for high-performance chemical sensors	GALSTYAN, Vardan
09:30	Colloidal quantum dots for low-power-consumption semiconductor gas sensors	LIU, Huan

Morning Session 2 - Chair: Vincenzo Guidi (University of Ferrara (Italy)) **(09:50-10:30)**

Invited Talk **(09:50-10:10)**

09:50	Multiscale modelling of complex dynamical processes in solids with MBN Explorer and MBN Studio	KOROL, A. V.

10:10	Channeling experiments at the Mainz Microtron MAMI	LAUTH, Werner

CoffeeBreak **(10:30-11:00)**

Invited Talk **(11:00-11:20)**

11:00	Advanced Channeling Technologies: Strong External Electromagnetic Fields to Guide Charged & Neutral Beams	DABAGOV, Sultan B.

Morning Session 2 **(11:20-12:40)**

11:20	Incoherent scattering reduction in crystals	TIKHOMIROV, Victor
11:40	Potential of parametric X-rays for application in particle identification detectors	LOBKO, Alexander
12:00	Progress towards an experiment for electromagnetic dipole moments of unstable particles at the LHC *	NERI, Nicola
12:20	Novel type of compact e.m. calorimeter based on oriented crystals for high-energy physics and astrophysics *	BANDIERA, Laura

Lunch (12:40-14:00)

Afternoon Session 1 - Renato Cucini (CNR-IOM - Istituto Officina dei Materiali, Trieste (Italy)) (14:00-15:20)

Invited Talk (14:00-14:20)

14:00	Using patchy particles to shed new light on the autocatalytic aggregation of soft matter	COREZZI , Silvia

14:20	Nucleation in Aqueous KCl Solutions Induced by Laser Pulses	TORRE, Renato
14:40	Dynamical properties of ice and water: a broadband dielectric spectroscopy study	ARTEMOV, Vasily

Invited Talk (15:00-15:20)

15:00	Hertz-to-terahertz dielectric response of nanoconfined water molecules	GORSHUNOV, B.

Afternoon Session 2 - Renato Cucini (CNR-IOM - Istituto Officina dei Materiali, Trieste (Italy)) (15:20-15:50)

15:20	Tuning the fast dynamics of PNIPAM-based systems with bio-cosolvents	ROSI, Benedetta Petra
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Abstract

Exploring the Third Dimension in Magnonic Crystals †

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Magnonic crystals (MCs) are materials with periodically modulated magnetic properties where the spin waves (SWs) band structure consists of intervals of allowed SW frequencies and forbidden gaps in which there are no allowed magnonic states.

In the recent past, most of the studies have been focused on planar nanostructures where the magnetic constituents have the same thickness, while, to the best of our knowledge, there are no reports of SW band structure in 3D MCs. This is mainly due to the difficulties associated with the fabrication of thickness modulated nano-elements by conventional nanofabrication techniques which require multilevel exposure process and alignment between successive fabrications steps.

Very recently, we proposed a new class of MCs constituted by closely packed thickness-modulated Permalloy, Fe/Permalloy and Fe/Cu/Permalloy nanowires. We show that this kind of structures support the propagation of collective SWs in the periodicity direction, thus demonstrating that layering structure and in-plane modulation are very effective for controlling the characteristics of the magnonic band [1].

Another possible approach to achieve a vertical control of the spin wave band structure is to have either an array of layered magnetic elements or an array of ferromagnetic dots deposited on top of a continuous ferromagnetic film. I will review the properties of the spin wave band structure, studied by wavevector-resolved Brillouin light scattering, in dense arrays of Py/Cu/Py nanowires [2,3] and 2D array of elliptical Py/Pt nanodots arranged into dense chains over the surface of a 20 nm thick Py continuous unpatterned film [4]. Particular emphasis is given to the reconfigurable dynamic response of these systems.

Finally, I will present some recent results on three-dimensional model of periodic meander-shaped ferromagnetic films and vertically coupled structures.

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Abstract

Near-Field THz Nanoscopy with Novel Accelerator-Based Photon Sources †

Lukas M. Eng [1,2,*], Frederik Kuschewski [1], Jonathan Döring [1], Lukas Wehmeier [1], Tobias Nörenberg [1], Thales de Oliveira [1], Hans-Georg von Ribbeck [1], Denny Lang [3], Bert Green [3], Sergey Kovalev [3], Nilesh Awari [3], Stephan Winnerl [3], Manfred Helm [3], Michael Gensch [3] and Susanne C. Kehr [1,2]

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This talk advertises scattering-type scanning near-field infrared/THz nanospectroscopy (s-SNIM) in the spectral range of 75 to 1.2 THz [1,2], as provided by the free-electron laser FELBE at the Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany. By combining s-SNIM with FELBE, we demonstrate a λ-independent optical resolution of ~10 nm only, by exploring structured Au samples, Graphene-nanotransistors, meta-materials [3,4], and local-scale ferroic phase-transitions [5–7] down to LHe temperatures [8]. Moreover, also the non-linear optical responses at IR wavelengths can be explored, as recently demonstrated when inspecting highly-doped GaAs/InGaAs core/shell nanowires [9]. Our THz-s-SNIM was also integrated into a THz pump-probe setup for the local analysis of excited states in structured SiGe samples. We developed a sophisticated demodulation technique that extracts pump-induced signals with a superior signal-to-noise ratio [10]. In addition, HZDR recently extended the available wavelength ranges down to the 100 GHz radiation, employing the novel super-radiant TELBE light source [11,12]. We adapted our s-SNIM to that novel TELBE photon source as well, achieving an equally high spatial resolution as with FELBE. This now allows to bridge the famous THz-gap in order to explore novel quantum phenomena of magnons, spin waves, and phonon polaritons in a various 2D and 3D materials.

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Invited Talks

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Abstract

Inelastic Neutron Scattering Study of Brønsted Acidity and Water Confinement in Zeolites †

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Zeolites, crystalline and microporous aluminosilicates, are one of the most important groups of functional materials. Zeolites are widely used as solid acid catalysts in petroleum refinery and petrochemical industries. Zeolites can be described as microcoporous polymorphs of quartz. Whilst quartz is SiO2, zeolites asmit the isomorphous substitution of Si by many tetrahedrally coordinated atom, typically Al (Si4+ à Al3+ + H+). In this way, the Si/Al ratio gives the number of acid sites, but not their location and strength.The catalytic properties of a zeolite depend strongly on its acidity, and this in turns depends on: the total number of acid sites, their individual strength, and their individual location. These three factors are strongly correlated. Geometric parameters that are defined by the location of the acid site (i.e., bond angles and lengths around the acid site) make a remarkable contribution to the acid strength. It was found that the strong acid sites have the trend to be found in relatively small micropores [1].

In the present work we study the zeolite LTA Si/Al = 40 (only one acid site per unit cell). The structure of LTA zeolite has the micropores consisting of large and small cavities. Inelastic neutron scattering (INS) has been used to study the acid sites of the LTA zeolite with different Si/Al ratios. There are two groups of bands: the first one found at 1050–1100 cm^{-1} that corresponds to the SiOH in-plane bending and another one found near 400–500 cm^{-1} which is attributed to the out-of-plane bending. These bending modes of the acid site are not no possible to measure with IR spectroscopy since these bands overlap with the strong bands from the zeolite framework. The combination of an extremely high quality of the samples and the sensitivity of the instrument allows to detect with high precision the acid sites of LTA Si/Al = 40 and obtain information about its position. In order to fully understand the INS spectra we performed *ab-initio* calculations [2,3].

In addition the polar properties of zeolites can be nicely tuned by selecting the appropriate chemical composition and concentration of structural defects in their frameworks. In the present study we were particularly interested about the mechanism of water adsorption on small pore zeolites and the influence of the polarity of the zeolite cavities in the clustering of water molecules when adsorbed in confined spaces, since there is controversy on the formation of hydroxonium cations when water is adsorbed on acid zeolites, and in case of hydroxonium formation, who many water molecules participate into the hydroxonium species. The simple framework of the chabazite makes this zeolite and ideal candidate for the INS study of adsorbed molecules with theoretical approaches in order to provide a deep understanding on the influence of the polarity of zeolite on the clustering of adsorbed water [4].

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Abstract

Polycrystalline Time-of-Flight Inelastic Neutron Scattering beyond the Density of States †

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Conventionally, experimental phonon dispersions are determined by inelastic neutron scattering on triple-axis spectrometers or by inelastic X-ray scattering, in both cases requiring single crystalline samples. When only polycrystals are available, the energy-dependent density of states (DOS) can be measured as an alternative.

Here I will make the point that the ($|\mathbf{Q}|$,E)-dependent spectral density, which is the primary quantity measured in coherent time-of-flight scattering on polycrystals, has a much greater information content than the DOS, to which it is customarily reduced, and that this information can be accessed by modelling the scattering signal. I will present applications of this technique to different systems and specifically show how the efficiency of the method makes it possible to perform temperature-dependent measurements with fine resolution, such as the behaviour of the phonon frequencies around the α-γ transition in elemental iron.

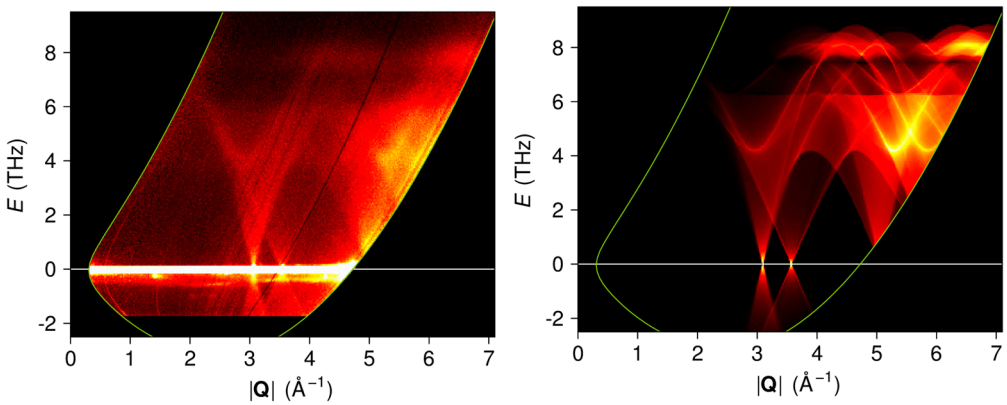

Figure 1. Time-of-flight spectra of polycrystalline Nickel: measured (**left**) and simulated (**right**).

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Abstract

Rubidium at Extreme Conditions †

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Transformations of alkali metals at high pressures is one of the hot topics of modern condensed matter physics. Exotic crystalline structures with very large and complex unit cells, unusual melting lines showing maxima and minima, pressure induced metal to non-metal transitions are some examples of this fascinating scenario. I will describe recent X-ray diffraction (XRD), Raman spectroscopy and Inelastic X-ray Scattering (IXS) studies on liquid and solid Rubidium at extreme pressures, up to several tens of GPa. XRD and IXS data in diamond anvil cells (DACs) consistently show a liquid−liquid transformation from a simple metallic liquid to a complex one, occurring at 6.5–8.5 GPa, which is slightly above the first maximum of the T−P melting line [1,2]. This transformation is traced back to the density-induced hybridization of highest electronic orbitals (s-d transition) leading to the accumulation of valence electrons between Rb atoms and to the formation of interstitial atomic shells, a behavior that Rb shares with Cs and is likely to be common to all alkali metals. Similarly, in the solid state, compressed alkali metals up to tens of GPa exhibit complex low-symmetry modifications, due to the density-driven transition of the valence electrons from the *s* state to states of higher angular momentum. We conducted challenging Raman spectroscopy measurements in DACs and *ab initio* computer simulations on the optical phonons of the low symmetry, high pressure crystalline phases of Rb up to 100 GPa [3]. The relative (relative to the normal condition value) density behavior of Raman frequencies of Rb is compared to that of Na and Li, once the frequencies of the two light alkali elements have been properly rescaled by their masses. Importantly, while the rescaled density behaviors of Na and Li agree with each other, Rb significantly differs, which highlights the different nature of the valence electron transition being of the *s-d* and of the *s-p* type in heavy and light alkali metals, respectively, a result that calls for further similar investigations of K and Cs. *Ab initio* simulations help the data analysis and show the evolution of the electronic, structural and dynamic properties in Rubidium extending to conditions still difficult to reach experimentally.

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Abstract

Magneto-Plasmonic Nanostructures and Crystals †

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Abstract: The fundamentals aspects of the key physics underlying the optical behavior of magneto-plasmonic nanoantennas are briefly introduced. A survey of applications to a variety of emerging technologies is presented as an example of their broad scientific and technological perspectives.

1. Introduction

Plasmons play a large role in the optical properties of metals. The rapidly developing field of magneto-plasmonics merges the concepts from plasmonics and magnetism to realize novel and unexpected phenomena and functionalities for the manipulation of light at the nanoscale. Magneto-plasmonics combines strong local enhancements of electromagnetic fields in surface plasmon excitations with magneto-optically active ferromagnetic materials. Owing to the intertwined optical and magneto-optical properties, magneto-plasmonics may offer a smart toolbox for actively magnetically tunable optical ultrathin surfaces and metasurfaces.

2. Content

Here we review fundamentals aspects of the underlying physics [1–3] and recent advances in the research on magneto-plasmonic nanoantennas and two-dimensional magneto-plasmonic crystals [4-16]. From the one side, they contributed to broaden the understanding and control of optics at the nanoscale. From the other side, magneto-plasmonic nanoantennas and surfaces have already shown a clear path towards applications to variety of emerging technologies as, e.g., ultrasensitive molecular sensing and ultrathin optical devices. A survey of applications to a variety of emerging technologies are presented as an example of the broad scientific and technological perspectives of magneto-plasmonic antennas and crystals, namely:

- magneto-plasmonic nanoantennas for ultra-sensitive and label-free molecular detection [4–8];
- ultra-thin 2D chiroptical surfaces, built on magneto-plasmonic bimetallic meta-atoms where chiral light transmission is modulated by the externally applied magnetic field [9];
- 2D magneto-plasmonic crystals, which support collective modes (surface lattice resonances) or surface plasmon polariton modes displaying a two-dimensional photonic band structure that can be engineered to obtain tailored and enhanced magneto-optical response [11–15];
- thermo-plasmonics based on bimetallic magneto-plasmonic nanoantennas, for harvesting electromagnetic radiation energy and convert it into heat, which can be used to finely tune the magnetization reversal in networks of interacting nanomagnets [16].

Challenges and future work will be briefly discussed.

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Abstract

The Influence of Non-Stoichiometry on the Order and Dynamics of Oxides Studied by Inelastic Neutron Scattering †

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Oxygen ionic conductors are materials of fundamental interest for the development of ambient temperature working devices for energy conversion, such as solid oxide fuel cells (SOFC).

Inelastic and neutron scattering experiments, coupled with ab-initio molecular dynamics simulations (AIMD), give the unique chance to unveil the presence of specific low-energy modes favoring diffusion events and so explaining the unusual high mobility down to moderate temperatures.

Experiments and AIMD on Nd_2NiO_4 systems [1,2] allowed to depict the on-site motion of the diffusive species and understand the impact of oxygen over-stoichiometry on the lattice dynamics of the Nd_2NiO_4 framework. A recent analysis on a single crystal allowed us to go beyond and verify that this partially disordered non-stoichiometric system show both correlated and uncorrelated dynamics, quite surprising for a crystalline compound [3].

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Abstract

Multiscale Modelling of Complex Dynamical Processes in Solids with MBN Explorer and MBN Studio †

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The multiscale modeling of complex molecular systems is a hot topic of the modern theoretical and computational research. To fully understand the dynamics of molecular systems and exploit it in different technological applications, such as hadron therapy, surface deposition and nanofabrication technologies, construction of novel light sources and others, one needs to consult many disciplines ranging from physics and chemistry to materials and life sciences, software engineering and high performance computing.

The MBN Explorer software package [1] is powerful and universal instrument of computational research that allows to build up, with the help of implemented algorithms operating at different space-and-time scales, multiscale models for the description of various molecular systems and processes therein for numerous biomedical and nanotechnology applications [2]. MBN Studio [3] is a graphical user interface for MBN Explorer that has been developed to facilitate setting up and starting MBN Explorer calculations, monitoring their progress and examining the calculation results.

There are several research areas in which multiscale simulations performed with the use of MBN Explorer and MBN Studio play an important role, e.g.in constructing of novel light sources based on charged particles propagation in crystalline undulators [4]. The talk will present novel theoretical and computational approaches and methodologies implemented in MBN Explorer and MBN Studio as well as related case studies.

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Abstract

Hertz-To-Terahertz Dielectric Response of Nanoconfined Water Molecules †

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Recently, considerable attention has been given to the properties of systems that contain interacting point electric dipoles. Such systems are expected to manifest rich variety of exotic phases resulting from competition between the dipole-dipole coupling and disordering effects, both dependent of various factors, like spatial symmetry and dimensionality of the dipoles locations, presence of defects and impurities, frustration, etc. An additional issue concerns the study of the dynamics of dipoles as interacting quantum rotors that experience a multi-well localizing potential in presence of hindering effects and quantum rotational tunneling. It is important, that the electrostatic coupling among the dipoles makes such systems qualitatively different from their magnetic counterparts. Since interacting spins have been thoroughly studied during last decades, significant progress has been achieved in understanding the underlying magnetic physics. In electric dipolar systems, the interplay of quantum tunneling, fluctuations and frustration provides with the possibility to realize new exotic phases, like (anti)ferroelectricity, quantum electric dipolar liquids and glasses, lead to quantum critical phenomena and quantum phase transitions. Understanding the nature of the corresponding phases, their formation and relations with magnetic counterparts is of great fundamental and technological interest, but is presently at its infancy.

Prospective playground for corresponding studies is provided by dielectrics whose crystal lattice contains voids filled with electric-polar molecules that only weakly interact with surrounding ions and are thus nearly free, but "feel" each other via long-range electric dipole-dipole interaction. Corresponding broad-band spectroscopic studies of the gemstone beryl with 0.5 nm sized pores hosting polar H_2O molecules (each carrying a dipole moment of ≈1.85 Debye) allowed to discover incipient ferroelectricity within the H_2O dipoles, along with a rich set of single-particle excitations at terahertz-infrared frequencies [1–5]. It was suggested that the (anti)ferroelectric phase transition into the macroscopically ordered state was suppressed by quantum tunnelling of H_2O molecules between 1 meV deep wells of the localizing six-fold potential. Here, we present detailed spectroscopic studies of single-particle and collective vibrational states of a network of H_2O molecules hosted by orthorhombic crystal lattice of cordierite. Unlike hexagonal beryl, water molecules in cordierite experience 2-well localizing potential while rotating 360° around the c-axis, with the wells separated by an order of magnitude higher energy barriers of ≈10 meV.

Using terahertz (THz), radio-frequency (RF) and microwave (μW) spectroscopies, we measure polarization-dependent (E-field component of the probing radiation parallel to a, b and

c axes) spectra of the complex dielectric permittivity $\varepsilon(\nu) = \varepsilon'(\nu) + i\varepsilon''(\nu)$ and AC conductivity $\sigma(\nu) = \sigma1(\nu) + i\sigma2(\nu)$ of hydrous cordierite in the range ν = 1 Hz–3 THz and at temperatures 0.3 K–300 K. Measurements on water-free (annealed in vacuum) crystals allowed us to extract the spectra determined exclusively by water molecules. In the THz range, 0.3 THz–3 THz, rich sets of highly anisotropic soft excitations are discovered. Applying density-functional and molecular dynamics analyses allowed us to associate the origin of the excitations with complex librational-rotational vibrations of the nanoconfined polar water molecules. In the RF-μW ranges, 1 Hz–1 GHz, for the E||a polarization we discover a strongly temperature-dependent overdamped excitation and assign its origin to relaxational dynamics of separate molecular dipoles within the confining cage. Below 3 K, we detect weak signatures of a phase transition into a glassy state formed by frozen water dipoles. We will perform comparative analysis of the results obtained on water dipoles arranged in hexagonal (beryl matrix) and in orthorhombic (cordierite matrix) arrays.

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Abstract

Resonant Inelastic X-ray Scattering Study of Excitations in Cuprate Superconductors †

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The mechanism of high-T_C superconductivity in cuprates remains an unsolved question since its discovery in 1986. Answering the question of its microscopic origin turns out to be a great challenge, complexity arises from the coexistence of several phases along with the superconductivity. Although electron-phonon coupling may not be the main origin of the Cooper pairing, its role across the phase diagram is still controversial, particularly in the under-doped region [1–3]. A direct way to probe the electron-phonon coupling has emerged thanks to the recent progress made in high resolution Resonant inelastic X-ray scattering (RIXS), which now allows to resolve phonons [4]. Theoretical studies suggested that the RIXS phonon cross-section directly reflects the momentum-dependent electron-phonon coupling strength [5,6]. In this talk, we will focus on the dynamical properties of the under-doped cuprate $Bi_2Sr_2CaCu_2O_{8+\delta}$. Low energy excitations were investigated using RIXS at the Cu L_3-edge with an energy resolution of 40–45 meV [4]. In the quasi-elastic region, an incommensurate charge density wave (CDW) was observed in this system, confirming its existence in this compound. In addition, this RIXS study resolved the bond-stretching phonon in the energy-momentum space. Importantly, it also revealed that the phonon dispersion changes at the CDW wave-vector indicating that the CDW unambiguously affects the lattice. RIXS measurements on another superconducting cuprate, $Ca_{2-x}Na_xCuO_2Cl_2$, will be also discussed.

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Abstract

Time-Resolved Investigations and Biotechnological Applications of Plasmonic Nanostructures †

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Plasmonics exploits the collective motion of conduction electrons in metals (plasmons), thus enabling light to couple with nanoscale objects, with the consequent generation of a plenty of novel and unexpected optical effects and functionalities. Plasmonic nanostructures have been deeply studied in the last decade due to their crucial impact on several areas of nanoscience and nanotechnology. Their unrivalled capability to squeeze light well beyond its diffraction limit, leading to extremely confined and enhanced electromagnetic fields on the nanoscale at optical frequencies, is of great interest for the prospect of real-life applications, such as energy harvesting and photovoltaics, wave-guiding and lasing, optoelectronics, fluorescence emission enhancement, plasmon-assisted bio-interfaces and nanomedicine. In this framework, traditional studies of the resonant behavior of plasmonic nanoantennas rely on standard intensity detection schemes. Up to date, the temporal dynamics of plasmonic nanoantennas remains challenging. In the first part of the talk we will show that, by combining femtosecond time-domain spectroscopy and high-resolution confocal microscopy, it is possible to measure full time- and field-resolved response of single plasmonic nanoantennas [1]. In the second part of the talk, we will then show practical applications of plasmonic nanostructures to single-molecule detection [2–4], enhanced spectroscopy on single-cells [5–7], optical trapping [8,9], enhanced Raman scattering [10–12] and resonant energy transfer [13].

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Abstract

Using Patchy Particles to Shed New Light on the Autocatalytic Aggregation of Soft Matter †

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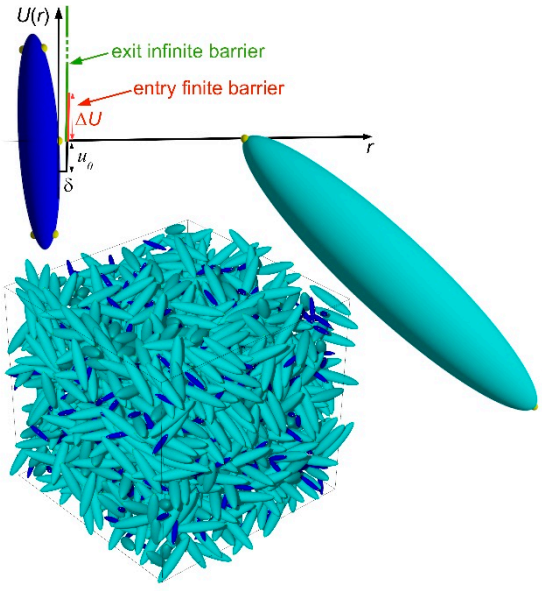
Autocatalysis, i.e., the speeding up of a reaction through the very same molecule which is produced, is common in chemistry, biophysics, and material science. Despite the pervasiveness of autocatalytic phenomena in nature and technology, autocatalytic aggregation has so far remained out of reach of realistic numerical simulations. Rate-equation-based approaches are often used to model the time dependence of products, but the key physical mechanisms behind the reaction cannot be properly recognized and then taken into account. On the contrary, patchy particles are designed learning from nature and can be thought of as an archetype of real monomers, but so far they completely lack autocatalysis. Here, building on previous studies on the subject [1–4], we report on a patchy particle model inspired by a bicomponent reactive mixture and endowed with adjustable autocatalytic ability [5]. Such a coarse-grained model captures all general features of an autocatalytic aggregation process that takes place under controlled and realistic conditions, including crowded environments. Simulation reveals that a full understanding of the kinetics involves an unexpected effect that eludes the chemistry of the reaction, and which is crucially related to the presence of an activation barrier. The resulting analytical description can be exported to real systems, as confirmed by experimental data on epoxy–amine polymerizations, solving a long-standing issue in their mechanistic description.



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Abstract

Advanced Channeling Technologies: Strong External Electromagnetic Fields to Guide Charged & Neutral Beams †

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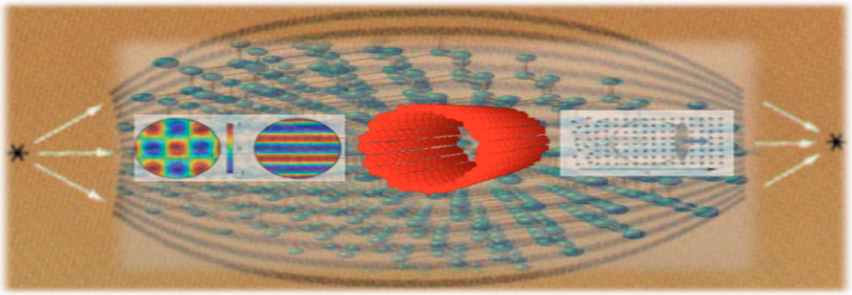
Channeling is the phenomenon well-known in the physics world mostly related to the propagation of the beams of charged particles in aligned crystals. Since the beginning of 1970s channeling of high-energy leptons (electrons/positrons of several MeV up to hundreds of GeV energies) and hadrons (protons/ions of tens GeV up to several TeV energies) has been applied at various famous world research centres within different national/international projects related to the phenomenon utilization to shape the beams as well as to produce high power x-ray and gamma radiation sources.

However, recent studies have shown the feasibility of channeling phenomenology application for description of other various mechanisms of interaction of charged as well as neutral particles beams in solids, plasmas and electromagnetic fields covering the research fields from crystal/laser/plasma based undulators [1] and collimators to capillary based x-ray and neutron optical elements [2].

This review talk is devoted to actual channeling-based projects that have been realizing since so-called renessiance of channeling studies started in the end of last century. The future possible developments in channeling physics will be analyzed within the presentation.



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Oral Presentations

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Abstract

Energy Scale of the Charge Density Wave in Cuprate Superconductors †

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The cuprate high temperature superconductors develop spontaneous charge density wave (CDW) order below a temperature T_{CDW} and over a wide range of hole doping (p). An outstanding challenge in the field is to understand whether this modulated phase is related to the more exhaustively studied pseudogap and superconducting phases [1]. To address this issue, it is important to extract the energy scale Δ_{CDW} associated with the CDW order, and to compare it with the pseudogap (PG) Δ_{PG} and with the superconducting gap Δ_{SC}. However, while T_{CDW} is well-characterized from earlier work, little is known about Δ_{CDW} until now. Here, we report the extraction of Δ_{CDW} for several cuprates using electronic Raman spectroscopy [2]. Crucially, we find that upon approaching the parent Mott state by lowering p, Δ_{CDW} increases in a manner similar to the doping dependence of Δ_{PG} and Δ_{SC} [2]. This indicates that the above three phases have a common microscopic origin [2]. In addition, we find that Δ_{CDW} and Δ_{SC} have the same magnitude over a substantial doping range, which suggests that CDW and superconducting phases are intimately related [2], as reported for example by fractionalized pair density wave [3].

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Abstract

Spin Dynamics and Phonons, Insights into Potential Molecular Qubits †

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Molecular spins are characterized by an effective electronic and magnetic tunability and this is a very relevant property for quantum computation applications [1]. In particular metal complexes have unpaired electrons located in the d orbitals, whose energy can be easily tuned using proper ligands; hence, metal complexes are very promising candidate to realize qubit devices. An accurate choice of the metal centre and of the ligands is able to substantially increase the spin coherence time [2], that is the basic requirement to implement operative qubits. In this framework, the effects of molecular and lattice vibrations, or phonons, on the spin relaxation mechanisms have been the focus of increasing attention. Thanks to our multi-technique approach, based on alternative current susceptibility, EPR and TeraHertz time-domain spectroscopy, we have evidenced correlation between low energy vibrations and spin relaxation time in molecular qubits [3,4]. Moreover, we have highlighted the role of the rigidity of the molecular structure and of the crystal lattice [4], together with the overall dimensionality [5], on phonons and on the spin dynamics. These recent results are here presented for a series of vanadyl-based compounds, where an appropriate choice of the ligand structure and of the coordination geometry allow to control the spin dynamics.

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Abstract

Sub-THz Raman Response and Critical Dynamics in $BaTiO_3$ †

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$BaTiO_3$ (BTO) is considered as a textbook material for the description of structural phase transitions (SPT) and the appearance of ferroelectricity. On cooling it undergoes successive cubic-tetragonal-orthorhombic-rhombohedral (C-T-O-R) phase transitions [1]. Various concepts such as soft phonon, central peak, relaxational mode, hard phonon are invoked to describe the dynamics of the lattice, the structural changes or the occurrence of ferroelectric state in this material [2–5]. The displacive or order-disorder (OD) character of the paraelectric-ferroelectric transition is long-standing object of controversies [4,6]. It is now admitted that both mechanisms co-exist [7,8]. It is to be underlined that up to now the simultaneous detection of both processes by the same technique was not so far reported. The possibility of existence of two critical degrees of freedom was only drawn by ab-initio calculations [9], or was indirectly derived from the discrepancy in dielectric permittivity between direct data and calculations via LST relationship [6,7]. Raman spectroscopy was widely used for investigate lattice dynamics and phase transition in BTO, but the very high damping of the soft phonon [3,10] impedes to extract the additional OD feature which should be located at lower frequency. Here we report new Raman spectra recorded as function of temperature in the tetragonal phase, using ultra low-frequency (ULF) set-up. This tool provides the measurement of Raman shift down to 5 cm^{-1} with respect of the Rayleigh line, providing therefore the detection of vibrational or relaxational modes centered around 200 GHz. Within the contribution we firstly discuss the differences and similarities in the various concepts used to describe lattice dynamics with link with SPT. Then we present new Raman data in BTO and highlight the occurrence of the additional peak lying at frequency lower than the soft phonon. The intensity and shape of this peak are strongly dependent on temperature. This feature is attributed to a local mode, related to Ti-off centering with a characteristic relaxation frequency showing a slowing down on approaching the T–C, and the T–O SPT as well.

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Abstract

Dynamical Properties of Ice and Water: A Broadband Dielectric Spectroscopy Study †

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Though the mechanical properties of ice and water differ, they still have much in common from the dielectric spectroscopy viewpoint. We analyze the spectra of dynamical conductivity of solid and liquid water (see Figure 1) as a signature of their molecular dynamics. The dynamics of ice and water are considered on the same footing. We introduce a model [1] that provides a clear interpretation of the experimental conductivity and dielectric constant over fourteen orders of frequency magnitude, thus extending the scope of the existing models. The model links together infrared vibrations with static conductivity and dielectric constant, gives the interplay between the electrical and thermodynamic properties of ice and water, and provides a new dynamical vision on the old problem of the water structure.

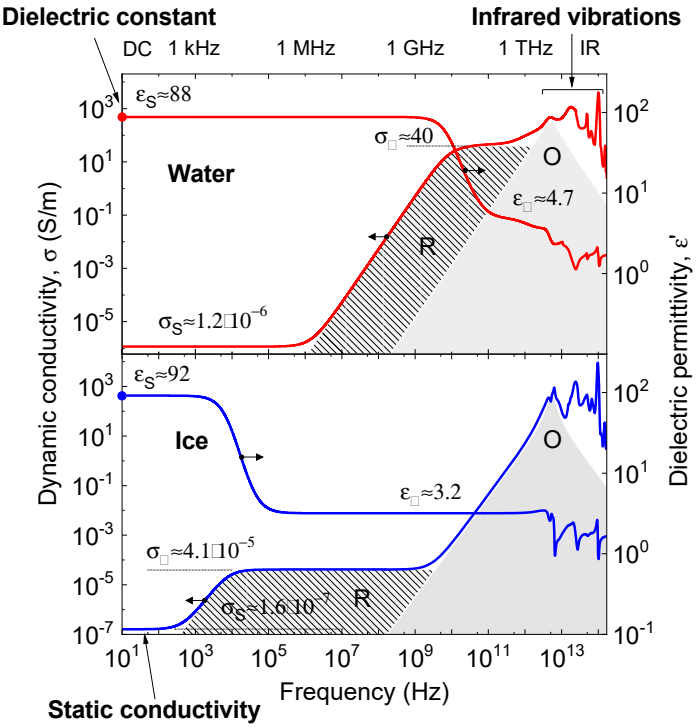

Figure 1. Broadband spectra of ice (blue) and water (red) in terms of dielectric permittivity (ε′) and electrical conductivity (σ).

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Abstract

Spin-Lattice Coupling in the Quantum Spin Ice Candidate $Tb_2Ti_2O_7$ Revealed by THz Spectroscopy †

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In geometrically frustrated magnetism, the very nature of the ground state of $Tb_2Ti_2O_7$, has remained a long standing conundrum. In this pyrochlore material, no conventional spin-ice or long-range magnetic order is stabilized, even at very low temperatures. Quantum fluctuations are suspected of being at the origin of such an exotic quantum phase, yet so far has lacked conclusive evidence. Using high-resolution synchrotron-based terahertz spectroscopy, we have probed the lowest energy excitations of $Tb_2Ti_2O_7$ (see Figure 1). It is revealed that a double hybridization of crystal-field-phonon modes is present across a broad temperature range from 200 k down to 6 K [1]. This so called vibronic process affects the electronic ground state that can no longer be described solely by electronic wave functions. We will present here new results obtained down to 250 mK in the exotic magnetic phase.

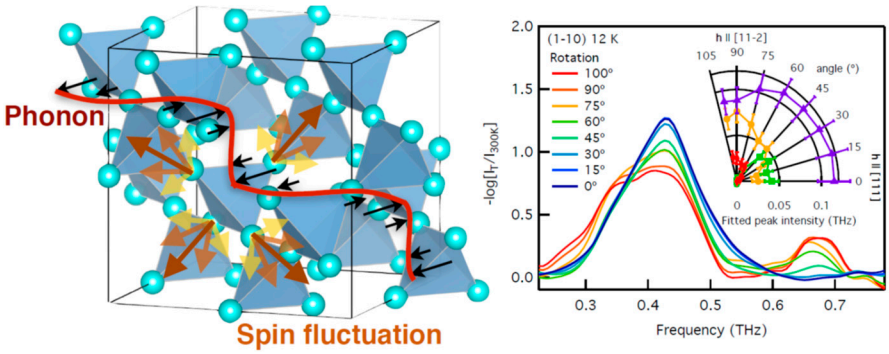

Figure 1. (**left**) Tb^{3+} Pyrochlore network and graphical description of the vibronic process that involves the hybridization between a phonon and a crystal field excitation. (**right**) Angular dependence of the THz spectra recorder at 12 K.

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Abstract

Electron Localizations in Alloy Exhibiting Nanotwinning †

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Ni_2MnGa is a ferromagnetic shape memory alloy in which a large spontaneous deformation up to 12% has been observed after application of an external magnetic field [1]. The key to such material functionality is the ferroelastic microstructure of martensite with deep hierarchical twinning up to nanoscale [2]. However, the microscopic origin of the martensitic transformation between the high temperature austenitic and low temperature martensitic phases is not fully understood to date as well as exact origin of nanotwining in martensitic phases. In present work we have used first-principles calculations based on density functional theory (DFT) to simulate magneto-optical (MO) Kerr spectra for different phases of Ni_2MnGa alloy: austenite, nonmodulated martensite without nanotwinning and nanotwined martensite represented by 4O structure [3]. The MO spectra provide a valuable insight into the mutual dependence of the the structure of the material and electronic structure and magnetic ordering.

The work of Himmetoglu et al. [4] suggests that the Hubbard treatment of the on-site Coulomb interaction of d-electrons localized on Mn sites (DFT+U) is required to describe correctly the electronic structure of Ni_2MnGa alloy. A comparison of the calculated and measured spectra allowed us to estimate the proper value of Coulomb interaction parameter U, which we found significantly smaller than the value proposed in previous works [4,5]. Using smaller U, we obtain a better quantitative agreement with experiment at least in case of elastic constants and lattice parameters in Ni_2MnGa. Comparison of the newly calculated densities of states covering the electron localization then provides a better insight into the origins of martensitic transformation and nanotwinning.

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Abstract

The Causality-Composition Law in the Non-Debye Relaxations Models †

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The standard approach to represent the experimentally measured data depending on some continuous parameter is to draw them as a curve, i.e. as a continuous function which fits the experimental points and hopefully follows some theoretical explanation. The most typical illustration of such procedure is a graphical representation of the time evolution of some physically relevant quantity. However, any time evolution pattern must satisfy a crucially important condition: its initial point may be chosen arbitrarily but has to be earlier than the final point. Thus, we can say that any result must not precede its cause and the fitted curve is to satisfy the causality law. This requirement leads also to the composition law. Namely if the system evolves from t0 to t such that t0 < t and if we choose an intermediate instant of time tint, t0 ≤ tint ≤ t, then the composition of evolution in the intervals (t0, tint) and (tint, t) must give the same result as the evolution in the interval (t0, t). This basic property, easily seen for the Debye, i.e. exponential law, is not so evident for non-Debye relaxation phenomena. We show explicitly how it is realized in two non-Debye relaxation patterns widely used in dielectric physics, namely the Cole-Cole model and the Kohlraush-Williams-Watts (stretched exponential) model observed in the photoluminescence.

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Abstract

Advances on the Modelling of Blood Flows and Pressures in Humans through a New Multiscale Mathematical Model †

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Many biophysical factors affect human circulation, so that a satisfactory understanding of its behavior is challenging [1]. Moreover, congenital vascular disease is the leading cause of pediatric death, and it is proven that physiological parameters such as cardiac output, cerebral blood flow, and arterial stiffness are related to age [2]. For these reasons, the assessment of cardiovascular structure and function is recognized as a main topic in the history of scientific research [3]. We developed a mathematical model to simulate cerebral and extracerebral flows and pressures in humans. The model is composed of an anatomically informed 1-D arterial network [4,5], and two 0-D networks of the cerebral circulation and brain drainage, respectively [6,7]. It takes into account the pulse-wave transmission properties of the 78 main arteries and the main hydraulic and autoregulation mechanisms ensuring blood supply and drainage to the brain. Proper pressure outputs from the arterial 1-D model are used as input to the 0-D models, together with the contribution to venous pressure due to breathing that simulates the drainage effect of the thoracic pump. The model is able to evaluate the effects of reduced/elevated carbon dioxide in the blood (hypo/hypercapnia) [8], and to compare adult and pediatric circulation through a straightforward calibration of the parameters. Proper MRI and ultrasound datasets were used to extract information about blood rheology (e.g., blood velocity and flow), and vessel status (hydraulic resistance and capacitance, inner pressure and cross section area). The model has the potential to predict important clinical parameters before and after physiological and pathological changes with focus on head and neck circulation, such as posture changes, vessel occlusions, venous thrombosis, and congenital diseases.

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Abstract

Molecular Dynamics of a Liquid Crystal with Highly Ordered Smectic E Phase under Different Forms of Confinement †

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Liquid crystals (LCs) confined in various host system have attracted great interest in recent years. New material properties originating from finite size of pores and interaction between molecules and pore surface have been reported, including optical properties, dynamic peculiarities and different phase diagram than in bulk. It was concluded that a change in the transition temperature origins from two competing effects: orientational order locally imposed by pore surface that increases the transition temperature and disordering effect resulting from the elastic forces and rearrangement of defect lines which cause the reduction of the transition temperature. One of our previous papers [1,2] discusses the dynamics and morphology of 4-heptyl-4′-isothiocyanatobiphenyl (7BT) confined in silica pores with average diameters of 4, 6, 7.5, 9.5 and 10.5 nm. While 7BT in bulk demonstrates a smectic E (SmE) phase characterized by an orthorhombic arrangement of molecules within the smectic layers, the order of 7BT molecules is imposed by a strong surface potential in nanopores. Consequently, molecular dynamics are significantly modified in nanopores compared to bulk. Two relaxation processes were detected by dielectric spectroscopy: one related to the "flip-flop" motions of molecules around their short axis, while the second was ascribed to the librational motions of molecules partially immobilized on pore walls. As the pore size decreases, the surface effect becomes more pronounced, with only librational motions observed in 4nm pores. An analysis of the temperature dependencies of specific IR absorption bands, in terms of their spectral position and integrated intensity, highlighted the varied influence of confinement on rigid and flexible molecular moieties: i.e., the gradual ordering of aromatic cores and amorphous-like behaviour of alkyl chains.

The purpose of this work is to exam the dynamic properties of 4-hexyl-4′-isothiocyanatobiphenyl (6BT) with a SmE phase experiencing different forms of confinement. *Hard* confinement was achieved by the infiltration of LCs into nanoporous aluminum oxide (AAO) templates with non-intersecting, cylindrical, channels. Other interesting, but as yet unexplored is *soft* confinement derived from the interactions between the polymer and guest liquid crystalline molecules. This was investigated on an example of electrospun polymer/liquid crystal composite fibers (see Figure 1). We prepared composite fibers for three different mass ratios of polycaprolactone (PCL) and 6BT. By a combination of broadband dielectric spectroscopy and Fourier-Transform Infrared (FTIR), the microscopic picture of the influence of *soft* and *hard* confinement on molecular dynamics is obtained. In this talk, I will discuss similarities and differences in the impact of hard and soft confinement on dynamic properties and crystallization kinetics of 6BT liquid crystal.

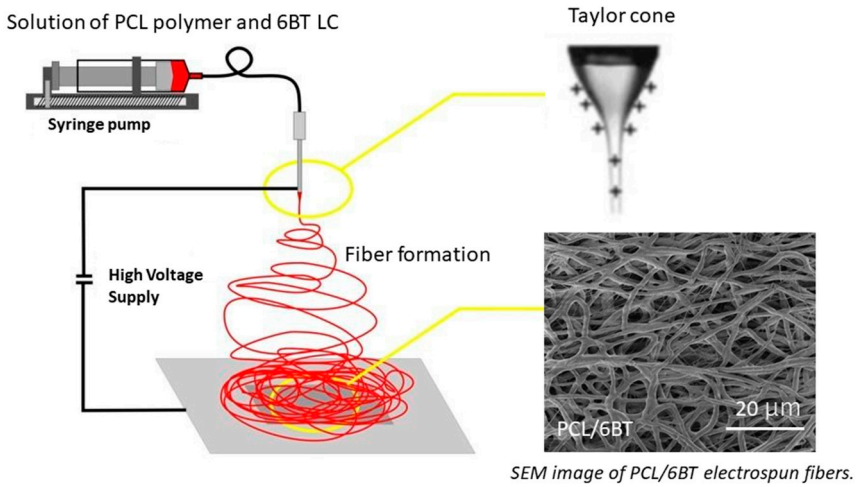

Figure 1. Sketch showing formation of composite PCL/6BT composite electrospun fibres.

Acknowledgments: M.J.-D. acknowledges the National Science Centre (Grant SONATA11: UMO-2016/21/D/ST3/01299) for financial support.

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Abstract

Domain Structure and Magnetization Reversal Mechanism in Co/Pd Nanopatterned Multilayer †

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Fabrication and modeling of patterned thin films with perpendicular magnetic anisotropy rise great interest due to their wide applications in magnetic storage, sensors and magnonic crystals. A good representative of such systems are well-ordered arrays of magnetic antidots and dots based on Co/Pd multilayers, where magnetic reversal mechanisms strongly depend on the array geometry [1,2]. We attempt to understand and reproduce the observed magnetic properties and domain structure appearing in the arrays by micromagnetic simulations performed using Mumax3 software [3]. In particular, changes in coercivity field, magnetic anisotropy constant and magnetic domain arrangement were studied and correlated with symmetry and size of nanostructures. The domain pattern simulations shed light on the details of formation the Néel domain walls, as compared to Bloch walls, depends on the distances between the antidots. The calculations show how edge effects, defects and inhomogeneity affect magnetization reversal and domain wall pinning mechanism, which helps to design similar patterned systems with the specific magnetic properties.

Acknowledgments: The numerical simulations were supported in part by the PL-Grid Infrastructure.

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Abstract

Edge Modes in the Switching Mechanism of Finite Chains of Macrospins †

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We study transitions of 1D systems of macrospins between their equilibrium configurations under a uniform magnetic field and under variations of the distances of the macrospins in such chains. A magnetic field opens a gap at the Brillouin zone border, giving room to bound edge states. If the number of macrospins in the chain is odd, two bound states, symmetric and antisymmetric, appear in the gap for the magnetic field parallel to the magnetization of the end macrospins and the instability is driven by a bulk soft mode. If the field is oriented antiparallel to the end macrospins no bound modes appear in the gap. In turn the instability involves softening of edge bound states as illustrated in Fig.1. The even-odd alternation of this behaviour will be presented, as well as the effect of variations of the macrospins mutual distances.

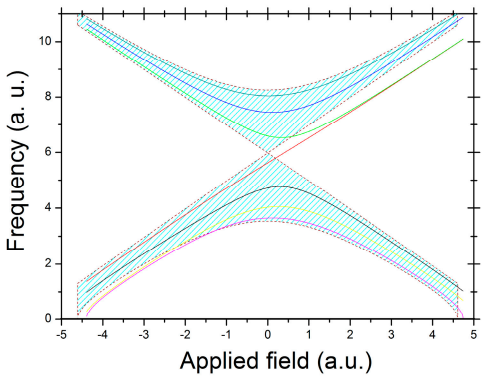

Figure 1. Bulk and bound states in a chain of seven macrospins in Stoner-Wohlfahrt model.

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Abstract

Nucleation in Aqueous KCl Solutions Induced by Laser Pulses †

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The nucleation processes are still today between the more intriguing problems of the condensed matter physics; they have been described by different models, but their understanding I still far to be complete [1]. In particular, we are missing the experimental investigations of the first nucleation events due to their unpredictable localization in the time and space coordinates.

The nucleation in saturated solutions can be induced by a short laser pulse of high intensity [2]; a series of experimental studies have proved that this phenomenon occur in aqueous solutions of very different nature, where the solutes can vary from simple salts to complex biological molecules [3]. Even if the NonPhotochemical Laser Induced Nucleation (NPLIN) is known from more than 20 years, several fundamental aspects of it remain open problems [4]. Nevertheless, the NPLIN enables the possibility to perform spectroscopic measurements during the first steps of crystal nucleation and growth, opening the harvesting of new valuable information on this elusive phenomenon.

We performed an experimental investigation of the nucleation phenomena induced by a 25 picosecond infrared laser pulse in a supersaturated aqueous KCl solution. In particular, we developed an experimental set-up able to perform a very fast imaging (up to 5×10^5 frame/s) of the solution modifications induced by the laser pulse. The fast imaging shows a series of physical processes taking place in the solution between the laser pulse arrival and the show up of the crystal nucleus, see Figure 1.

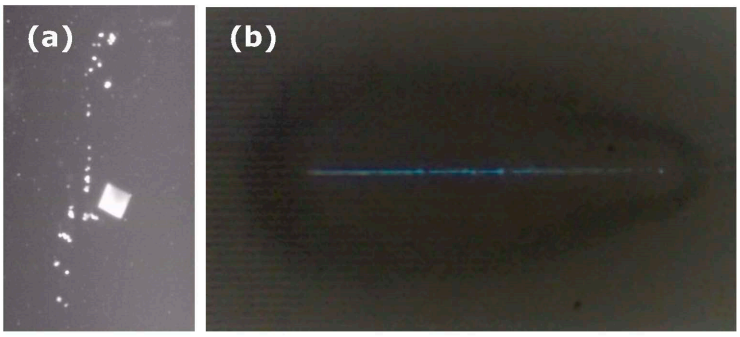

Figure 1. (**a**) KCl crystals induced by a laser pulse of 25 ps; (**b**) plasma line and shockwave preceding the nucleation phenomena, captured by an ultrafast camera with a 25 μs shutter time.

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Abstract

Spin Wave Modes in a Cylindrical Nanowire in Crossover of Dipolar-Exchange Regime †

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Although the magnetic wires have been [1] broadly investigated, some of their dynamical properties, like: (anti)crossing between the spin wave modes and the impact of the magnetic field on the spin wave spectrum, still need to be explored. In our studies [2] we identify the dispersion branches and their (anti)crossings (see Figure 1) in crossover of the dipolar-exchange regime by plotting the spatial profiles of spin waves and respective magnetostatic potentials. We also check how we can tune the spectrum of the modes by application of the external magnetic field and how it affects the dominating type of interaction. We use two approaches for solving the Landau-Lifshitz equation: semi-analytical calculations and numerical computations based on the finite element method.

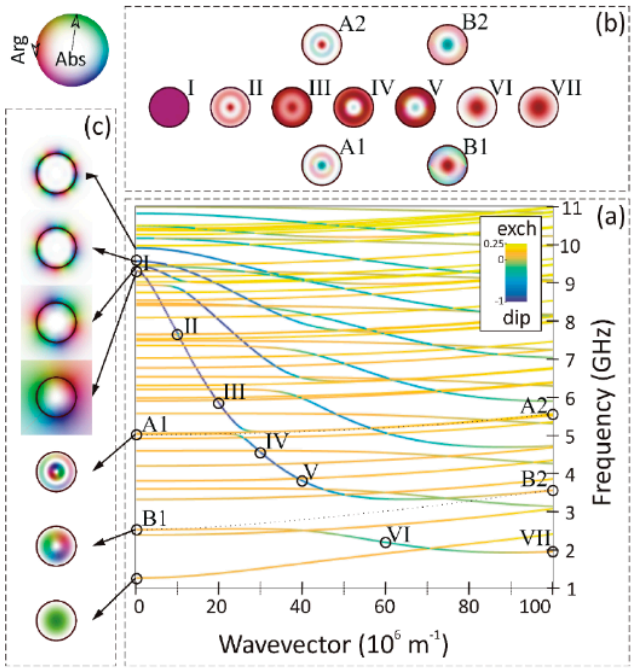

Figure 1. (**a**) Dispersion relation of cylindrical (60 nm-radius) Ni nanowire magnetized along its axis in the absence of an external field and the profiles of (**b**) dynamic magnetization, and (**c**) magnetostatic potential for selected spin wave modes.

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Abstract

Low-Dimensional Composite Material Based on Modified Graphene and Metal Oxide for High-Performance Chemical Sensors †

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Low-dimensional chemical sensors based on metal oxides have received great attention for the applications in security and medical diagnoses. Transition oxide nanomaterials exhibit promising sensing performance owing to their large surface area and good chemical stability. However, the sensing performance of these materials have yet to reach to their full potential in capabilities and usage. The fabrication of composite materials based on metal oxides is an effective way to enhance their sensing properties. TiO_2 nanotubes (TNTs) have received extensive attention for gas sensing applications due to their large surface area, unique physical and chemical properties. Graphene with its modified forms, high specific surface area and excellent electronic properties can revolutionize performances of the functional devices. Herein, we report an efficient strategy to improve the sensing properties of TNTs. We fabricated composite structures by coupling of TNTs and modified-graphene. The morphological, structural and elemental analyses of samples were carried out. The sensing properties of obtained materials were tested towards H_2, NH_3, CO, ethanol and acetone (Figure 1). We studied the effect of each material on the sensing performance of composite structures. The studies have shown the variation of mixture material concentration and the modification of graphene layers have a crucial effect on the response and the selectivity of the obtained composite materials. The obtained results demonstrate that we have developed an efficient method for the preparation of composite structures and the obtained materials can be applied for the fabrication of high-performance sensing systems.

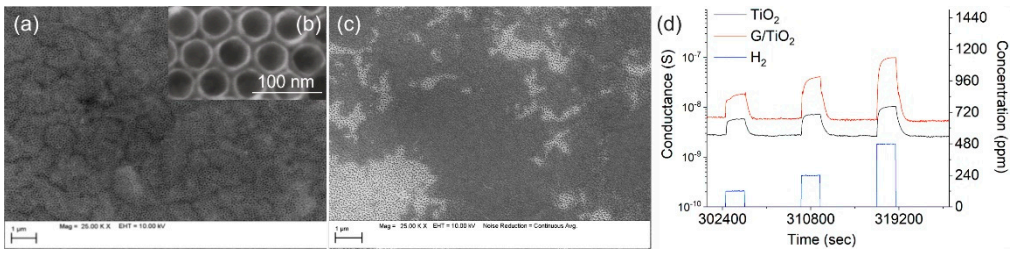

Figure 1. (**a**,**b**) SEM images of the TNTs, (**c**) SEM micrograph of the composite (G/TiO_2), (**d**) dynamical response of the composite (G/TiO_2) and pure TNTs towards 120, 240 and 480 ppm of H_2 at 300 °C.

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Abstract

Ensamble Sampling for Lattice Dynamics †

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Computational investigation of anharmonic and temperature-dependent aspects of lattice dynamics requires, among other things, replication of the conditions of thermal equilibrium. This requirement is very challenging when performing quantum mechanical calculations. Typically, it involves large number of atoms and long simulation times needed to approximate thermodynamical limit conditions. This is usually achieved by running a long molecular-dynamics calculation on the system, to thermalize all degrees of freedom, and selecting well-separated (independent) configurations from the obtained trajectory. While this approach provides good sampling of the configuration space of the system it is computationally very expensive and exceptionally wasteful. To obtain independent samples the selected times in the trajectory must be separated by multiple time steps—often tenths or hundreds. Thus, we are throwing away a large amount of computational time, often above 80%, to obtain good sampling of the probability distribution in the configuration space. Furthermore, in the case of lattice-dynamical calculations, we are using only the positions from the trajectory—since we have usually no use for the velocity information. Together, this makes the described procedure limited to fairly small systems.

In this work we present an alternative scheme for creating a representation of the probability distribution in the configuration space, which aims to faithfully reproduce densities generated by the molecular dynamics, while being much more effective in terms of computational time. This approach uses well-known techniques of probability distribution modelling, and apply knowledge of the behaviour of the system in thermodynamic equilibrium to obtain low sample rejection rate in the procedure. This method, coupled with the effective-potential modelling of the interatomic forces provides a promising path to tackle problems of anharmonic and temperature-dependent lattice dynamics even in systems with large and complicated unit cells.

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Abstract

On Some Enigmatic Properties of Relaxation Functions †

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The Debye model of dielectric relaxation provides us with the simplest shape of spectral functions, i.e., relations connecting characteristics of polarized dielectric medium and the frequency of the polarizing electric field. An example of such a relation is $\chi(i\omega) = (1 + i\omega\tau^*_D)^{-1}$ which shows how the complex susceptibility $\chi(i\omega)$ depends on ω and on a single material dependent parameter called the characteristic time τ^*_D. As expected, such a spectral function transformed to the time domain leads to the exponential decay law. In contemporary dielectric physics the Debye model finds only a little application and to fit the experimental data it is usually replaced by phenomenologically rooted modifications among which the Cole-Cole, Cole-Davidson, Havriliak-Negami and the "excess wing" models play dominant roles. The first three of them, similarly like the Debye pattern, still depend on a single characteristic time τ^* but involve insertion of fractional powers $0 < \alpha, \nu \leq 1$ according to $\chi(i\omega) = (1 + (i\omega\tau^*)^\alpha)^{-\nu}$. Meanwhile, the "excess wings" model introduces additional characteristic times, e.g. through the ansatz $\chi(i\omega) = (1 + (i\omega\tau_2)^\alpha)/(1 + (i\omega\tau_2)^\alpha + i\omega\tau_1)$. All the above mentioned spectral functions, if treated as functions of a complex variable $\omega \to z$, share a common behavior—for suitably adjusted, but physically well justified values of parameters, they are analytic in the lower half of the complex plane and map it into the upper half plane. On first sight this property seems negligible but appears to have important mathematical consequences. Functions which obey it have uniquely determined integral representations given as weighted sums of Debye's spectral functions (in mathematics equivalent to the so-called Stieltjes transforms of such weight functions) and, if transformed to the time domain and taken for $t > 0$, are completely monotone, i.e., representable as the Laplace transforms of nonnegative locally integrable functions. This means that widely accepted models of non-Debye dielectric relaxation phenomena may be obtained through summing up elementary Debye relaxations with different, continuously distributed characteristic times. In the talk we are going to provide arguments if this statement should be treated either as a mathematical artifact or as a physically based conjecture.

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Abstract

Direct Detection of Multiple Backward Volume Modes in Yttrium Iron Garnet at Micron Scale Wavelengths †

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Spinwave propagation in yttrium iron garnet (YIG) films has a long history [1] but has recently attracted renewed attention due to the observation of an unusual coherent phenomenon [2] in a heavily pumped magnon gas in the backward volume geometry [3] where the spectrum displays a minimum. The effect has been termed Bose condensation or, from a more classical perspective, a Rayleigh-Jeans condensation. The time dependence of the observed behavior has recently been simulated and shown to arise from a dynamic equilibrium state of a classical magnon gas interacting through three and four magnon scattering processes [4].

The measurements cited above utilized the Brillouin scattering technique which has the advantage allowing studies over a broad spectral range, but for which the resolution is limited. To better understand the properties of magnons in the vicinity of the minimum in the spectrum (where the condensation occurs) we have patterned a set of wave-vector-specific, multi-element, "ladder" antennas, with which we can *directly couple* spin waves with micron and submicron wavelengths to a microwave generator and determine the resulting absorption. Our measurements, which are shown in the Figure 1, were carried out on a 2.84 micron film and have resolved the dispersion relations of multiple (ten or more depending on the wavelength) low lying backward volume modes for wavelengths of 10, 3, 1 and 0.6 microns. Overall the data are in excellent agreement with theoretical predictions based on a Heisenberg model Hamiltonian [5]. Data are also compared with solutions of Landau-Lifshitz equation that include both dipolar and exchange effects [6].

We will also report our recent experiments in which we use our one micron antenna to detect *coherent spin waves* at the minimum which arise via a Suhl two magnon decay processes where we pump at twice the detected frequency; this is the first time such modes have been detected to our knowledge. Other parametric pumping experiments will also be described.

The techniques developed in this work now facilitate the characterization of spin waves at length scales limited only by available lithography and with a spectral resolution that greatly exceeds that of Brillouin scattering.

Dispersion curves of magnons in a 2.4 micron thick film in the backward volume geometry.

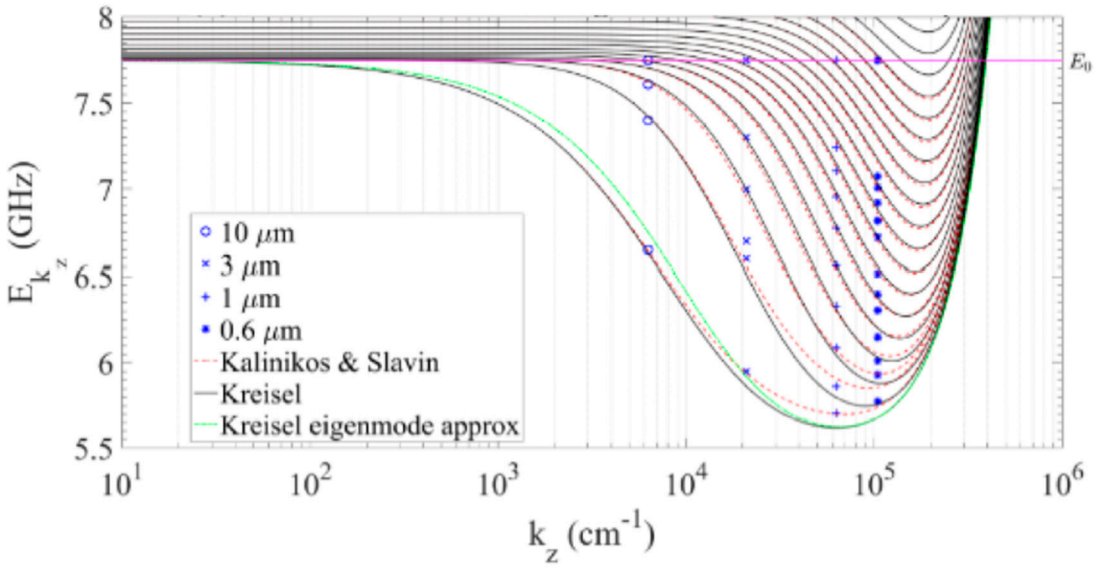

Figure 1. Dispersion curves of magnons in a 2.4 micron thick film in the backward volume geometry.

Acknowledgments: The magnetic resonance measurements were performed at Northwestern University under support from the U.S. Department of Energy through grant DE-SC0014424. Device fabrication was carried out at Argonne and supported by the U.S. Department of Energy, Office of Science, Materials Science and Engineering Division. Lithography was carried out at the Center for Nanoscale Materials, an Office of Science user facility, which is supported by DOE, Office of Science, Basic Energy Science under Contract No. DE-AC02-06CH11357.

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Abstract

Proton Momentum Distributions in Strong Hydrogen Bonds in the Solid State †

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Neutron Compton scattering (NCS) is a unique experimental technique made possible by the development of epithermal neutron sources, such as the ISIS source of the Rutherford Appleton Laboratory in the UK [1,2]. Dynamic structure factors, measured in NCS, are solely determined by the nuclear momentum distribution (NMD). In the picture of purely classical nuclei, the NMD shape is determined by whole energy spectrum of the motional modes, including translational and rotational modes, followed by lattice and internal molecular vibrations. However, more and more experimental evidence has been accumulated over the years that nuclear quantum effects, such as nuclear zero point motion, delocalisation and tunnelling, determine the shapes of NMDs of lightweight isotopes such as protons and deuterons. At sufficiently low temperatures, all nuclear quantum systems are cooled down to their ground states. In this low-temperature limit, the NCS recoil peak shape for a given nucleus is proportional to the square of the absolute value of its nuclear wave function, which is dictated by the shape of the local, effective Born-Oppenheimer (BO) potential [1,2]. Furthermore, different shapes of the BO potentials can be selected by applying Bayesian approach to fitting data obtained from an NCS experiment [3]. Such statistical tests can detect traces of self-interference of a nuclear wave function in effective BO potentials, a prerequisite of nuclear quantum tunnelling in condensed matter systems.

Molecular crystals exhibiting strong hydrogen bonds seem as natural fit for the NCS technique. In this contribution, the results of recent NCS investigation of the solid solutions of equimolar water-phosphoric acid mixture and its deuterated counterpart, will be presented. The analysis of the NMDs, augmented with Bayesian inference methodology, reveals line-shape features characteristic for proton tunnelling in the water-H_3PO_4 mixture below 160 K but shows no such features in the case of the deuterated water-D_3PO_4 mixture. Taken together, these observations suggest the existence of the so-called tunnelling effect in the kinetics of the proton transfer below 160 K, most likely involving concerted proton tunnelling along Grotthuss chains. It is the interplay between the amount of the ZPE and the height of the activation barrier for the proton transfer, which in consequence leads to a non-trivial nuclear quantum isotope effect, whereby kinetic rate constants of protons are orders of magnitude higher than those for deuterium. The presented methodology paves the way for a novel experimental screening protocol for the presence of the signatures of nuclear quantum tunnelling in condensed matter systems.

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Abstract

Investigation of High Pressure Phase Transition by Means of Infrared Spectroscopy in the Cairo Frustrated Pentagonal Magnet $Bi_2Fe_4O_9$ †

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$Bi_2Fe_4O_9$ is a common by-product in the synthesis of the multiferroic compound $BiFeO_3$ and has been claimed itself to display multiferroic properties [1]. The lattice formed by the two different sites of four iron Fe^{3+} magnetic atoms is quite remarkable as it materializes the first analogue of a magnetic pentagonal lattice [2]. For its peculiar lattice geometry it has attracted interest in the field of geometrical frustration. At room temperature and atmospheric pressure, the crystal structure is orthorhombic within the *Pbam* space-group and the compounds undergoes a magnetic phase transition at 238 K from a paramagnetic state toward a non collinear magnetic state characterized by a propagation vector k = (1/2, 1/2, 1/2) and a large degree of frustration ($\theta_P/T_N \sim 7$) [2]. Recently it has been shown that $Bi_2Fe_4O_9$ undergoes a structural transition under pressure at 6–8 GPa toward the maximal non-isomorphic subgroup *Pbnm*, with $c' = 2c$. The driving force of the phase transition is the displacement of the O1 oxygen atom from fully constrained Wyckoff position *2b* to a less-constrained *4c* one [3]. Previous studies have reported the investigation of dynamical properties by mean of Raman spectroscopy both at ambient condition and at high pressure in a diamond anvil cell [3,4]. However, the vibrational modes involving O1 oxygen atoms are not Raman active but infrared active.

We will report the first polarized infrared spectroscopy measurement of $Bi_2Fe_4O_9$ performed in a DAC from 1 to 20 GPa in the far-infrared range [60–800 cm^{-1}] and at low temperature. The measurements have been performed at the AILES beamline of synchrotron SOLEIL exploiting the high-pressure/low-temperature set-up [5] coupled with the high brilliance of the radiation source in a wide spectral range on a very thin sample (~50 μm) placed between diamonds with culets of 500 μm diameter. From our high quality spectra, we are able to identify the B_{3u} and B_{2u} modes within the (ab)-plane. Interestingly, while all phonon frequencies increase with pressure, the phonon mode around 200 cm^{-1} undergoes an anomalous softening with increasing pressure. In order to assign the phonon modes and reveal the microscopic mechanism of the high-pressure transition we also have performed DFT calculation at different pressures. The calculation mostly accounts for the measured phonon modes allowing the assignation of atomic motions.

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Abstract

Vibrational Properties of *Closo*–Borane Anions in Superionic Conductors †

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Metal closo-borate compounds have attracted recent attention as superionic lithium or sodium conductors. In $Na_2B_{12}H_{12}$ or $Li_2B_{12}H_{12}$ the superionic phases are related to the temperature induced phase transitions [1]. Modification of the crystal structure or ion substitution provide the means of tuning their cation conductivity. Spectroscopic fingerprint of internal *closo* anion ($B_{12}H_{12}^{2-}$) vibrations provides unique opportunity to study influence of such modification in the crystal properties. Dynamical fingerprint of anion vibrations is related to the nature of cation–anion interactions.

We report on theoretical calculations of the change of IR and Raman modes of $B_{12}H_{12}$ structure upon deformation along the high symmetry axes as well as interaction of such anion with model configuration of cations. These anions are aromatic structures and even smallest deformations are related to changes in B–H stretching frequencies of entire structure. Deformation is related to change of the electronic structure that extends over entire anion, Figure 1. Our systematic studies of anion dynamical properties are confronted with experimental evidence of Raman modes and cation conductivity.

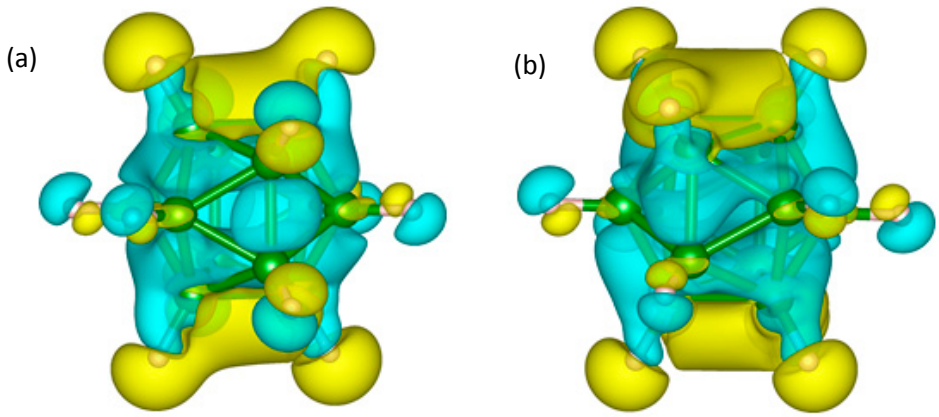

Figure 1. The charge density difference of $B_{12}H_{12}$ *closo* anion deformed along C_3 symmetry axis (**a**) and C_2 axis (**b**). Yellow colour is for charge accumulations, cyan–charge depletion. Yellow balls are for colour, grey–hydrogen.

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Abstract

Dimensionality Effects and Phase Transition Dynamics in Spintronics Materials as Seen by X-ray Electron Spectroscopies †

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Hole-doped rare-earth manganites, like $La_{0.66}Sr_{0.33}MnO_3$ (LSMO), display peculiar phenomena such as colossal magnetoresistance and half-metallicity, originating from the competition between charge, spin, and orbital order parameters [1]. Optimally doped LSMO thin films can be used to realize fully spin polarized currents (the spin polarization at the Fermi level reaches about 100% for $T<T_{Curie}$ [2]), a feature which, combined with the ferromagnetic order that persists up to about 350 K [3] renders such system a most technologically attractive material for spintronics. Hard X-ray PhotoElectron Spectroscopy (HAXPES) extends the probing depth of PES to the bulk of the solid (tens of nm), and therefore does not suffer of the modification induced by the surface electronic relaxation, revealing specific bulk-only features responsible of electron and metallic properties [4,5]. Furthermore, pump-probe HAXPES experiments reveal spin-dynamics extending up to several hundreds of picoseconds after the IR pumping [6,7]. By comparison with all-optical techniques we are able to attribute the observed quenching to a collapse of magnetic order related to double exchange and half-metallicity of the system [6,7].

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proceedings

Abstract

Advanced Diffusion Strategies for Junction Formation in Germanium †

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The investigation of innovative dynamical processes for the fabrication of highly doped and high quality Ge layers is currently a hot topic in many applicative fields such as nanoelectronics, photonics and radiation detectors. Challenges that require a deep physical and material science investigation are: (i) the high electrical activation in narrow region that can be obtained by out of equilibrium processes but has not to introduce lattice damage that may deteriorate the electrical properties. High concentration of the active dopant may transform germanium in a plasmonic material for sensor applications, or in an optical active material thanks to the direct gap transition that occurs at high doping and high strain. (ii) The control of the amount of doping at nanoscale (deterministic doping) is fundamental to meet the request of nanodevices production. Traditional methods as ion implantation are difficult to manage due to statistical fluctuations. In particular, this task has to be solved in germanium to exploit such material as a high mobility material in nanoelectronic. (iii) The preservation of the material purity during doping processes is a relevant problem especially when high purity germanium (HPGe) is used for gamma detector for nuclear spectroscopy and gamma imaging applications.

In this talk we will present some example of our recent research on germanium to contribute to the above challenges. Molecular doping process i.e., the production of monolayer self- assembled source of dopants on the devices surface is a promising way toward deterministic doping. We recently investigate the use of both P and Sb monolayer to this aim [1,2]. The effectiveness of such monolayers as diffusion sources is investigated. A very promising way to obtain very high doping is pulsed laser melting (PLM), this is a highly out equilibrium process that melts the extreme surface of the crystal and allows for dopant diffusion into the melt and its incorporation during fast regrowth. The application of this method to Ge allows for record activation of the dopants. Finally, we investigated the contamination induced by this laser process in the bulk of the material and we understood that it is a very promising method for doping of HPGe making possible fast and cheap processing for next generation gamma detectors [3,4].

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Abstract

A New Beamline for Advanced Photoelectron Spectroscopy Based on Extreme Ultraviolet High Harmonics at High Repetition Rate †

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Spectroscopy in the femtosecond time domain can both reveal fundamental insight in the properties of materials and provide relevant experimental tests for functional systems. The quest for sources of ultrashort photon pulses (~100 fs) in the Extreme Ultraviolet (EUV) region operating with an adjustable repetition rate up to the MHz range has led, in this last years, to the development of high harmonic generation (HHG) coherent sources based on table-top lasers. In particular, a comprehensive characterization of the photoelectron final state in ordered solids requires measurement, with a sub- picosecond time resolution, of energy, momentum and spin-polarization of the photo-emitted current, with an energy and a momentum resolution comparable to those achieved using advanced synchrotron radiation sources.

We have built and characterized a versatile twin-beamline for advanced photoemission experiments based on a table-top laser HHG source operating in the EUV range up to 200 kHz repetition rate. The beamline is able to provide 10^{12} photons/sec in the range 15–35 eV, and 10^{9} photons/sec up to 75 eV, with variable repetition rate, allowing one to measure shallow core level photoemission spectra in combination with valence band ones.

Experiments on metal and topological insulator have been performed to test the capabilities of the beamline, showing a pulse duration shorter than 100 fs and an energy resolution lower than 35 meV. The possibility to choose the optimal repetition rate for a given experiment (up to at least 200 kHz, or lower) makes it possible to explore a wide excitation-fluence range in pump-probe experiments, minimizing sample heating when relevant.

The twin-branch beamline operates as a user's facility. It represents a unique instrument for dynamical "all resolved photoemission experiments" to study excited states and transient electronic and magnetic configurations at surfaces, nanostructures and solids, with the possibility of covering the full Brillouin zone of complex materials.

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Abstract

Reciprocal Relation between Spin Peltier and Spin Seebeck Effects †

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In recent times, the interaction between magnetization and heat currents in a magnetic material has gained a renewed interest thanks to the observation of the spin Seebeck effect (SSE) [1,2]. The SSE is the spin counterpart of the Seebeck effect that corresponds to the generation of a pure magnetization current in a magnetic insulator as consequence of a thermal gradient. This is electrically detected by means of the inverse spin Hall effect [3], that rises in a high spin orbit coupling heavy metal deposited on the magnetic insulator. Equally to the ordinary thermoelectricity, the SSE has its reciprocal effect that is the spin Peltier effect [4,5]. In this work we provide an experimental proof of the reciprocal relations between SSE and SPE [6,7] in a single bulk sample of yttrium iron garnet (YIG) covered by a platinum thin film. For both the SSE and the SPE experiments, we employ a measurement system designed for the detection of heat currents exchanged between the thermal reservoirs and the sample under test. The sample-specific value for the characteristics of both effects measured on the present YIG/Pt bilayer is $(6.2 \pm 0.4) \times 10^{-3}$ KA^{-1} at room temperature, that corresponds to the analogous for spins of the Thomson relation between thermoelectric effects.

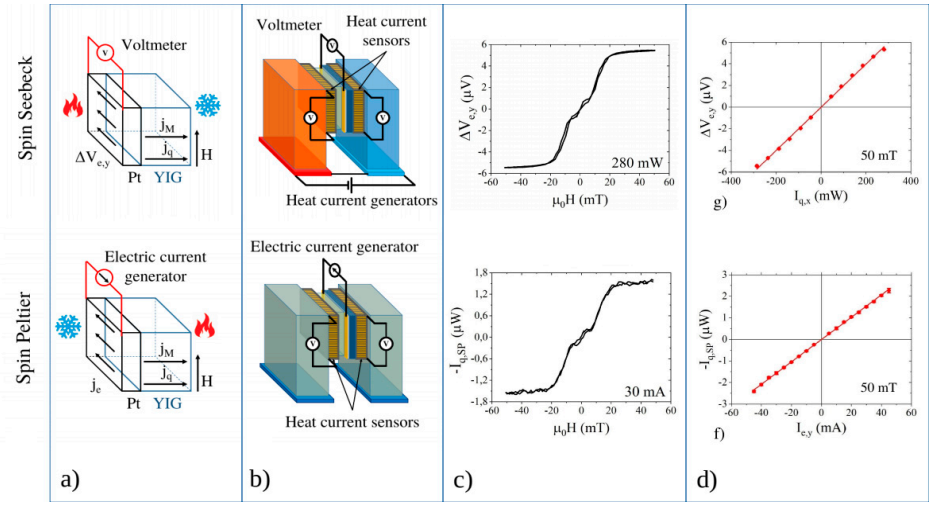

Figure 1. SSE and SPE heat-current-based measurements. (**a**) Schemes of the YIG-Pt device. (**b**) Sketches of the experimental setups. (**c**) Examples of SSE and SPE hysteresis loops. (**d**) Results at magnetic saturation of the SSE voltage as function of the heat current and SPE heat current as function of the electric current.

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Abstract

Measuring Interfacial Dzyaloshinskii-Moriya Interaction: A Review †

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Topology is known to stabilize rather exotic states in condensed matter and in magnetic materials. A recent example is the formation of particle-like excitations of continuous fields, as predicted by Skyrme. These so called skyrmions occur in presence of inversion symmetry breaking and indirect exchange, both favouring chiral magnetic structures via the Dzyaloshinskii-Moriya Interaction (DMI) [1,2]. Recently, the DMI received broad attention from the magnetism community as it was found to occur in systems appealing for spintronic applications composed of a heavy metal (HM) layer and an ultrathin ferromagnetic (FM) film with perpendicular magnetic anisotropy (PMA). Here the inversion symmetry breaking is induced by the interface and the exchange interaction is mediated by the spin-orbit coupling in the HM layer. Chiral domain walls and skyrmions are emerging as promising information carriers for future spintronic technologies, as they can be driven by electric currents with an unprecedented level of efficiency [3]. A measure for the stability of chiral magnetic structures and the strength of the DMI is the related energy coefficient D [2]. Although DMI-based phenomena have created an extremely active research field, an established and reliable method to measure D is still lacking. As a matter of fact, a lot of disagreement is currently present in the literature, especially regarding measurements of small DMI ($D < 0.5$ mJ/m^2). Not only different measuring techniques are found to provide contradictory values for D, but controversies are also present when utilizing the same method on nominally identical stacks. We present here a review of interfacial DMI measurements, considering not only the different measurement techniques as domain wall based [4,5] and spin wave based [6] measurements, but also different compositions of the stacks investigated (e.g., FM: Co, CoFeB; HM: Pt, Ta, Ir, W). We try to clarify the differences of the various techniques describing their advantages and limitations and define a set of rules to be able to compare the data, quantitatively define the role of HM layer, considering its thickness, the production methodology, the annealing, etc. We also aim to introduce a standard coordinate system for the experimental quantities in order to define uniquely the sign of D.

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Abstract

Incoherent Scattering Reduction in Crystals †

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Despite the large strength of the coherent effects of particle deflection and radiation in crystals, all their applications are essentially limited by the incoherent scattering process. Though the difference of the latter from the scattering process in amorphous media was, in fact, envisaged by both the x-ray diffraction and coherent bremsstrahlung theories, the relational effect of multiple scattering reduction in crystals is scarcely known, has not been clearly observed, despite some attempts, and is usually missed in interpretation of the abundant experimental data. At the same time, this effect is presently important for the problems of particle deflection by long crystals, for both channeling and crystal undulator radiation, etc., and needs to be implemented in theory.

Since multiple scattering reduction arises in crystals due to correlations of particle collisions with the strings or plane atoms, it can be observed at any high energy in the wide angular regions. At the same time, this effect can be clearly observed only under the rear conditions of any coherent scattering effect complete suppression. To reveal the latter, we applied the quantum Born approximation theory, being also equivalent to the classical one in straight trajectory approximation, and found a particular conditions of 1 GeV particle incidence at the angles of 2 degree and 3 mrad with respect to the ‹001› axis and (110) plane of Si crystal, respectively, making possible to observe the multiple scattering reduction under the complete absence of coherent scattering, as Figure 1 illustrates.

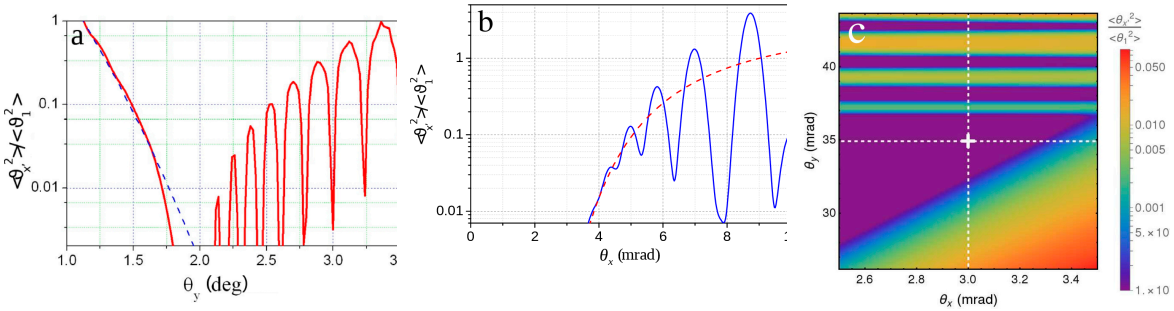

Figure 1. Dependence of multiple scattering mean square angle on in incidence angle θ_y w.r.t. the Si ‹001› axis at $\theta_x = 3$ mrad (**a**); on that of θ_x w.r.t. the Si (110) plane at $\theta_y = 34.9$ mrad (2ϵ) (**b**) and on both θ_x and θ_y (**c**), in units of ‹θ_1^2›, corresponding to the maximum incoherent scattering reduction.

To treat the effect of multiple scattering reduction in general case, one has to abandon Born approximation, preserving at the same time a quantum treatment of the particle scattering by separate crystal atoms. Applying the Wigner function approach, we introduced accordingly some new quantum incoherent particle scattering treatment, applicable on a classical trajectory [1].

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Abstract

Potential of Parametric X-rays for Application in Particle Identification Detectors †

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Cerenkov counters and transition radiation detectors are particle identification detectors (PID) used in many HEP experiments [1,2]. Study and development of new accelerator facilities such as Future Circular Colliders (CERN), NICA (JINR) and others formulate new needs for particle identification in conditions of very high energies and luminosities. Parametric X-rays (PXR) [3] have big potential to be applied in particle identification detectors as radiation mechanism combining many properties of Cerenkov radiation and transition radiation in high kinematics range $\gamma > 1000$. PXR mechanism well developed to date, both theoretically and experimentally. Many experiments were performed with electron beams. Key experiment with first observation of PXR from 70 GeV protons was reported in [4]. Later, PXR has been studied with 5 GeV protons and 2.2 GeV/u carbon nuclei in a silicon crystal on the external beams of the Nuclotron at JINR [5] and with 400 GeV/c protons in bent crystals at CERN SPS [6].

So, we may state, that the community reached good understanding of the PXR properties by now and it is ready for the feasibility study of PXR application in particle identification. In contribution we will present and discuss characteristic features of PXR potentially applicable for PID including time dependences as timing requirements are of high importance for future colliders due to their increased collision rates. As first step for PXR application for high energy particle detection, implementation of PXR simulation tool to the GEANT4 toolkit can be proposed.

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Abstract

Channeling Experiments at the Mainz Microtron MAMI †

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The electron accelerator MAMI is multilevel racetrack microtron with a beam energy from 180 MeV up to 1.6 GeV and a continiuous beam current of more than 20 μA. The excellent beam quality due to the low emittance in transveral and longitudinal direction is well suited for channeling experiments and related radiation investigations.

The possibility to produce undulator-like radiation in the hundreds of keV up to the MeV region by means of channeling in periodically bent crystals is well known (see [1] for a review). The usual schemes of making crystalline undulators involve some method of bending the planes or axes of the crystal, altering the usual channeling. One scheme, the large-amplitude, large-period, bends the planes such that the bending amplitude and period of the planes are significantly larger than the amplitude and period of the channeling motion. A second scheme consists of having a short-amplitude, short-period configuration. The bending of the planes only slightly perturbs the channeling motion trajectory, leading to increased radiation emission at higher photon energies than the usual channeling radiation.

In recent years, experiments have been carried out at MAMI to investigate the radiation emission of channelled electrons in periodically bent silicon and diamond crystals. The results will be discussed for several epitaxially grown strained layer $Si_{1-x}Ge_x$ crystals and boron doped diamond crystals at electron beam energies between 270 and 855 MeV.

Funding: Work supported by the European Commission (the PEARL Project within the H2020-MSCA-RISE-2015 call, GA 690991).

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Abstract

Colloidal Quantum Dots for Low-Power-Consumption Semiconductor Gas Sensors †

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Gas sensors are becoming increasingly important for the safety and quality of human life. In the past decades, semiconductor gas sensors employing high-temperature ceramics technology have been intensively investigated, and higher sensitivity as well as selectivity have been achieved. Silicon-based micro-electro-mechanical system (MEMS) hotplates have also been utilized to reduce both the volume size and power consumption of semiconductor gas sensors. Colloidal quantum dots (CQDs) possess a highly sensitive and programmable surface, combined with excellent solution processability, which make them ideal building blocks for next-generation gas sensors compatible with silicon-based or flexible substrates. Through the controllable synthesis with the surface and interface engineering strategy of CQDs, we have demonstrated sensitive and selective semiconductor gas sensors with lower power consumption based on metal sulfides [1,2] and oxides [3,4], respectively. In addition to traditional rigid substrates including ceramics and Si-based MEMS hotplates, soft substrates, being flexible and stretchable, were successfully used for CQD gas sensors, which may open up a powerful new degree of freedom for semiconductor gas sensors being more intelligent and integratable.

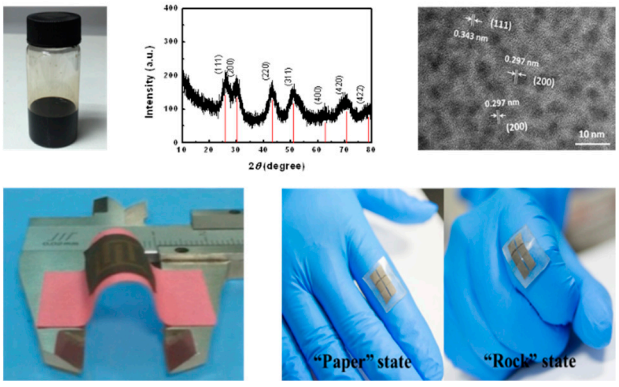

Figure 1. Colloidal quantum dots for low-power-consumption semiconductor gas sensors. Reproduced with permission from Huan Liu; *Physically flexible, rapid-response gas sensor based on colloidal quantum dot solid* [1] and *Fully stretchable and humidity-resistant quantum dot gas sensors* [2]; published by Wiley (2014) and the American Chemical Society (2018), respectively.

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Student Communications

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Abstract

Non-Debye vs. Debye Dielectric Relaxation: How Does Memory Effect Arise? †

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The Debye model presents an essential and elegant description for the relaxation phenomena based on statistical mechanics. However, this model describes systems characterized by a single relaxation time as perfect liquids and crystals, quite far for the complexity which affects almost all amorphous and glassy materials.

The Debye model has been used as a starting point for other dielectric relaxation theories, named non-Debye (or anomalous) relaxation models, as for example the Havriliak-Negami relaxation model.

All these models show a power law decay behaviour for the response function as experimentally proved. A useful and powerful mathematical tool for investigating this behaviour is the fractional calculus.

The present study deals with a novel approach involving a fractional generalization for the time and frequency variables.

This approach allows us to generalize the Debye's idea to more complex systems addressing the problem from another point of view complementary to the well-known one ruled by fractional calculus.

In particular this method examines the time-domain response function defined in terms of a Gamma distribution. The complete monotonicity of the pulse response function follows directly from our investigations.

Moreover, this method encourages the emergence of the fading memory effects as an intrinsic feature of these complex systems due to the presence of the Gamma distribution.

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Abstract

Ab-Initio Study of the Electron-Phonon Interaction of a Single Fe Adatom on the MgO/Ag(100) Surface †

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Controlling the magnetic moment of individual atoms is a technologically important challenge, with applications as high density storage devices. Breakthrough experimental studies have recently shown that it is possible to create stable magnetic quantum states in individual adatoms [1–3]. While the role of electronic interactions on the magnetic stability has been thoroughly investigated theoretically [4–6], the coupling with phonons has attracted much less attention. The aim of this work is to study, via ab-initio calculations, the effect of the electron-phonon interaction (EPI) in Fe adatoms deposited on MgO/Ag(100), a benchmark system where the EPI is believed to determine to large extent its magnetic stability [3]. Here we present the calculated electronic structure and vibrational dynamics of this system, including the local vibrations of the adatom. Furthermore, we analyze the effect of the EPI on the magnetic stability via the renormalization of the electronic properties of the adatom.

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Abstract

Efficient Calculation of Anisotropic Fermi Surface Problems through Helmholtz Fermi Surface Harmonics †

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In metals, the details of the Fermi surface and the magnitude of the matrix elements connecting different points defined on it determine most of their transport properties, which are limited by the electron-phonon coupling and the scattering by impurities. Typically, the calculation of an anisotropic physical property defined on the Fermi surface, say in an impurity or Boltzmann transport problem, requires the consideration of several thousands of points on the surface. In contrast, the Helmholtz Fermi Surface Harmonics (HFSH) technique allows us to accurately treat these problems considering few elements of the HFSH set.

Here we introduce the recent developments we have implemented in this direction, including the symmetry treatment and the derived selection rules. We also show a representative benchmarking list of examples, illustrating the potential of this method.

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Abstract

Tuning the Fast Dynamics of PNIPAM-Based Systems with Bio-Cosolvents †

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Smart polymers as poly-N-isopropylacrylamide (PNIPAM) are well known due to their fast response to variations of parameters like temperature, pH, and pressure. PNIPAM phase behavior results from the competition between hydrophobicity of methyl and methylene groups and the ability of amide groups to make strong hydrogen bonds. When the temperature increases above a lower critical solution temperature (LCST) ~32°C, molecular agitation disrupts hydrogen bonds and leads to a coil-to-globule transition which is reminiscent of the *folding transition* of proteins. Different environments can impact on this delicate balance between hydrophilic and hydrophobic interactions and strongly affect the LCST [1], in the same way that the addition of cosolvents can lead to stabilization or denaturation in protein folding. Interestingly, these are not the only thermodynamic conditions in which there are analogies between protein and PNIPAM behaviors. The onset of anharmonic dynamics on the picosecond scale observed at ~250K in concentrated PNIPAM samples has been recognized as an analogue of the protein *dynamical transition* [2]. As in proteins [3], it is interesting to observe how different solvents can change the features of this intriguing phenomenon. We use a multi-technique approach to study how different solvent mixtures can affect the dynamics of PNIPAM-based systems under different thermodynamic conditions. The use of Raman and IR spectroscopy is well suited to investigate the role of protic and aprotic cosolvents in the changes in hydration state of PNPAM across the LCST, while neutron scattering techniques give access to information on the effect of protein stabilizers on the PNIPAM "dynamical transition".

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Posters Presentations

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Abstract

The Structural Origin of Composition-Driven Magnetic Transformation in $BiFeO_3$-Based Multiferroics †

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Perovskite-like compounds are widely known as model systems for studying the relationships between crystal structure and physical properties. Among them, magnetically-ordered ferroelectric oxides have attracted much attention in recent years. Such materials combine spin and electric dipole ordering in the same phase, thus providing the technologically important possibility to control magnetism with an electric field. While $BiFeO_3$ is the most thoroughly studied magnetic ferroelectric compound, the properties of its solid solutions remain a matter of intensive debate. In this work we show how variation in the chemical composition of $Bi_{1-x}AE_xFe_{1-x}Ti_xO_3$ (*AE*= Ca, Sr, Ba) multiferroics affects their crystal structure and magnetic behavior. The polycrystalline samples have been studied by X-ray diffraction, neutron powder diffraction, VSM-magnetometry, electron microscopy, and scanning probe microscopy techniques. It has been found that Ca/Ti and Sr/Ti substitutions suppress the cycloidal antiferromagnetic structure specific to the parent compound, thus stabilizing a weak ferromagnetic and ferroelectric state. The Ba/Ti-doped solid solutions retain the magnetic behavior characteristic of the pure $BiFeO_3$. The composition-driven changes in the magnetic properties of the $Bi_{1-x}AE_xFe_{1-x}Ti_xO_3$ perovskites correlate with the structural evolution, confirming the existence of a tight coupling between the type of magnetic ordering and electric polarization/magnitude of oxygen octahedra tilting in these materials. The magnetostructural correlations reflect the pattern of chemical substitution-induced changes in the polarization- and oxygen octahedra rotation-related components of the Dzyaloshinskii-Moriya interaction affecting the magnetic structure. The investigation sheds light on the conditions favoring the coexistence of spontaneous magnetization and polarization in $BiFeO_3$-based multiferroics.

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Abstract

Magnetic Ordering of Three Thiosemicarbazonecopper(II) Complexes †

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During the last decades, metal-organic compounds constitute an active field of research, and among them, complexes that combine thiosemicarbazone ligands with copper(II) are appealing from the point of view of material science due to their interesting structural and magnetic properties [1]. Complementary, they are also extensively studied due to biological and pharmacological applications that rely on their rich coordination and redox chemistry [2].

We present a first principles density-functional theory calculation of three thiosemicarbazone copper complexes: [{CuLX}$_2$], with X = Cl, Br and I (Figure 1). All of them crystallize in isomorphous triclinic structures that contain one dimer per unit cell [3,4]. In order to study their magnetic structure, we have calculated the energies for the ferromagnetic and all the antiferromagnetic orderings compatible with a supercell containing 2 × 2 × 2 crystallographic unit cells (Figure 2). Results show that energy differences between the most stable structures for each X halide are very small (several meV/dimer/), and as a consequence, the ground state cannot be assigned unambiguously to a single ordering, any of the low energy structures being a valid candidate for the ground state.

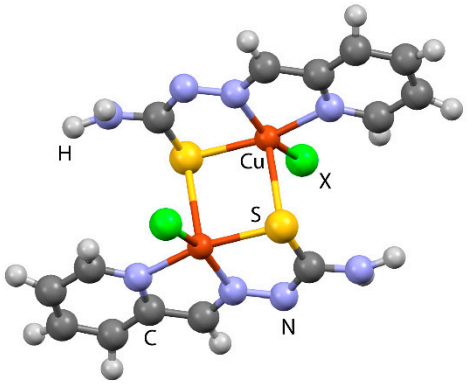

Figure 1. [{CuLX}$_2$] complex.

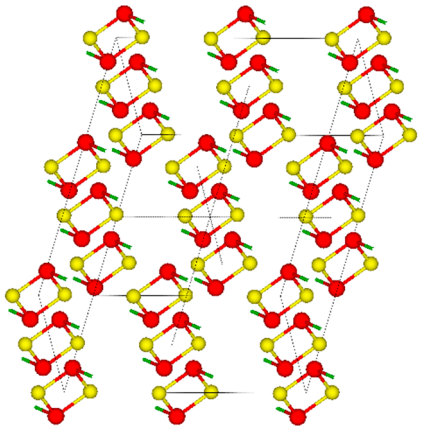

Figure 2. Schematic view of the supercell. Only Cu and S atom are showed.

We have also evaluated the magnetic exchange interactions by mapping the calculated energies of all the magnetic orderings to the Ising model taking into account couplings between the first and second neighbours. It can be concluded that the competition between ferro/antiferro and intra/interdimeric interactions is the origin of the complex magnetic energy landscape present in these materials.

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Abstract

Radioisotope Production through Accelerators in Crystalline Targets †

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Abstract: The production techniques of radioisotopes for medical purposes is a valuable and important field in nuclear medicine. In particular, the expensive cost of the prime materials for the production via cyclotron obliges the search for new solutions to enhance the production rate with minor upgrades of the current instrumentation. Oriented ordered structure can modify particle trajectories inside a medium leading to a sensible variation of the interaction rate with atomic nuclei. Under specific orientations of the target with respect to the incident beam, the probability of inelastic interaction with nuclei can be enhanced with respect to the standard rate. This effect is called anti-channeling and leads to an increase of the radioisotope production yield. A dedicated set of experimental measurements were carried out at the CN accelerator of the INFN Legnaro Laboratories to investigate nuclear reactions under channeling experiments. In particular, the production of the Arsenic-74 radioisotope through a proton beam delivered to a natural single-crystal Germanium target was monitored via γ-spectroscopy of the prompt γ-rays upon de-excitation of produced nuclei, in order to quantify the production rate variation as a function of the incident angle.

1. Introduction

The current wealth of radioisotopes has been made possible especially through nuclear reactors. This allowed the development of several applications in modern nuclear medicine, biology, and other fields. At the same time, great efforts have been made for the development of accelerators devoted to the production of radioisotopes [1]. Indeed, production through accelerators is spreading worldwide, despite its higher cost with respect to the production via nuclear reactors, due to some advantages such as the high specific activity that can be obtained through the (p,xn) and (p,α) reactions, the smaller amount of radioactive waste, and the possibility to produce radioisotopes very close to hospitals in compact facilities.

In this contest, the research of new technological solutions to obtain a more efficient radioisotope production is of special interest. One possible way to improve production efficiency with a minor upgrade of the existing technology is the usage of a crystalline target. Indeed, ordered and oriented

structures, such as crystals, can modify the trajectories of incoming beam particles interacting with them. Compared to the motion into an amorphous medium, ions interacting with a crystal are subject to coherent interactions due to the periodicity of the atoms in the crystalline structure. This phenomenon is capable of modifying particle trajectories inside the medium, causing the variation of the interaction rate with the atomic nuclei.

An interesting effect can be observed when charged particles enter a crystal at an angle close to the critical angle for channeling θ_C with respect to an atomic plane [2] ($\theta_C = \sqrt{U/E}$, which depends on the interplanar potential well with depth U, and the particle energy E). In such a case, almost all the beam particles, even those entering in the middle of two planes, undergo a motion above the maxima of the potential barriers, where the nuclei of the lattice atoms are located, thus resulting in a higher probability of interaction with nuclei with respect to the motion into an amorphous medium with the same density [3]. In particular, the enhancement of the $^{18}O(p,\alpha)^{15}N$ reaction obtained with protons at 642.5 keV (i.e., just above a sharp resonance at 628 keV) impinging a Al_2O_3 crystal has been observed through a dedicated experiment performed at the INFN-Legnaro Laboratories [4]. This result suggested the development of a crystalline target for the production of radioisotopes of interest for medical applications. In this paper, a measurement of the enhancement of the production of the Arsenic-74 isotope, which is used in tumor imaging [5], via the $^{74}Ge(p,n)^{74}As$ reaction in antichanneling condition, is shown.

2. The Experimental Setup

The LNL-CN is a Van Der Graaf electrostatic accelerator with a maximum voltage terminal of 5.5 MV, thus being ideal for investigating nuclear reactions in the first layers of a material. As shown in Figure 1, a rectangular Ge sample (10x10x1 mm, with the main surface oriented along the (111) crystallographic planes) is installed onto a goniometer with angular resolution of 0.01° and a minimum pressure inside the chamber of approximately 10^{-7} mbar. This goniometer allowed the alignment of the crystal axis with respect to the incoming beam, to study the transition from channeling to antichanneling condition. Beam divergence and goniometer resolution—both of the order of 0.01°—are perfectly suitable for channeling studies at these energies, taking into account that θ_C for channeling between Ge (100) planes for 4 MeV protons is of the order of 0.2°.

The alignment of the samples was done through a silicon detector for Rutherford Backscattering analysis (RBS), i.e., by measuring the backscattered particles as a function of the angle between the beam and the samples. The RBS detector was placed at 115 mm and at an angle of 160° from the target. A HPGe detector was placed outside the chamber in order to measure the prompt γ-radiation emitted by the target during the irradiation with the proton beam.

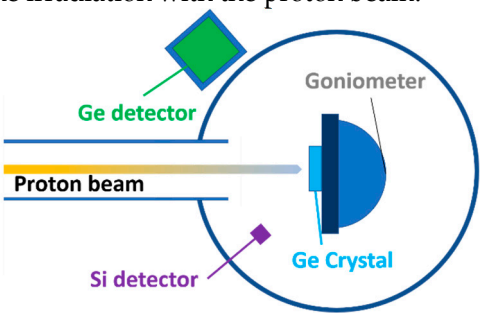

Figure 1. Experimental setup. A proton beam is delivered by the LNL-CN accelerator to a germanium single crystal installed onto a goniometer. Backscattered protons are detected through a silicon detector, while the γ-radiation is measured through a HPGe detector.

The beam energy was set at 3.80 MeV, i.e., a value slightly above the threshold of production of the Arsenic-74 radioisotope through the $^{74}Ge(p,n)^{74}As$ reaction, in order to confine the production of the radioisotope in the first few micrometers of thickness of the target, where the antichanneling effect is concentrated. The amount of ^{74}As produced can be determined by considering the prompt γ-rays

from the low-lying excited states of the ^{74}As in the measured γ-spectra. The scheme of the nuclear reaction and of the γ-radiation studied is shown in Figure. 2

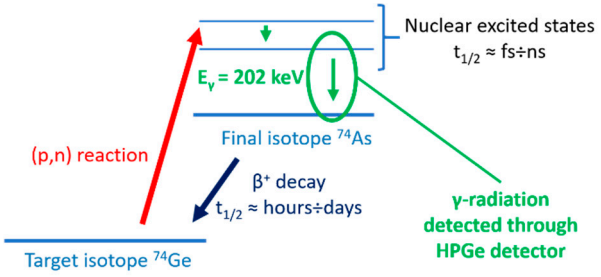

Figure 2. Scheme of the nuclear reaction studied. Prompt γ-radiation from the low-lying 202 keV state of ^{74}As is measured through the HPGe detector to determine online the ^{74}As production rate.

3. Results

Firstly, the threshold energy for protons for populating the low-lying excited levels of Arsenic-74 was determined. For this purpose, measurements of the γ-spectra for a proton beam at different energies (3.75, 3.80 and 3.85 MeV) were performed. In particular, by looking at the integral of the γ-peak at 202 keV (see Fig. 3b, as an example, the γ-spectrum for protons at 3.80 MeV) emitted by the excited ^{74}As we extrapolated a threshold energy E_{Th} = 3.72±0.01 MeV. This result allowed to find the maximum depth for the production reaction through protons incident at E_{In} = 3.80 MeV by means of a simulation of the energy loss of protons into germanium via SRIM software, obtaining a depth $d_{Th, Ein=3.80\ keV}$ = 2.75±0.05 μm. Then, those protons which suffer backscattering into the target as they are at the threshold energy, will reach the Si detector having an energy of $E_{Th,RBS}$ = 3.44±0.01 MeV. As shown in Fig. 3(a), after finding the alignment for axial channeling condition in which backscattering is at its minimum (black line), a comparison of the integral of the RBS spectra above the $E_{Th,RBS}$ energy shows an enhancement in backscattering efficiency in antichanneling condition of 9.1±0.3% with respect to the randomly oriented case. At the same time, the integral of the 202-keV peak (see Figure 3(b)) shows that the production of the ^{74}As in antichanneling is increased of the 9.8 ± 0.6% with respect to the random case.

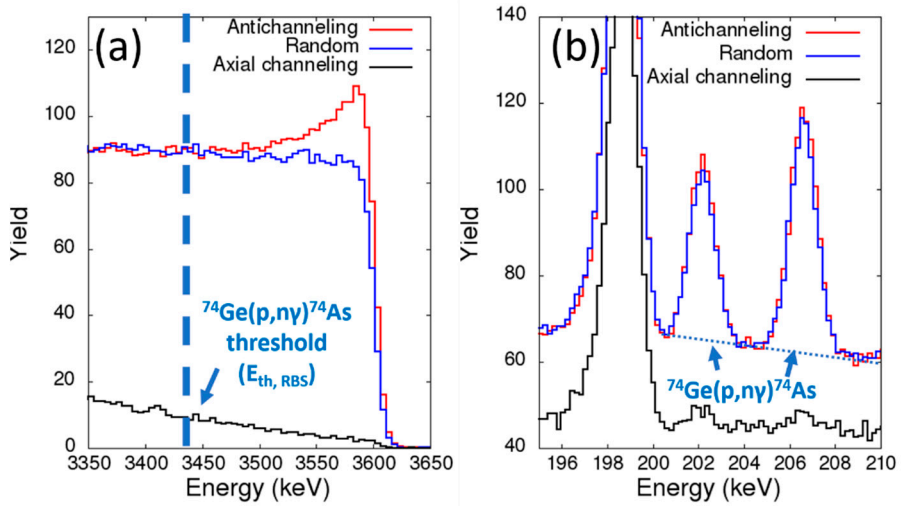

Figure 3. Rutherford Backscattering of protons incident at 3.80 MeV (RBS, a) and γ-radiation (b) measured online at different alignment conditions (antichanneling, random orientation, axial channeling). Yield is normalized to 1 μC of incoming protons.

4. Conclusions

In this work, the enhancement of the production of a radioisotope for medical applications due to the antichanneling effect is shown. The measurement was performed through γ-spectroscopy online, i.e., during the irradiation of the target with a proton beam, after performing the alignment of the target by means of the Rutherford Backscattering of the proton beam. In particular, the increase of the amount of backscattered protons above the reaction threshold in antichanneling condition with respect to the case of a randomly oriented target is found to be in good agreement with the enhancement of the production of the Arsenic-74 radioisotope, as one can observe looking at the 202 keV line in the γ-spectra. Both the effects are due to the higher nuclear density experienced by the beam particles undergoing the quasi-channeled motion. This result confirms the possibility to improve the production of radioisotopes for medical applications via antichanneling.

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Abstract

Manufacturing of Bent Silicon Crystals for Steering of Particle Beam at Ultra-High Energy Synchrotrons †

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Since the '70, physics of interaction between bent crystals and heavy particles (protons or ions) is investigated at various worldwide particle accelerators, driven by the possibility to use bent crystals as optical elements for steering or focusing charged particle beams.

Recent improvements in crystal manufacturing techniques, joined with a deeper understanding of the physics behind crystals-particle beams interactions lead to a discovery of numerous interactional effects appearing as crystal planes or axis are aligned to a charged particle beam. The technology readiness level is mature enough to allow the use of crystals even in the Large Hadron Collider (LHC) of CERN, where crystals are being experimented as primary collimators of the protons or ions circulating beam, and are suggested as core elements of fixed-target experiments. The crystals, that operates without the need of a power source, does not require a cryogenic environment and are extremely compact and lightweight, can represent a reliable alternative to the use of magnets or other optical elements in ultra-high energy and intensity particle modern particle accelerators.

The purpose of this work is describe manufacturing and characterization solutions of crystals suitable for installation in the LHC as primary collimators of the proton or lead ions circulating beams. Successful development of such crystals is based on a merging of ultra-modern technologies used in microelectronics, X-ray science, ultra-precise optical and mechanical machining. Availability of this innovative generation of crystals makes to envisage innovative possibilities for particle beam steering at ultra-high energy and intensities particle accelerators.

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Abstract

Structures, Optical and Mechanical Properties of PLA/ZnO SiO_2 Al_2O_3 Composite Elaborated by a Solvent Casting Method †

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Keywords: Polylactic Acid; ZnO; SiO_2 and Al_2O_3 powders; crystallinity; optical and mechanical properties

In this study, granulated polylactic acid and ZnO, SiO_2 and Al_2O_3 powders were mixed to form PLA/ZnO and PLA/ZnO SiO_2 Al_2O_3 composites with different concentrations using a solvent casting method. The influences of ZnO, SiO_2 and Al_2O_3 particles on the physical and mechanical properties of the PLA films were investigated. Chemical and crystal structures are characterized by FTIR-ATR, Crystallinity of PLA/ZnO SiO_2 Al_2O_3 composites are analyzed by X-ray diffraction techniques and Mechanical properties (tensile strength and young modulus) are determined by traction test. The result show an improvement of crystallinity of PLA composites compared of pure PLA and enhanced mechanical properties of module young value and tensile strength value that varied from 2.01 to 3.05 GPA and from 21, 67 to 28,92 MPa, respectively.

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Abstract

Structural, Morphological and Magnetic Properties of $Fe_{60-x}Co_x(Al_2O_3)_{40}$ Nanocomposite Coating Deposited by Thermal Spraying †

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Abstract: $FeCo/Al_2O_3$ nanoparticles thermal sprayed on a steel plate with different Co concentration from 0 to 20% by means of a thermal spraying process, $Fe_{60-x}Co_x(Al_2O_3)_{40}$ powder alloy was synthesized using planetary ball mill for different Co concentration at 20 h of milling. The aims of this work are to study the effect of Co concentration and milling time on the magnetic, structural behavior and mechanical properties of the $FeCo/Al_2O_3$ coating. Appearance of FeCo magnetic Solid solution phase after 20 h of milling, the crystallite sizes reduced from 18nm to 7nm and lattice strains increased from 0.36 to 0.56%, this variation are caused by the diffusion of Co atoms in iron lattice. For the coating, various phase of magnetic domains observed on surface by Atomic Force Microscopy (AFM), apparition the new phases, Al_2FeO_4 at 0%, $CoAl_2O_4$ at 5%, $CoFe_2O_4$ at 10% and CoFe at 20%. Saturation magnetization is max at 20 wt% of Ni and coercivity is min at 10 wt% of Co. Microhardeness and Young module were characterized by Nanoidentation techniques that shows an improvement in mechanical properties

Keywords: $FeCo/Al_2O_3$ nanostructured; mechanical alloying; thermal spray; MEB; AFM; DRX; VSM; Nanoidentation testing

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Abstract

Enhancement of Bremsstrahlung Radiation Generated by Electron Beam Interaction in an Axially-Oriented Scintillator Crystal (Poster) †

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Since their discovery, scintillator materials have played an important role in nuclear and particle physics, as well as in medical and industrial imaging. In particular, inorganic scintillator crystals are widely exploited for the realization of homogeneous electromagnetic (e.m.) calorimeters for high-energy physics (HEP) and astrophysics to measure the energy of $e^{\pm}$ and of γ-rays. Since for primary particles of multi-GeV or TeV energies the shower results to be ten or more radiation lengths (X_0) long, high-Z scintillator crystals with X_0 of about 1 cm have been introduced to realize compact calorimeters.

Despite these materials are crystalline, the lattice influence on the e.m. shower is usually completely ignored both in detector design and simulations. On the other hand, it is well known since 1950s that the crystal lattice may strongly modify the e.m. shower.

In this poster, we present an experimental investigation of the dependence of the e.m. radiation generated by a 855 MeV/c electron beam as a function of the alignment of a Lead Tungstate ($PbWO_4$) crystal with respect to the electron beam, passing from random alignment to axial alignment. The measurements, performed at the line MAMI-B (Mainz, Germany), demonstrated that in case of axial alignment the photon production increased with respect to the random-alignment case. This effect could be advantageously exploited to reduce the amount of scintillator material in future e.m. calorimeters and γ-telescopes [1].

The $PbWO_4$ scintillator crystal was also tested through hard X-ray at the ID11 and BM05 beamlines at the European Synchrotron Radiation Facility (ESRF) of Grenoble (France) to test its lattice quality. Indeed, the crystallographic perfection is mandatory to exploit axial effect for the enhancement of electron beam interaction in an oriented scintillator crystal.

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