INTERNATIONAL CONFERENCE

4 – 6 SEPTEMBER, 2017

FMS 2017

FRONTIERS IN MATERIALS SCIENCE

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Alfried Krupp Wissenschaftskolleg Greifswald

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Wissen lockt. Seit 1456

Aim of the conference

Aim of the conference is to bring together researchers from Europe and Asia with focus on Vietnam and Japan, as a communication platform to discuss novel fast emerging fields. Areas will be nanostructured materials for magnetism, spintronics and optics, photonic materials and computational materials science. The talks will cover the fields from nano-scale characterization to first-principles calculations. Special focus at Greifswald will be also given to novel techniques and the interdisciplinary field of nanotechnology and biophysics.

We hope you will enjoy the maritime atmosphere of the city old University City of Greifswald, historic name -Academia Gryphica-, University founded in 1456, the modern environment and support of the enjoyable and stimulating Alfried Krupp Kolleg within the center of the city.

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We thank the generous support by the Alfried Krupp Kolleg foundation
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Program „Frontiers in Materials Science FMS2017“

Sunday 3. September	
	Arrival

Monday 4. September	
9am- 10:30am	***Welcome*** *Session 1:* **Plenary Talks** Manganese-based Spintronics *Shigemi Mizukami (WPI Advanced Institute for Materials Research, Tohoku University)* Designing Quantum Spin-Orbit-Coupled Materials: A Source for Exotic States *Roser Valenti (Institut für Theoretische Physik, Goethe-Universität Frankfurt)*
10:30am- 11am	*Coffee*
11am- 12:30am *A and B run as parallel sessions!*	*Session 2 A:* **New methods from Nanoscale to Biology** Common Principles in Synthetic Mechanophores and Mechanoresponsive Biomolecules *Kerstin G. Blank (Mechano(bio)chemistry, MPI of Colloids and Interfaces, Potsdam)* Real-Time Deformability Cytometry: Spatiotemporal Polymer and Cell Response in Microfluidic Systems *Oliver Otto (ZIK HIKE, University of Greifswald)* Atomic Force Microscopy, What Else? *José L. Toca-Herrera (Institute for Biophysics, Dep. of Nanobiotechnology, University of Natural Resources and Life Sciences Vienna (BOKU))*
11am- 12:30am	*Session 2 B:* **Synchrotron Research** Inversion Symmetry Breaking by Oxygen Octahedral Rotation in A-site-ordered n=1 Ruddlesden-Popper Phases AA'TiO_4 (A=alkaline, A'=rare earth) and the cation size effects *Hirofumi Akamatsu (Dep. of Applied Chemistry, Kyushu University)*

	Comparison Between the Ultrafast Optical Responses and Ultrafast Structural/ Atom Dynamics in Novel Perovskite Solar Cell Prototypes *Simone Techert (Göttingen University)* Crystal Structure of Anion Changeable Layered Double Hydroxides by Synchrotron Radiation X-ray Diffraction *Chikako Moriyoshi (Graduate School of Science, Hiroshima University)*
12:30am-2:30pm	*Lunch*
2:30pm-4pm 2:30pm-4pm	*Session 3 A:* **Plasmonics** Plasmon Induced Photoemission from Individual Small Silver nanoparticles: Role of the Substrate *Ingo Barke (Institute of Physics, University of Rostock)* Direct Laser Writing of Plasmonic Nanostructures *Ngoc Diep Lai (Laboratoire de Photonique et Moléculaire, Université Paris-Saclay)* Looking for Synergies in Molecular Plasmonics by Hybrid Functional Nanostructures *Tobias A.F. König (Leibnitz-Institut f. Polymerforschung Dresden,Technical University Dresden)* *Session 3 B:* **Polymers and Molecules** Applications of 3D Lithography *Christian Denker (Institute of Physics, University of Greifswald)* Reticular Solids with Adamantane-type Building Blocks *Fabio Pichierri (Dep. Of Applied Chemistry, Tohoku University)* In situ Control of Solid-State [2+2] Photodimerization in the Molecular Crystal of a Cobalt Complex *Akiko Sekine (Dep. of Chemistry, Tokyo Institute of Technology)*
4pm-5pm	*Coffee and Poster Session*
5pm-6:30pm *C and D run as parallel sessions!*	*In Parallel Poster Session* *Session 3 C:* **Photocatalytic Nanomaterials** Photocatalytic Nanomaterials and their Applications *Nguyen Thanh Binh (Institute of Applied Physics and Scientific Instruments, VAST)*

5pm- 6:30pm	Structure-Activity Relationships for Quadrupole Perovskite Catalysts *Ikuya Yamada (Dep. of Materials Science, Osaka Prefecture University)* Novel Structural, Electronic, and Reactive Properties of Nano Ceramic Materials: Theoretical Study *Shin'ichi Higai (Murata Manufacturing Co., Ltd.)* *Session 3 D:* **Physics of Nanostructures** Magnetic Core-Shell Nanostructures *Huynh Dang Chinh (Hanoi University of Science and Technology, Ha Noi)* Phase Transitions in Ferroelectric Thin Films Described by Ising Model in Transverse and Longitudinal Fields *Cong Thanh Bach (Faculty of Physics, VNU University of Science)* Interplay of Magnetism and Dynamics in Graphene Nano-Flakes *Andreas Honecker (Laboratoire de Physique Théorique et Modélisation, Université de Cergy-Pontoise)*

Tuesday 5. September	
9am- 10:30am	*Session 4 A:* **New methods from Nanoscale to Biology** Microfluidic Single-Cell Analysis and Manipulation *Stefano Pagliara (Living System Institute, University of Exeter)* Polymeric and Hydrogel Coatings – Particle and Capsule Functionalization *André Skirtach (Gent University, Institute for Solid State Physics,TU Dresden)* Cell-like Hydrogel Beads as Mechanical Probes for Biophysical Applications *Salvatore Girardo (Biotechnology Center, TU Dresden)*
9am- 10:30am	*Session 4B:* **Molecular Junctions and Devices** In Situ Generation of Open Shell Phenalenyl: Towards Designing Novel Multifunctional Materials *Swadhin Mandal (IISER Kolkata)* Future of Organic Solar Cells and Organic Light Emitting Diodes: Materials, Processing and Application *Nguyen Nang Dinh (University of Engineering and Technology, Vietnam National University)* Spin Transport and Molecular Orientation in Hybrid magnetic Tunnel Junctions *Tae Hee Kim (Dep. of Physics, Ewha Womans University)*

10:30am-11am	*Coffee*
11am-12:30am 11am-12:30am	*Session 5 A:* **First principle and High Throughput Calculations** Computational Nano-Materials Design: From Basics to Actual Application *Hideaki Kasai (National Institute of Technology, Akashi College)* Application of Crystallography to High-Throughput Calculations *Yoyo Hinuma (Dep. of Materials Science and Engineering, Kyoto University, National Institute for Materials Science, Center for Frontier Science, Chiba University)* First-principles and Semi-empirical Methods of Calculations of Optical Properties of Functional Materials *Mikhail G. Brik (College of Sciences, Chongqing University of Posts and Telecommunications, Institute of Physics, University of Tartu)* *Session 5 B:* **Topological Insulators and Spin Physics** Topological Insulators: Magnetism, Strong Electron Correlation and Ferroelectricity *Oliver Rader (BESSY II Helmholtzzentrum)* Ultrafast Spin Dynamics in CoFeB/MgO/CoFeB Magnetic Tunnel Junctions *Jakob Walowski (Institute of Physics, University of Greifswald)* Ultrafast Laser Pulse Switching the Magnetization of FePt Nanoparticles Deterministically for Data Storage Application *Robin John (Institute of Physics, University of Greifswald)*
12:30am-2:30pm	*Lunch*
2:30pm-4pm	*Session 6 A:* **THz Dynamics** Spintronic Emitters of Ultrashort Terahertz Pulses *Tobias Kampfrath (Fritz-Haber-Institute Berlin, Germany)* Active and Passive Control of Dissipation in Light-induced Coherent Ultrafast Dynamics *Henning Ulrichs (I. Physical Institute, University of Göttingen)* Modelling THz Spin Dynamics *Ulrich Nowak (Konstanz University)*

2:30pm-4pm	*Session 6 B:* **Oxides and Spectroscopy** Development of Functional Dielectric Materials in Silicates and Aluminates *Hiroki Taniguchi (Dep. of Physics, Nagoya University)* Strain Disorder: a New Degree of Freedom to Control Structurally Dissimilar magnetic Phase Separation in $La_{5/8-y}Pr_yCa_{3/8}MnO_3$ Epitaxial Thin Films *Dileep K. Mishra (Mat. Science Program, Indian Institute of Technology, Semiconductor Physics and Devices Lab, Raja Ramanna Centre for Advanced Technology)* Ab-initio Multiplet Calculations for X-ray Absorption Spectroscopy: Application to Cathode Materials *Hidekazu Ikeno (Nanoscience and nanotechnology Research Center, Osaka Prefecture University)*
4pm-5pm	*Coffee and Poster Session*
5pm-6:30pm	*In Parallel Poster Session* *Session 6 C:* **Hard Magnets for Applications** Magnetic Field-Induced Synthesis of Mn-Based Ferromagnetic Alloys *Keiichi Koyama (Graduate School of Science and Engineering, Kagoshima University)* First-Principles Study on the Magnetic Anisotropy of Ga-Added Nd-Fe-B Magnets *Yasutomi Tatetsu (Dep. of Materials Science and Engineering, Tokyo Institute of Technology)* Magnetic Materials from an Industry Perspective *Peter Siegle (Veekim AG)*
5pm-6:30pm	*Session 6 D:* **Dielectric Properties and Thermoelectrics** Dielectric Properties of $BaTiO_3$ by Molecular Dynamics Simulations Using a Shell Model *Tamotsu Hashimoto (Research Center for Computational Design of Advanced Functional Materials, National Institute of Advanced Industrial Science and Technology)* Complex Field Induced Phases in the Frustrated Quantum Spin Chain Linarite, $PbCuSO_4(OH)_2$ *Stefan Süllow (Institute for Condensed Matter Physics, TU Braunschweig)*

	Thermoelectric Properties of Spinel Sulfide $ZnCr_2S_4$ and Electron Transport Calculation Using Open MX and BoltzTraP *Masanobu Miyata (School of Materials Science, Japan Advanced Institute of Science and Technology)*
7pm	**Public evening Lecture** Correlated Electrons – a Molecular Approach *Michael Lang (Physics Institute, Goethe-University Frankfurt)* **The talk will be followed by a reception with drinks and food.**

Wednesday 6. September	
9am – 10:30am	*Session 7 A:* **Spin- and Orbitronics** Materials for Spin-Orbitronics *Mathias Kläui (Institute of Physics, Johannes Gutenberg-University Mainz)* Increase of Pulse Laser-induced Terahertz-wave Intensity in Ta/CoFeB/MgO Films by Annealing Process *Yuta Sasaki (WPI Advanced Institute for Materials research, Tohoku University, Dep. of Applied Physics, Tohoku University)* Spin Absorption Effects Due to Various Functional Materials *Takashi Kimura (Dep. of Physics, Kyushu University)*
9am – 10:30am	*Sessions 7 B:* **Hybrid Nanosystems** Rocking at the Nanoscale: Controlling and Probing Optically Active Nanosystems by Nanoquakes on a Chip *Hubert J. Krenner (Chair of Experimental Physics 1, University Augsburg)* Evidence for Electronic Phase Separation in the Diluted Magnetic Semiconductors (Ga,Mn)As and (Ga,Mn)P *Martin Lonsky (Institute of Physics, Goethe-University Frankfurt)* Theoretical Design of ZnO Nanoporous Crystalline Structures *Vu Ngoc Tuoc (Institute of Engineering Physics, Hanoi University of Science and Technology)*
10:30am – 11am	*Coffee*

11am – 12:30am	*Sessions 8 A:* **Towards Neuromorphic Computing** Neuron Networks in Artificial Landscapes *Robert Blick (Hamburg University)* Memristor-Based Neural Networks *Andy Thomas (IFW Dresden)* Reservoir Computing with Spin-Torque Nano-Oscillators *Flavio Abreu Araujo (Unité mixte de Physique CNSR/Thales)*
11am – 12:30am	*Session 8 B:* **Spin- and Spinwaves** Mutually Synchronized Spin Torque and Spin Hall Nano-Oscillators *Johan Akerman (University of Gothenburg)* Gold-based Magnetic Alloys: Fe-Au Thin Films by Heavy Ion Implantation *Hoang-Nam Nhat (Fac. of Engineering Physics and Nanotechnology, VNU-University of Engineering and Technology)* Micro-Hall Magnetometry Studies 2D and 3D Magnetic Nanostructures *Jens Müller (Institute of Physics, Goethe-University Frankfurt)*
12:30am-2:30pm	*Lunch*
2:30pm-4pm	*Session 9 A:* **Advanced Imaging Techniques** Ultrafast STM Driven By THz Fields *Tyler L. Cocker (Dep. of Physics, University of Regensburg)* Nanoscale Magnetic Imaging Using High-Harmonic Radiation *Sergey Zayko (IV. Physical Institute, University Göttingen)* Ultrafast Spin Dynamics Probed By Fs Lasers *Daniel Steil (I. Physical Institute, University of Göttingen)*
2:30pm-4pm	*Session 9 B:* **Transport in Nanostructures** InAs Nanowire-Based Devices for Applications in Quantum Information Technology *Thomas Schäpers (Peter Grünberg Institute 9, Forschungszentrum Jülich, JARA-Fundamental of Future Information Technology, Forschungszentrum Jülich)* 1D and 2D hybrid materials for nanoelectronics *Laëtitia Marty (University Grenoble Alpes, Inst. NEEL)*

	Electrochemical Deposited ZnO/Magnetic-Metal Hybrid Core/Shell Nanowires for Spintronic Device Application *Masashi Akabori (Japan Advanced Institute of Science and Technology (JAIST))*
4pm-5pm	*Coffee*
5pm-6:30pm	*Session 10 A:* **Advanced Imaging Techniques** Phase-Locked Dynamics Wide-Field Magneto-Optical Microscopy *Jeffrey McCord (Institute for Materials Science, Kiel University)* Advanced Spectroscopy Methods: Magnetic Dichroism in Transmission Electron Microscopy *Bernd Rellinghaus (IFW Dresden)* Ultrafast Nanoscale Dynamics Probed by Time-Resolved Transmission Electron Microscopy *Sascha Schäfer (IV. Physical Institute- Solids and Nanostructures, University of Göttingen)*
5pm-6:30pm	*Session 10 B:* **Materials Science** Influence of Cu Addition on Precipitation and Growth Behavior of MnS in Silicon Steel: Experimental Observation and KWN Modeling *Nobufumi Ueshima (Dep. of Metallurgy, Tohoku University)* First-principles Calculations on Point Defects in Semiconductors *Yu Kumagai (Materials Research Center for Element Strategy, Tokyo Institute of Technology,PRESTO, Japan Science and Technology Agency)* Ca Substitution Effect and Relation Between the Dielectric Relation Time and Piezoelectric Property of $Ba_{1-x}Ca_xTiO_3$ (BCTx) and $BaZr_{0.2}Ti_{0.8}O_3$-$Ba_{1-x}Ca_xTiO_3$ ($BZT-BCT_x$) *Le Van Hong (Institute of Materials Science, VAST)*

	Farewell and Dinner in Theater Café Restaurant

Poster

1. Experimental study on background signal in lateral a spin valve
   T. Ariki, T. Nomura. K. Ohnishi [1,2], T. Kimura[1,2], [1] Department of Physics, Kyushu University, Fukuoka, [2] Research Center for Quantum Nano-Spin Science, Kyushu University, Fukuoka, 819-0395, Japan

2. Heat transport in GMR nanowires: Evidence for Thermal Magneto Resistance
   N. Asam[1], K. Yamanoi[1] and T. Kimura[1,2], [1] Dept. of Physics, Kyushu University Motooka 744 Nishi-ku Fukuoka Japan 819-0395, [2] Research Center for Quantum Nano-spin sciences, Kyushu University, Fukuoka Japan.

3. Photocatalytic Ability Of G-C_3n_4nanosheets Loaded Ag Clusters To Use As Catalyst In Degradation Of Rhodamine B
   Do Danh Bich[1],, Nguyen Quynh Mai[1], Le Thi Mai Oanh[1], Lam Thi Hang[2], and Nguyen Van Minh[1], [1]Center for Nano Science and Technology , Department of Physics, Hanoi National University of Education, Hanoi, 100000, Vietnam, [2]Hanoi University of Natural Resources and Environment, Hanoi, 1000000, Vietnam*

4. Influence of annealing temperature on physical properties and photocatalytic ability of g-C_3N_4 nanosheets synthesized through urea polymerization in air
   Lam Thi Hang[1, 2], Dao Viet Thang[3], Nguyen Manh Hung[3], Do Danh Bich[2, 4], Nguyen Van Minh[2, 4], Le Thi Mai Oanh[2, 4], [1]Faculty of Basic Sciences, Hanoi University of Natural Resources and Environment, Vietnam, [2]Center for Nano Science and Technology, Hanoi 100000, Vietnam, [3]Faculty of Basic Sciences, Hanoi University of Mining and Geology, Duc Thang ward, Hanoi 100000, Vietnam, [4]Department of Physics, Hanoi National University of Education, Hanoi 100000, Vietnam

5. Weak localization of magnons in chiral magnets
   M. Evers[1], C. A. Müller[1], U. Nowak[1], [1]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

6. Electronic structure of Cu-doped hydroxyapatite/β-tricalcium phosphate composite
   K. Fukui[1] and T. Yamamoto[1,2],[1]Faculty of Science and Engineering, Waseda University, Shinjuku, Tokyo 169-8555, Japan
   [2]Institute of Condensed-Matter Science, Waseda University, Tokyo, 169-8555, Japan

7. EXAFS Debye-Waller Factors of Transition Metals
   Under High Pressure
   Nguyen Ba Duc[1], Vu Quang Tho[1] and Ho Khac Hieu[2], [1]Tan Trao University, Tuyen Quang, Vietnam, [2]Duy Tan University, Da Nang, Vietnam

8. Phenalenyl-Cu for organic Magnetic Tunnel Junctions (MTJ)
   N. Jha[1], C. Denker[1], Anand Paryar[4], P. K. Vardhanapu[4], B. Das Mohapatra[2], H. Mohamad[1], M. Medvidov[3], U. Martens[1], C. Helm[1], S. Mandal[4] and M. Münzenberg[1], [1] Institut für Physik, Ernst-Moritz-Arnd-Universität Greifswald, Germany,[2] National Institute of Science and Research, Bhubaneshwar, India,[3] ZIK HIKE, Ernst-Moritz-Arndt Universität Greifswald, Germany,[4] Department of Chemical Sciences, IISER, Kolkata, India

9. Laser induced photocurrents in a FM/TI-heterostructure analyzed by 2D maps for VIS
   Tobias Kleinke, Thomas Schumann, Markus Münzenberg, Institute of physics, Ernst-Moritz-Arndt University Greifswald, Greifswald, Germany

10. Fabricating a microlense to build a THz emitter
    Finn-F. Lietzow[1], Nina Meyer[1], Jakob Walowski[1], Christian Denker[1], Markus Münzenberg[1], [1]Institute of Physics, Greifswald University, Greifswald, Germany

11. Thermovoltage generation by inhomogeneous laser heating of magnetic tunnel junctions
    U. Martens[1], J. Walowski, T. Huebner[2], A. Boehnke[2], G. Reiss[2], Timo Kuschel[2], A. Thomas[3], M. Münzenberg[1], [1]Institut für Physik, Ernst-Moritz-Arndt Universität, 17489 Greifswald, Germany, [2]CSMD, Physics Department, Bielefeld University, 33615 Bielefeld, Germany, [3]Leibniz Institute for Solid State and Materials Research Dresden (IFW Dresden), Institute for Metallic Materials, 01069 Dresden, Germany

12. Simulation of Nanoscale Femtosecond Acoustics in Phononic Superlattices
    Dennis Meyer, Henning Ulrichs, I. Physikalisches Institut, Universität Göttingen, Germany

13. Determining the spotsize of a microlense to build a THz emitter
    Nina Meyer[1], Finn-F. Lietzow[1] Jakob Walowski[1], Christian Denker[1], Markus Münzenberg[1], [1]Institute of Physics, Greifswald University, Greifswald, Germany

14. Metal-Insulator Transition with Structural Distortion in a Layered Perovskite $La_3Ni_2O_7$: A First-Principles Study
    Yasuhide Mochizuki[1], Hirofumi Akamatsu [1], Yu Kumagai [2], and Fumiyasu Oba [1,2], [1] Laboratory for Materials and Structures, Institute of Innovative Research, Tokyo Institute of Technology, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan, [2] Materials Research Center for Element Strategy, Tokyo Institute of Technology, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan

15. Crystal Structure and Soft Phonon Mode in Improper Ferroelectric $BaAl_2O_4$
Yuki Nakahira[1], Chikako Moriyoshi[1], Yoshihiro Kuroiwa[1], Hiroki Moriwake[2], Yui Ishii[3], and Shigeo Mori[3], [1]Department of Physical Science, Graduate School of Science, Hiroshima University, Hiroshima 739-8526, Japan, [2]Department Japan Fine Ceramics Center, Nagoya 456-8587, Japan, [3]Department of Materials Science, Osaka Prefecture University, Osaka 599-8531, Japan

16. Fe-embedded g-C_3N_4: effective catalyst for Rhodamine B decomposition
Le Thi Mai Oanh[1,], Danh Bich Do[1], Lam Thi Hang[2], Pham Manh Cuong[1], and Nguyen Van Minh[1], [1]Center for Nano Science and Technology , Department of Physics, Hanoi National University of Education, Hanoi, 100000, Vietnam, [2]Hanoi University of Natural Resources and Environment, Hanoi, 100000, Vietnam*

17. Electronic structure of topological point- and line-node semimetals
Seigo Souma[1,2], Zhiwei Wang[3], D. Takane[4], K. Nakayama[4], C.-X. Trang[4], H. Kotaka[5], K. Yamauchi[5], T. Oguchi[5], K. Segawa[6], T. Sato[1,4], T. Takahashi[1,2,4], and Yoichi Ando[2], [1]Center for Spintronics Research Network, Tohoku University, Sendai 980-8577, Japan,[2]WPI Advanced Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan, [3]Institute of Physics II, University of Cologne, Cologne 50937, Germany,[4]Department of Physics, Tohoku University, Sendai 980-8578, Japan, [5]Institute of Scientific and Industrial Research, Osaka University, Ibaraki, Osaka 567-0047, Japan,[6]Department of Physics, Kyoto Sangyo University, Kyoto 603-8555, Japan

18. Three-Dimensional Twinning of GaAs Nanowires on Hydrogen-Silsesquioxane Covered GaAs(001) Using Molecular Beam Epitaxy
Dat Q.Tran, Huyen T. Pham, Koichi Higashimine, Yoshifumi Oshima, Masashi Akabori, Japan Advanced Institute of Science and Technology (JAIST), Japan

19. Electronic properties of noncentrosymmetric superconductor Th_7Ni_3
M. Sahakyan and V. H. Tran, Institute of Low Temperature and Structure Research, Polish Academy of Sciences, 50-422 Wroclaw, Poland

20. Exchange bias properties in A_2-Mn_2VAl/Fe bilayers
Tomoki Tsuchiya[1], Ryota Kobayashi[1], Takahide Kubota[1, 2], Koki Takanashi[1, 2], [1] Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan.[2] Center for Spintronics Research Network (CSRN), Tohoku University, Sendai 980-8577, Japan

21. Enhancement of the sensitivity of magnetic field sensor based on anisotropic magetoresistance effect in NiFe thin films
B.D. Tu, L.K.Quynh, L.V. Cuong, P.D.Thang, D.T.H.Giang, N.H.Duc, Faculty of Engineering Physics and Nanotechnology, VNU University of Engineering and Technology, Hanoi, Vietnam

22. Electronic Structure of Mn-doped oxide phosphor materials
Mekhrdod Subhoni[1], Kholmirzo T. Kholmurodov[2,3], Tomoya Murai[4], Kentaro Mori[4], Daisuke Yamada[4], and Tomoyuki Yamamoto[4,6],[1]Academy of Science, Dushanbe, Republic of Tajikistan,[2]Joint Institute for Nuclear Research, Dubna, Russia, [3]Dubna State University, Dubna, Russia, [4]Faculty of Science and Engineering, Waseda University, 169-8555, Tokyo, Japan, [5]Institute of Condensed-Matter Science, Waseda University, 169-8555, Tokyo, Japan

Abstracts Talks

Manganese-Based Spintronics

Shigemi Mizukami

WPI Advanced Institute for Materials Research, Tohoku University, Sendai, 980-0075, Japan

The exploration of new materials is one of the important issues in material science. This is also the case for spintronics. Although iron-cobalt alloys have been mainly used for various spintronic applications, it is demanded to find new materials to overcome some limitations in current spintronic applications. Here, we focus on manganese, which has fascinating properties as known from the past. The elemental Mn metal does not show any strong magnetism; however Mn element gives various interesting physical properties when it forms alloys or compounds with other elements. Over the past decade, we have studied various Mn-based magnetic alloys for spintronic device applications [1-3]. Recently we have demonstrated to fabricate ultrathin epitaxial manganese alloys using some ordered alloy templates, which offers a good playground to study physical phenomena related to the spin transport and spin-orbit interaction [4,5].

In this talk, I will overview our past studies on manganese alloys and shows the recent progress of study on manganese nano-layer mentioned above, and discuss the possibility for future memory and THz applications. This study was partially supported by the KAKENHI and the ImPACT program.

References

[1] F. Wu, S. Mizukami, D. Watanabe, H. Naganuma, M. Oogane, Y. Ando, and T. Miyazaki, *Appl. Phys. Lett.*, 94, 122503 (2009).
[2] S. Mizukami, F. Wu, A. Sakuma, J. Walowski, D. Watanabe, T. Kubota, X. Zhang, H. Naganuma, M. Oogane, Y. Ando, and T. Miyazaki, *Phys. Rev. Lett.*, 106, 117201 (2011).
[3] Q. L. Ma, S. Mizukami, T. Kubota, X. M. Zhang, Y. Ando, and T. Miyazaki, *Phys. Rev. Lett.*, 112, 157202 (2014).
[4] K. Z. Suzuki, R. Ranjbar, J. Okabayashi, Y. Miura, A. Sugihara, H. Tsuchiura, and S. Mizukami, *Sci. Rep.*, 6, 30249 (2016).
[5] M. Takikawa, K. Z. Suzuki, R. Ranjbar, and S. Mizukami, *Appl. Phys. Express*, accepted.

Designing quantum spin-orbit-coupled materials: a source for exotic states

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The realization of the so-called Kitaev spin liquid as a ground state in edge-sharing d^5 materials appears to represent a very significant synthetic challenge. In this talk I will revisit the magnetic interactions and excitations in hexagonal iridates (Na_2IrO_3, Li_2IrO_3) and $RuCl_3$ by a combination of ab initio density functional theory calculations and nonperturbative exact diagonalization methods and from this analysis I will discuss the potential for realizing exotic spin liquid phases in real materials. [1,2,3,4]

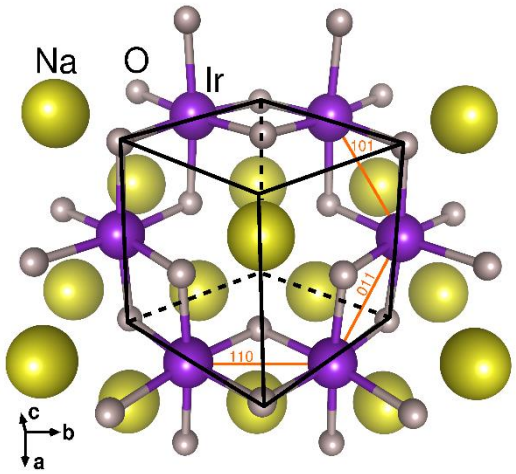

FIG. 1. Structure of Na_2IrO_3

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Common Principles in Synthetic Mechanophores and Mechanoresponsive Biomolecules

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Much effort is currently invested in the development of (bio)materials with well-defined mechanical properties. This is motivated by the desire to measure cell generated forces *in situ* at the molecular level and to direct cellular behaviour using controlled mechanical stimuli. In parallel, materials scientists aim at the development of self-reporting and self-healing materials that respond to mechanical force in a pre-defined way. Key to all these efforts are mechanosensitive molecular building blocks, such as synthetic, small-molecule mechanophores and mechanoresponsive biomolecules [1, 2].

Focussing on common principles that guide the design of mechanosensitive molecules, I will introduce our current set of synthetic and biological mechanical building blocks. Following a mechanical calibration at the single-molecule level, these building blocks are equipped with a fluorescent reporter system that reports on the mechanical state of the molecule. This allows us to directly observe the force acting on an individual molecule using a fluorescence readout so that a molecular force sensor is obtained [1, 2]. Considering the above applications, such sensors report on mechanical material deformation in a highly sensitive manner down to the single-molecule level. Our approach further opens up new routes toward correlating the bulk and molecular mechanical properties of a material and for the development of tuneable extracellular matrix mimics whose mechanical properties are controlled at the molecular level.

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Real-Time Deformability Cytometry: Spatiotemporal Polymer and Cell Response in Microfluidic Systems

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With the development of real-time deformability cytometry (RT-DC), we have introduced a high-throughput method for quantitative and continuous mechanical single-cell classification of heterogeneous cell populations at rates of several hundred cells per second [1]. Cells are driven through the constriction zone of a microfluidic chip leading to cell deformations due to hydrodynamic stresses only. The ensuing deformations can be quantified and an analytical model based on linear elasticity theory enables the derivation of cell material properties [2].
Here, we demonstrate the extension of RT-DC towards a multi-parameter label-free biological assay where data acquisition is based on real-time image analysis only. Performing RT-DC on whole blood we highlight its potential to identify subsets in heterogeneous cell populations and to characterize specific mechanical phenotypes after drug-induced alterations of the cytoskeleton. Inside these samples the dynamics of single cells can be monitored with sub-millisecond temporal resolution giving access to cellular viscoelastic properties on short time scales. Using mixture model statistics a subset of governing parameters partitioning a dataset can be identified and linear mixed model analysis allows for computation of statistical significance. Based on the RT-DC platform we also study rheological properties of non-Newtonian fluids on phase boundaries. We show that controlling flow rate is sufficient to actively adjust the hydrodynamic system.

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Atomic Force Microscopy, what else?

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In this talk, the versatility of the atomic force microscopy (AFM) for investigating questions related to soft matter, biophysics or biology will be presented.
In particular, I will show the way AFM is utilized as a high resolution imaging device to characterize (macro)molecules at different interfaces (e.g. crystallization processes or lipid-protein interactions) and what information can be obtained from it [1]. Furthermore, I will point out the advantages (and troubles) of the AFM when it is used as a mechanical device [2]. In this part, I will talk about molecular/colloidal forces, elasticity of macromolecules, force spectroscopy and cell mechanics.
Finally, I will point out different possibilities to combine the scanning probe microscopy with other microscopy techniques, such as fluorescence microscopy and RICM.

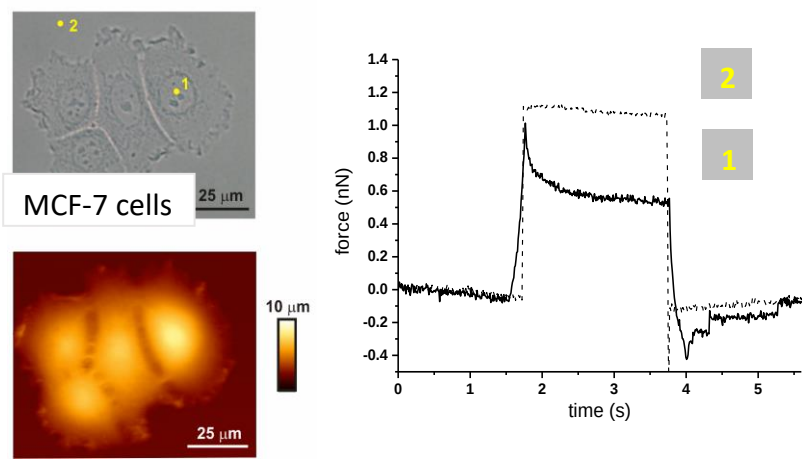

FIG. 1. Force relaxation experiment on breast cancer cells (MDF-7) at constant height. (1) The applied force is relaxed by the cell after two seconds. (2) On the contrary, the substrate behaves like a hard surface: it does not relax the force. This method in combination with creep experiments can be used to obtain a full mechanical description of biomaterials [3].

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Inversion Symmetry Breaking by Oxygen Octahedral Rotation in Asite-Ordered n=1 Ruddlesden-Popper Phases AA'TiO_4 (A=alkaline, A'=rare earth) and the Cation Size Effects

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Recently, a lot of attention has been paid to layered perovskite oxides exhibitingnoncentrosymmetry due to oxygen octahedral rotations (OORs) towards the development of new series of ferroelectrics and multiferroelectrics.[1] We have reported the OORinduced noncentrosymmetry of A-site-ordered n=1 Ruddlesden-Popper phase NaA'TiO4 (A'=rare earth),[2] in which inversion symmetry is broken by OORs represented by a–b^0c^0/b^0a–c^0 in Glazer notation.[3] The Na ions can be replaced by different monovalent cations such as H, Li, K, and Ag, possibly leading to the discovery of large piezoelectric family. It would be expected that smaller A-site cations induce larger OOR in the framework of concept of tolerance factor. Here we report experimental and theoretical work showing, however, that the K substitutes also exhibit the OOR-induced noncentrosymmetry and, surprisingly, the OOR instability is enhanced with substitution of larger K ions for smaller Na ions. Synchrotron x-ray diffraction (SXRD) and second harmonic generation (SHG) measurements for polycrystalline KA'TiO_4 (A'=Sm, Eu) samples revealed that KA'TiO_4 (A'=Sm, Eu) belongs to a noncentrosymmetric P-42_1m space group with an a–b^0c^0/b^0a– c^0-type OOR at room temperature similarly to the Na substitutes.[2] The variabletemperature SXRD and SHG measurements showed that KA'TiO4 has higher structural phase transition temperatures relevant to the OOR than the Na substitutes (Fig. 1), while the transition temperatures are higher for smaller rare-earth ions.[2] It was found from detailed crystallochemical analyses of the results of first-principles calculations that the rare-earth and alkaline ions play different roles in the OOR although both the ions occupy the same sites in a crystallographic viewpoint: the rare-earth ions strongly attract O_2– ions to optimize their oxygen coordination due to the trivalent positive charge, while the alkaline oxide layers impose in-plane strain on the other layers so as to tune the OOR instability.

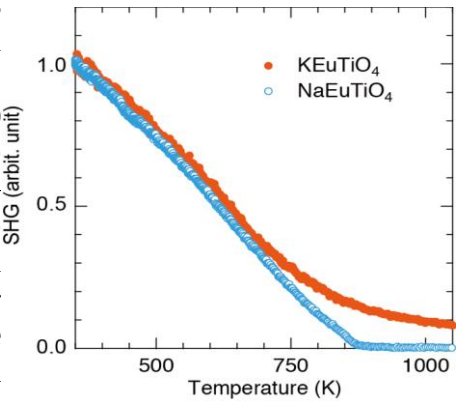

Figure 1. Temperature dependence of SHG intensity for AEuTiO4 (A=Na and K).

H.A. was financially supported by JSPS KAKENHI Grant-in- Aid for Research Activity Start-up (Grant No. 16H06793). H.A. also thanks Murata Science Foundation for their financial support.

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Comparison between the Ultrafast Optical Responses and Ultrafast Structural / Atom Dynamics in Novel Perovskite Solar Cell Prototypes

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Ultrafast optical spectroscopy and ultrafast structural dynamics studies based on high flux and pulsed X-ray methods based on synchrotron and Free Electron Laser sources are complementary tools for studying real time structure-function relationships of opto-electronic devices such as photo-switches, photo-switchable ferroelectrics or novel types of solar cells.
The manganite Pr0.65Ca0.35MnO3 presents such a material with photovoltaic, thermoelectric, and electrocatalytic activities. This perovskite solar cell material is characterised through strong correlations. In particular, the optical control of the relaxation process of the optically excited charge carriers in the solids is one of the parameters allowing for tuning light conversion efficiencies. In the current work we have utilized the effect of the so-called photo-induced phase transition to create transient nanosecond long living charge carrier species of the type of polaron states. Usually, optically excited electrons in a solid thermalize rapidly on a femtosecond to picosecond timescale, due to their interactions with other electrons and phonons. In the current work, we have studied these mechanisms with ultrafast optical and ultrafast X-ay methods and exploited new mechanisms to slow down these non-desired thermalization features. In consequence, the efficiencies of the light energy conversion in these photovoltaic devices have increased.
The electronic and structural dynamics of $Pr_{0.65}Ca_{0.35}MnO_3$ reveals an ultraslow recombination dynamics on a nanosecond-time scale. The strong correlation between the excited polaron and the octahedral dynamics of its environment appears to be substantial for stabilizing the found hot polaron.

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Crystal Structure of Anion Changeable Layered Double Hydroxides by Synchrotron Radiation X-ray Diffraction

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Layered double hydroxides (LDH) $[M^{2+}_{1-x}M^{3+}_{x}(OH)_2][A^{n-}_{x/n}]\cdot mH_2O$ (A^{n-}: n-valent anion, m: number of hydration water) have attracted much attention owing to its anion-exchangeability. One of the interesting characteristics of LDH is anion-selectivity, i.e., which anion can exist in an LDH crystal depends on a combination of anions in LDH and an aqueous solution [1]. The anion-selectivity can be applied to purifying the environmental water. Many studies on the anion-selectivity have been done but the mechanism is still unclear. To find a key to understanding the mechanism, we have studied the relationship between the anion-selectivity and the accurate crystal structures (atomic positions, atomic thermal displacement parameters, and electron density distributions) of the LDH materials with many combinations of M^{2+}, M^{3+}, x, and A^{n-}. Powder diffraction data were obtained at powder diffraction beamline BL02B2 of the synchrotron radiation facility SPring-8. The crystal structure and electron density distribution in crystals were analyzed by the maximum entropy method (MEM)/Rietveld method.

The crystal structure and electron charge density distribution of $[Mg_{2/3}Al_{1/3}(OH)_2][Cl^-_{1/3}]\cdot mH_2O$ are shown in FIG. 1 as an example of our study [2]. The hydrate structure (m = 0.52) at room temperature changed to the anhydride one (m = 0) by heating. The Cl ion position was delocalized in the hydrate structure while localized in the anhydride one. These results indicate the smaller thermal vibration even in the high temperature region. Thus the structure analyses revealed that the water molecules controls the anion mobility in LDH crystals. The further discussion on relationship between the structure and the anion exchangeability will be given.

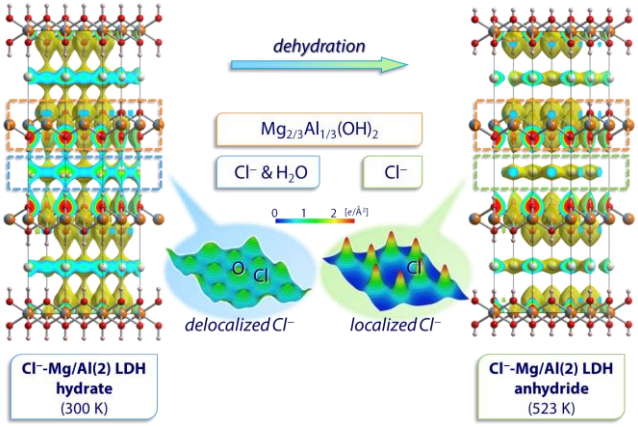

FIG. 1. Crystal structure and electron density distribution (surface level: 0.5e Å^{-3}) of anion exchangeable $[Mg_{2/3}Al_{1/3}(OH)_2][Cl_{1/3}]\cdot mH_2O$ (Cl^--Mg/Al(2) LDH) in hydrate and anhydride forms [2]. Both structures have rhombohedral ones of space group R-3/m.

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Plasmon Induced Photoemission from Individual Small Silver Nanoparticles: Role of the Substrate

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The plasmonic response of metal nanostructures not only depends on material, shape and size but also on coupling phenomena to the environment. Compared to ensemble techniques single particle spectroscopy is beneficial for addressing the role of such interactions, because inhomogeneous broadening is avoided and spectroscopic and geometric properties can be more precisely correlated. Here we use two-photon photoemission electron microscopy (2P-PEEM) with optical excitation close to the plasmon resonance which leads to efficient emission of electrons [1] that can be analyzed regarding their spatial, energetic, and angular properties. We measured the electron intensity as a function of photon energy for individual silver nanoparticles in the size range between 5 and 30 nm. The data are correlated with geometric properties obtained by atomic force microscopy (AFM). Clusters were produced in the gas phase and soft-landed onto natively oxidized Si(111) as well as on clean Si(111)-(7x7) to access the role of cluster-surface interaction. Compared to the oxidized substrate we find a pronounced mode splitting on clean Si(111)-(7x7) instead of the expected simple shift of the plasmon resonance. We attribute this behavior to the formation of complex plasmon modes which are caused by the optical properties of the substrate: the large polarizability of Si gives rise to induced image dipoles such that higher-order multipoles can be formed [2]. Implications of this effect on the observed size-dependent distribution of plasmon energies and lifetimes are discussed.

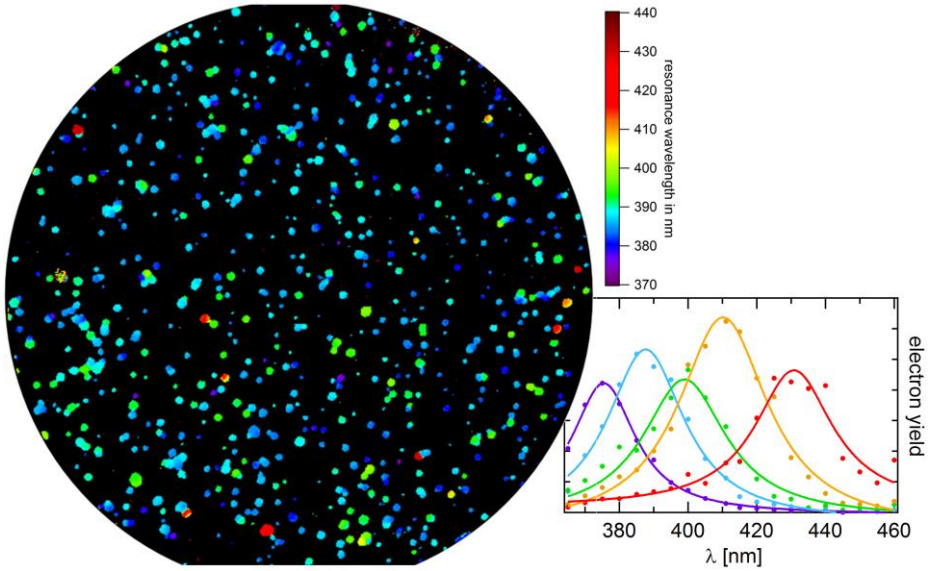

FIG. 1. Left: Color-coded map of plasmon energies of individual Ag nanoparticles on silicon covered with a native oxide layer. Right: Excitation spectra of some selected particles.

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Direct Laser Writing of Plasmonic Nanostructures

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We demonstrate that high-temperature annealing leads to transformation of continuous gold thin film into isolated nanoparticles thanks to the dewetting effect, which exhibit remarkably enhanced and localized plasmon resonance spectra. The strong dependence of the resonance band spectra on the annealing temperature, the initial metallic film thickness and supporting substrates was experimentally investigated. Moreover, we demonstrate a direct way to realize arbitrary gold nanostructures via a local dewetting method. This technique was based on the optically induced local thermal effect at the focusing region of a direct laser writing (DLW) system employing a green continuous-wave laser. The local high temperature allowed the creation of gold nanoparticles only at the focusing area of the optical system. By moving the focusing spot, this DLW method allowed us to "write" desired 2D gold patterns, with a feature size down to sub-lambda. A heat model was also proposed to theoretically explain the localized heating process of the absorbing gold layer. We also demonstrate that this technique is an excellent method for data storage and color printer applications.

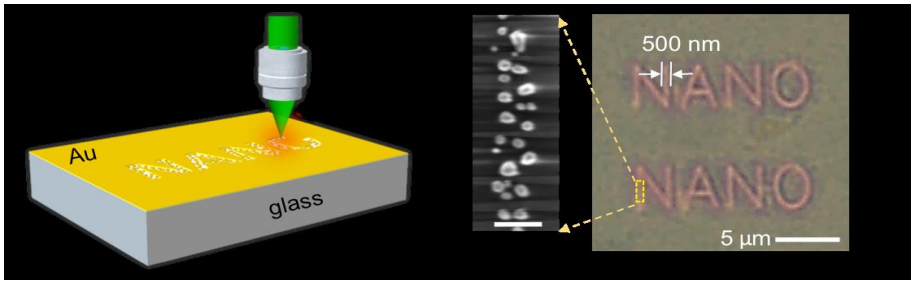

FIG. 1. (a) Illustration of the DLW technique used to realize desired gold nano-islands pattern. (b) Optical microscope and SEM (inset) images of fabricated gold nanopattern (letter ``NANO").

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Looking for Synergies in Molecular Plasmonics by Hybrid Functional Nanostructures

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Keywords: plasmonics, self-assembly, macroscopic

For the next generation of optical devices, the possibility of cost-efficient manufacturing requires both tailored control of the nanoparticle building blocks as well as an up-scaleable self-assembly method for macroscopic areas. We address these demands using bottom-up directed self-assembly of plasmonic nanoparticles to achieve collective plasmonic resonances in high quality plasmonic modes.[1] A first step toward these tailored modes are the controlled synthesis of the plasmonic building blocks with specific mintage materials (gold or silver), subwavelength dimensions and morphologies with less symmetry axis (cubic shape). For instance, we have recently been able to fabricate core shell nanoparticles with a specific dielectric spacer for controlled electric field enhancement.[2] As a second step, we use a directed self-assembly technique to align these building blocks to achieve collective plasmonic excitations such as constructive interference between plasmonic and diffraction modes (Fano resonance). Finally, we go one step further and use our directed self-assembly approach to discuss a magnetic metasurface. This magnetic mode could be excited using a plasmonic film coupled nanoparticle system.[3] This extraordinary electric field enhancement opens up new possibilities in ultra-sensitive sensing applications, plasmon-induced charge separations and the tailored control of the electric as well as magnetic field is important for energy conversion, super-absorber and metamaterial applications.

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Application of 3D Lithography

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3D 2-Photon-Lithography, originally developed for 3D photonic crystals, opens a wide range of new possible applications in many other fields, e.g. life sciences, micro-optics and mechanics [1].

We will present our recent applications of 3D 2-Photon-Lithography and show infra-red laser light focusing lenses directly fabricated on optical fibers, 3D evaporation masks for in-situ device fabrication using different deposition angles, tunnel structures for guiding growth of elongated cells, pillars for investigation of cell mechanics and master-mold fabrication for Polydimethylsiloxane (PDMS) micro-fluidic channels.

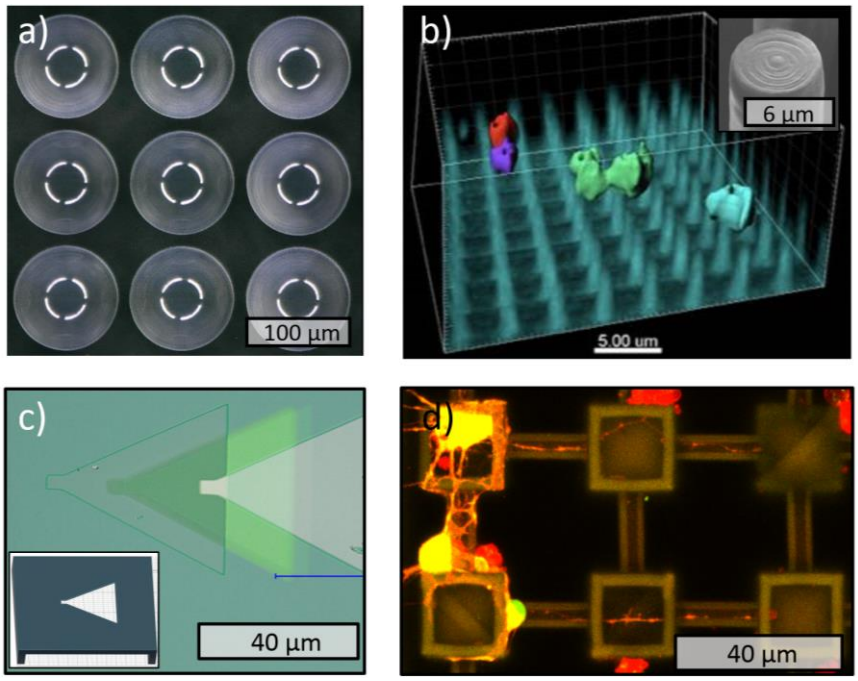

FIG. 1. a) Micro-lenses on a glass plate, b) Platelets on pillars (1µm diameter and 5µm height), the inset shows the top of a 6 µm pillar, c) In-situ structured organic tunnel junction, d) Guided growth of neuron axons in 4µm channels

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Reticular Solids with Adamantane-Type Building Blocks

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Synthetic chemists have so far produced thousands of organic molecules bearing one or more functional groups with the ability to form non-covalent interactions (e.g. H-bonds) in the solid state. By selecting the right combination of such building blocks and metal ions, the syntheses of several molecular organic frameworks (MOFs) have been achieved in the recent years [1,2]. These crystalline solids do possess large cavities that can host small molecules such as CO_2, H_2, acetylene, and many others, thereby paving the way to the development of functional materials for energy and environmental applications. Furthermore, computational quantum chemistry methods and molecular simulation are currently playing an important role in the design of novel MOFs.

In this contribution, I will give an overview of the research field of MOFs along with recent results concerned with the computer-aided design of reticular solids based on adamantane-type building blocks. Adamantane ($C_{10}H_{16}$) is a cage hydrocarbon with the same carbon framework as in diamond (Fig. 1a). Several functionalized derivatives of adamantane have been synthesized along with heteroatom-containing analogues such as hexamethylenetetramine ($C_6N_4H_{12}$) shown in Fig. 1b. The latter has the ability to coordinate metal ions via the nitrogen lone-pair and hence it represents a useful building block for the design of MOFs.

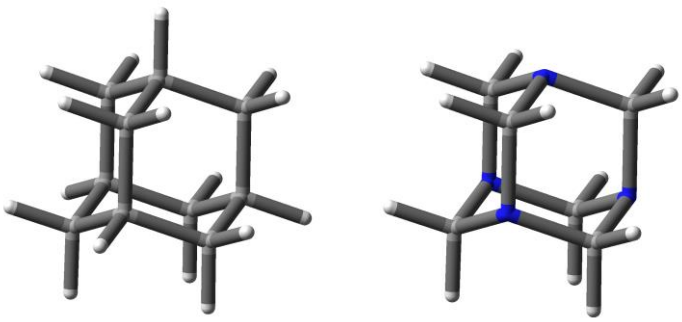

FIG. 1. Molecular structures of (a) adamantane and (b) hexamethylenetetramine.

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In situ Control of Solid-State [2+2] Photodimerization in the Molecular Crystal of a Cobalt Complex

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Solid-state [2+2] photodimerization of olefins is a well-known topochemical reaction where the structure of the reaction product is pre-determined by the molecular arrangement in the initial crystal. On the other hand, there are cases in which we would like to avoid the [2+2] photodimerization reaction such as in thermal paper and the thymine in DNA complex. *In situ* control of the reactivity of the photodimerization seems challenging because the reaction depends on the initial structures. However, if another reactive group is present in the crystal, it can trigger a change of the crystal structure or crystalline environment around the reactant molecule, thus the photodimerization reactivity can be controlled *in situ*, which is called "dual reactive strategy" [1,2].

In this study, the control was realized in a "dual photoreactive crystal" by using the strategy to design (3-cyanopropyl)(4-styrylpyridine)cobaloxime (**1**), shown in Fig. 1, which was synthesized as a dual photoreactive complex with two photoreactive groups, 3-cyanopropyl and 4-styrylpyridine, coordinated to the central metal. After the visible light irradiation, the 3-cyanopropyl group isomerized to 2- and/or 1-cyanopropyl by keeping the single crystalline form. On the other hand, [2+2] dimerization occurred between the 4-styrylpyridine moieties of adjacent molecules by UV light irradiation. Therefore, these two kinds of photoreactions, which we call "dual photoreaction", are wavelength-selective and proceed independently from each other. Interestingly, after the 3-cyanopropyl group isomerized with visible light irradiation, the [2+2] dimerization of 4-styrylpyridine moieties by UV light irradiation was suppressed. Thus, the *in situ* control of solid-state [2+2] dimerization reactivity of **1** was achieved by using another photoreaction.

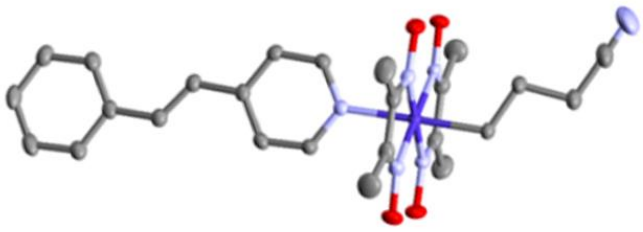

Fig.1 Molecular structure of **1**

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Photocatalytic Nanomaterials and their Applications

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Abstract: In this report, titanium dioxide nano particles and thin films were prepared by sol-gel method and/or hydrothermal technique using titanium isopropoxide as a precursor containing Ti(IV). Atomic-force microscopy (AFM), scanning electron microscopy (SEM), X-ray powder diffraction (XRD), porosity and contact angle measurements were carried out to investigate the physical and chemical properties of the particles as well as the fabricated thin films. The photocatalytic activity of prepared materials was examined by the degradation of methylene blue, methyl orange under UV-VIS irradiation. Moreover, the hydrophilic properties of TiO2 thin layers were studied under the influence of porosity of the films. Some potential applications of the nano photocatalyts such as bacteria killing, self-cleaning effect based on their photocatalytic and hydrophilic properties were also reported.

Structure-Activity Relationships for Quadruple Perovskite Catalysts

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Oxygen evolution/reduction reaction (OER/ORR) catalysis is of importance for energy conversion technology. ABO_3-type perovskite oxides have been extensively investigated as promising candidates for functional materials [1]. Quadruple perovskite oxide series, $AA'_3B_4O_{12}$, is a derivative of ABO_3-type perovskites consisting of specially ordered *A*-site ions. This series has been also widely investigated because of various properties and phenomena such as magnetoresistance, multiferroicity, charge disproportionation/ordering/transfer, and negative thermal expansion. The Fe^{4+}-based quadruple perovskite $CaCu_3Fe_4O_{12}$ (CCFO), which is synthesized under high pressure, displays a charge disproportionation ($2Fe^{4+} \rightarrow Fe^{3+} + Fe^{5+}$) [2]. simultaneously with a Fe-to-Cu electron charge transfer [3]. CCFO also exhibits a highly active catalytic activity for oxygen evolution reaction (OER, $4OH^- \rightarrow O_2 + 2H_2O + 4e^-$ in alkaline conditions) [4]. OER is an essential process for energy conversion like water splitting and charging of rechargeable metal-air batteries although platinum-based catalysts like IrO_2 and RuO_2 are currently used.

The OER activity of CCFO exceeds those of the simple Fe^{4+}-based perovskites (Ca/Sr)FeO_3 and state-of-the-art catalyst $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$ (BSCF) (Fig. 1) [4]. Also, the $CaCu_3B_4O_{12}$ perovskite series (*B* = Ti, V, Cr, Mn, Fe, and Co) showed higher OER activity compared with the corresponding (Ca/Sr)BO_3. This indicates that the Cu substitution for Ca at *A*-sites induces structural and/or electronic transformations, leading to higher catalytic activity. However, possible complex effects by Cu insertion hinder essential factors enhancing activity. Hence, we investigated Mn-based perovskite series $AMnO_3$ and AMn_7O_{12} (*A* = Ca, La) [5]. AMn_7O_{12} consists of elements/ions nominally identical with the corresponding $AMnO_3$ (Ca^{2+}, La^{3+}, and $Mn^{3+/4+}$) thus reasonably excludes synergistic effects between different constituent metals. Fig. 2 shows linear sweep voltammograms for $AMnO_3$ and AMn_7O_{12} (*A* = Ca, La). AMn_7O_{12} displayed higher OER catalytic activity than the corresponding $AMnO_3$. According to the first principle calculations of bulk electronic states, no considerable differences between $LaMnO_3$ and $LaMn_7O_{12}$ were found [5]. In contrast, possible changes in OER mechanism are proposed based on the Mn-Mn interatomic distances. In the presentation, structure-activity relationships for quadruple perovskite catalysts are discussed.

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Novel Structural, Electronic, and Reactive Properties of Nano Ceramic Materials: Theoretical Study

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Great numbers of studies have been done on nano inorganic materials with much expectation for expression of novel functional properties. Precise understanding of their fundamental properties, i.e., structural, electronic, and reactive properties is very important for both basic materials science and applied industry. However, the details had hardly been clarified. I have investigated these properties of nano ceramic clusters (NCC) for barium titanate ($BaTiO_3$) and related perovskites, which have been the most representative ferroelectric materials, by first-principles theoretical calculations for the first time, and found their quite interesting properties [1-4]. First, for the structural properties, amorphized structures are formed on these NCC surfaces. Second, for the electronic properties, the values of energy gaps are widely varied from almost zero to the values larger than those for the bulks depending on their structures. Third, for the reactive properties, I have examined the adsorption stability for H_2O, CO_2, and related molecules on both $BaTiO_3$ solid and NCC surfaces, and made clear a remarkable enhancement of the adsorption stability on the NCC surfaces compared with that on the solid surfaces. In addition, the size dependence of NCC on the adsorption stability was also revealed.

In the present talk, I show these novel and interesting properties of the perovskite NCC. Furthermore, I review the recent research progresses for NCC [5] and make discussion on them.

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Phase Transitions in Ferroelectric thin Films described by Ising Model in Transverse and Longitudinal Fields

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Finite temperature order-disorder phase transition in ferroelectric thin films (intermediate case between 2d and bulk cases) described by Ising model in transverse and longitudinal fields is investigated using mean field [1] and Gaussian fluctuation of the order parameters approximations. Dependence of the components of the order parameters, critical transverse field, and phase diagram … on the film thickness is obtained and analyzed. Quantum phase transition case is obtained directly in the zero temperature limit. Calculation for some ferroelectric titanate perovskite ultrathin films [2] is carried out for comparison with experimental results.

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Interplay of Magnetism and Dynamics in Graphene Nano-Flakes

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The production of a single layer of carbon atoms called "graphene" in 2004 was a big surprise and triggered a still growing research activity that aims at replacing silicon by graphene or similar materials for fabrication of nano-devices. On the one hand, the single-atom resolution is attractive as it constitutes the ultimate limit for the structuring of materials, on the other hand, graphene-type materials offer other favorable physical properties for technological applications. Recent developments of the field include an explosion of the number materials such as MoS_2 that –like graphene– consist of single layers of atoms forming a honeycomb lattice, but may vary in their physical and electronic properties.

Coulomb interactions are known to induce magnetism at "zig-zag" edges of nano-structures cut from such honeycomb-lattice materials, a phenomenon that is highly relevant to potential spintronics applications. In this contribution, we will revisit a Hubbard-model description for static and dynamic properties of such magnetic nano-structures. In particular, we will present a benchmark of the performance of a static mean-field approach, a more sophisticated "dynamical" mean-field theory (DMFT), and numerically exact quantum Monte Carlo results, using hexagonal nano-flakes as a test bed.

Microfluidic Single-Cell Analysis and Manipulation

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Micro- and nano-scale bioengineering and biomedical technologies are becoming pivotal in health sciences. In particular, single-cell analysis has recently allowed the discovery of novel antibiotics (1), the cultivation of microorganisms from the Human Most Wanted Taxa (2) and an enhanced understanding of key biological phenomena such as antibiotic susceptibility in bacteria, gene expression and stem cell pluripotency (3). In the first part of my talk I will introduce a microfluidic-microscopy platform to mechanically phenotype live mammalian cells including embryonic stem cells. I will show that the nuclei of some embryonic stem cells display a unique material property that is they are auxetic exhibiting a cross-sectional expansion when stretched and a cross-sectional contraction when compressed (4). In the second part of my talk I will present a microfluidic platform for isolating single bacteria and investigating their response to environmental stress in terms of changes in their physiological state and in the expression of key genes.

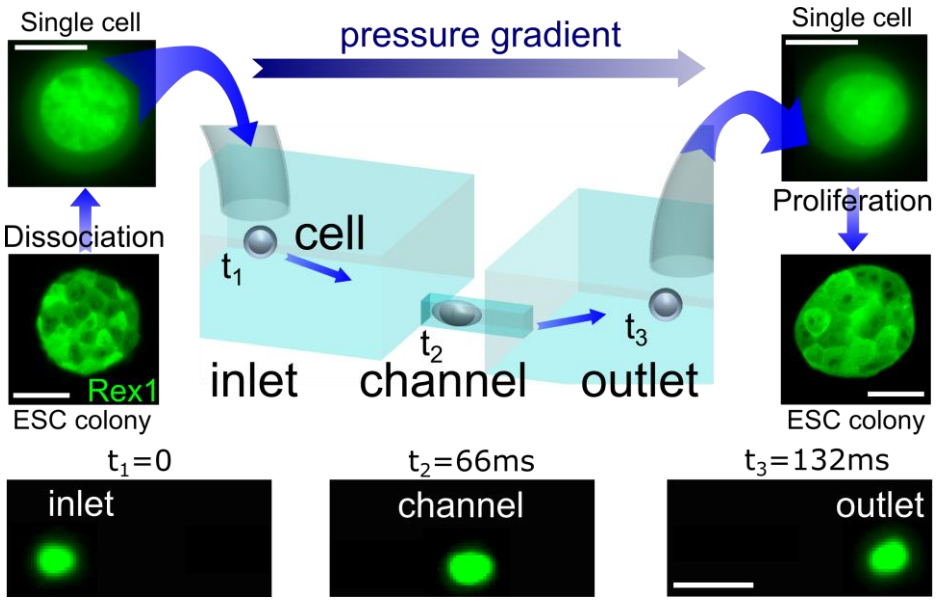

FIG. 1. Schematics illustrating mechanical phenotyping of single live embryonic stem cells.

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Polymeric and Hydrogel Coatings – Particle and Capsule Functionalization

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Soft matter materials are becoming essential components in designing advanced biomedical devices and applications. Drug delivery is an area where development of particles is sought, but particles find important applications in functionalization of coatings, which is essential for understanding cell and cell-surface interaction and for tissue engineering, in general. Two different, but complementary approaches, in regard with polymer state, hydrogels and polyelectrolyte multilayers coatings will be discussed. Functionalization of such soft matter materials with particles brings important functionalities allowing to control the cross-linking process and mechanical properties, while adding capabilities of capsule functionalization of the coatings. We shall discuss physico-chemical analysis of the above mentioned coatings with an eye on applications of the developed structures in cell cultures and in-vivo.

Cell-Like Hydrogel Beads as Mechanical Probes for Biophysical Applications

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Cells and tissues mechanical properties are receiving growing interest in biomedical research. It has been demonstrated how such properties can be used as a marker-free way of quantifying physiological and pathological changes in cells [1]. Following these findings, different technologies have been developed to measure cell stiffness [2]. The basic idea is based on the opportunity to induce and measure deformation (strain) in cells applying a certain force (stress). Due to their complexity, variation and viscoelastic properties, cell lines cannot be used as standard samples. Furthermore, the results obtained with one technology cannot be validated by another one, leading to an uncertainty on the efficiency of the model employed for the data analysis. In this scenario, the development of synthetic, pure elastic particles that can be used to validate the mechanical measurements would be beneficial. Such artificial probe has to provide the same results independently from the employed technology. Hydrogels represent suitable materials for this purpose, and, among them, polyacrylamide gel (PAAm) has been accepted as a linearly elastic material. Nevertheless, different factors can affect the network formation, leading to heterogeneities that affect gel physical properties such as swelling, elasticity, transparency and permeability [3]. Here, we illustrate the production, characterization and functionalization of different PAAm micro-beads, obtained by using a flow focusing microfluidic device. We investigated different gel compositions keeping the cross-linker (bis-acrylamide) to monomers (bys-acrylamide+acrylamide) ratio concentration constant and changing the total monomers concentration. Size distribution, swelling and refractive index were measured in order to analyze beads homogeneity and structural properties (cross-link density and mesh size). AFM [4] indentation and RT-DC [5] analysis of beads elastic properties, showed that, under specific correction to the employed models, these techniques provide comparable values of microgel bead stiffness. Furthermore, we demonstrated that beads polydispersity in stiffness (due to the intrinsic incorporated defects) can be reduced through FACS sorting. Finally, NHS-acrylate was introduced to the gel composition to allow for beads functionalization with proteins. To demonstrate their applicability as stress tensors in developmental biology, PLL-functionalized beads were injected in zebrafish embryos, where their interaction with the surrounding cells was showed by beads deformation during embryo development.

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In Situ Generation of Open Shell Phenalenyl: Towards Designing Novel Multifunctional Materials

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Open shell phenalenyl chemistry started more than 50 years back and the first solid state phenalenyl radical was realized only 15 years ago highlighting the synthetic challenges associated in stabilizing carbon based radical chemistry though it has great promise as building blocks for molecular electronics and multifunctional materials.[1] Alternatively, we developped in recent years that a stable closed shell phenalenyl has tremendous potential as this can be utilized to create in situ open shell state by external spin injection. In this way we have prepared new route to closed shell phenalenyl based organometallic catalysts for various organic transformations, organocatalysts and molecular spin memory device. In this presentation, I shall emphasize on our recent effort in developping novel materials based on phenalenyl molecules.[2-4]

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Future of Organic Solar Cells and Organic Light Emitting Diodes: Materials, Processing and Application

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Recent achievements on the use of nanocomposites such as nanostructured composites with a structure of nanoparticles embedded in polymers (NIP) and nanocomposites with a structure of polymers deposited on nanoporous thin films (PON) for Organic Light Emitting Diodes (OLED) and Solar Cells (OSC) are presented in this work. For the hole transport layer (HTL), nanocrystalline TiO_2 nanoparticles were embedded in polyethylenedioxythiophene: Poly(4-styrenesulfonate) (PEDOT"PSS). The influence of nanooxides on the photoelectric properties of the NIPs is explained with regard to the fact that TiO_2 particles usually form a type-II heterojunction with a polymer matrix, which essentially results in the separation of nonequilibrium electrons and holes. Conjugate polymer luminescence quenching is strongly dependent on the nature of nanostructural particles embedded in polymer matrice. Actually, the higher quenching of the polymer fluorescence observed in presence of TiO_2 nanoparticles proves that the transfer of the photogenerated electrons to the TiO_2 is more efficient for rods. Characterization of the nanocomposite films showed that both the current-voltage characteristics and the photoluminescent properties of the NIP nanocomposite materials were significantly enhanced in comparison with the standard polymers. OLEDs made from these layers demonstrate high photonic efficiency. PON structure are suitable for use in a reverse OLED, where the light goes out through a transparent or semi-transparent cathode; moreover, it is much easier to make Ohmic contact to the metallic Ti electrode. The output power, the luminous efficiency, the peak wavelength and the full width at half-maximum (FWHM) of the deep-blue OLED were 1.5 mW, 1.0 cd/A, 455 nm and 100 nm, respectively, at a forward current of 30 mA.
For OSCc, the operating-temperature range for photovoltaic device parameters can be improved due to the addition of nc-TiO_2 in the polymeric photoactive layer, for instance, a P3HT+nc-TiO_2. The photovoltaic conversion efficiency was reached a value of 1.72%. The enhancement in the photoelectrical conversion efficiency of the solar composite-based cells is attributed to the presence of nano-heterojunctions of TiO_2/P3HT. For the temperature range of (30 – 70) ^oC, the decrease of the open-circuit potential was compensated by an increase of the fill factor; and the increase in the short-circuit current resulted in an overall increase of the energy conversion efficiency. At elevated temperatures of 60 – 80^oC the efficiency of the pure P3HT-OSC and SCC cells reached a maximum value of 1.6% and 2.1%, respectively. Over this temperature range the efficiency of P3HT-based cell decreased strongly to zero, while for the composite cells it maintained a value as large as 1.2 % at a temperature range of (110 – 140) ^oC. The improved thermal stability of the composite-based device was attributed to the lowered thermal expansion coefficient of the nanocomposite photoactive layer.

Keywords: Nanocomposite, Organic light emitting diode, Organic Solar Cell, Photoluminescence, PL-quenching, Current-Voltage characteristics.

Spin Transport and Molecular Orientation in Hybrid Magnetic Tunnel Junctions

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A Spin transport phenomena through a Cu-phthalocyanine (CuPc) barrier with and without an ultrathin MgO(001) layer were investigated systematically as a function of CuPc thickness ranging from 1 to 10 nm. An epitaxial Fe(001)/MgO(001) layer was utilized as a spin injector, while a polycrystalline Co film as a spin detector. By using new model combined with tunneling and hopping, we analyzed the spin transport across the MgO/CuPc hybrid barrier. For the MgO/CuPC hybrid barrier with a total thickness of ~ 3 nm, we observed mageneto-resistance (MR) values of ~ 120 and ~ 10 % at 77 and 300 K, respectively. To our knowledge so far, it is the largest MR value reported at 77 K in organic-based magnetic tunnel junctions.

In order to understand the role of MgO(001) thin layer in the spin transport properties of these MTJs, the interfacial electronic structures were investigated by using the surface sensitive technique of spin-polarized metastable de-excitation spectroscopy (SP-MDS). These findings have significant implications for the understanding of spin injection from a ferromagnetic (FM) layer into an organic semiconductor (OSC), and highlight the importance of adsorption geometry and interfacial exchange coupling in the process of spin injection.

Our results provide significant new insights into the spin injection phenomenon at the FM/OSC interface and the operation of molecular spintronic devices.

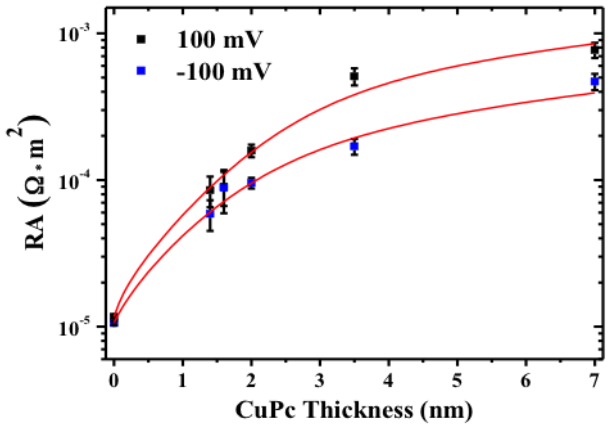

FIG. 1. Resistance-area product as a function of CuPc barrier thickness measured on magnetic tunnel junctions with MgO(001)/CuPc hybrid barriers

Computational NanoMaterials Design: From Basics to Actual Application

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The increasing demand for more advanced technology, coupled with the astonishing development of nanotechnology in the 21st century, necessitates the more advanced techniques in the elucidation of material function formation mechanisms and realization of new generation functional materials. With the advent of advanced computational facilities and techniques, Computational Materials Design (CMD®) [1] is now a reality. Here, the fundamental properties of materials are accurately calculated through first-principles (*Ab-Initio*) calculations; that is, the properties of materials are calculated accurately from fundamental equations of quantum theory without empirical parameters. It's impact on industrial research and development has become very significant in the past years and is expected to grow in the coming years with the explosion of the number of granted patents purely based on CMD.

In the conference, the current state-of-the-art facilities in Materials Design, esp., efforts being made to employ CMD techniques (cf., e.g. [1,2]), together with the associated (Surface) Reaction Design (CRD) techniques [3] will be discussed; highlighting benchmark systems such as bio-inspired materials design, role of inducing spin polarization, surface design through alloying and controlling the dynamics of reaction partners, with special attention to Fuel Cell, Spintronics, Gas Purification System, Steam Methane Reforming and Memory Device applications [1-10].

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Application of Crystallography to High-Throughput Calculations

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Data-oriented materials research is becoming more and more common, with many studies employing high-throughput first-principles calculations based on density functional theory. However, systematic calculations on surfaces remain a blue ocean. One huge complication is polarity, where "polar" surfaces must be stabilized in a case-by-case scenario [1]. The "crystal form" and "isometry" concepts in crystallography can be applied to create an algorithm that, once a crystal structure of any space group type is given, automatically identifies whether a surface orientation always gives polar slabs or not and derives a set of nonpolar and stoichiometric slab models, if any exist [2]. For instance, a nonpolar stoichiometric slab model for β-Ga_2O_3 with the $(20\bar{1})$ orientation can be built using the algorithm (Fig. 1), which would be difficult to make by hand.

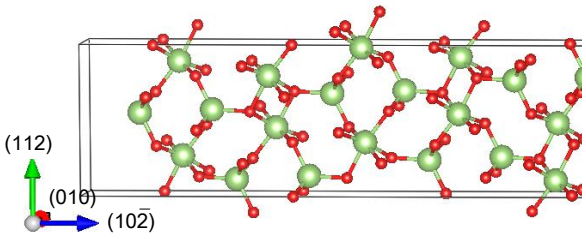

Fig. 1. β-Ga_2O_3 slab with $(20\bar{1})$ orientation. Box shows a supercell to be used in calculations.

Determination of a recommended band path when drawing electronic structure diagrams is not as trivial as it looks. The symmetry of the crystal and restrictions on the electronic band structure at Brillouin zone boundaries, which are independent characteristics, must be taken into account, and points and lines with high symmetry are to be included in the band path. Remarkably, the recommended band path depends on the point group in some Bravais lattices because of orbit splitting with symmetry reduction within the same Bravais lattice (example in simple cubic lattice shown in Fig. 2) [3].

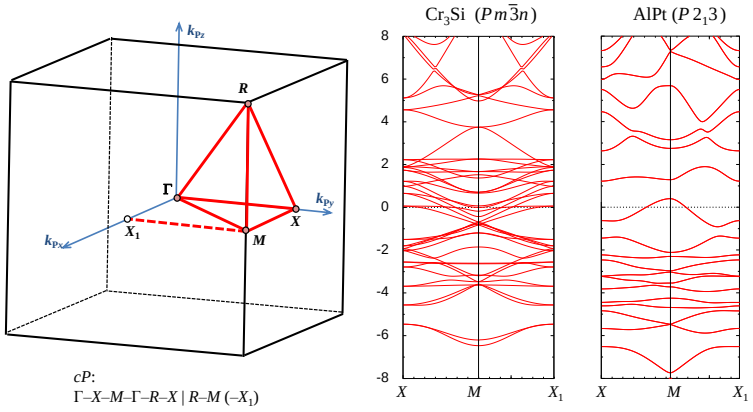

Fig. 2. Recommended band path and electronic band diagrams (same segments within the recommended path) for Cr_3Si and AlPt.

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First-principles and Semi-empirical Methods of Calculations of Optical Properties of Functional Materials

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Combination of the first-principles and semi-empirical methods of calculations of optical properties of solids with impurity ions (such as transition metal or rare earth ions) is a useful approach to gain a deeper understanding of interaction between impurities and host materials [1-3]. Special attention should be paid to the position of the impurity ions energy levels in the host band gap, since it determines the application potential of a particular material. By combining the crystal field theory with the first-principles calculations of the electronic structure of solids it is possible to plot complete energy level diagrams that includes electronic band structure of the host and impurity energy levels (Fig. 1). Several examples of calculations and analysis of optical and electronic properties of doped materials will be presented and discussed in details

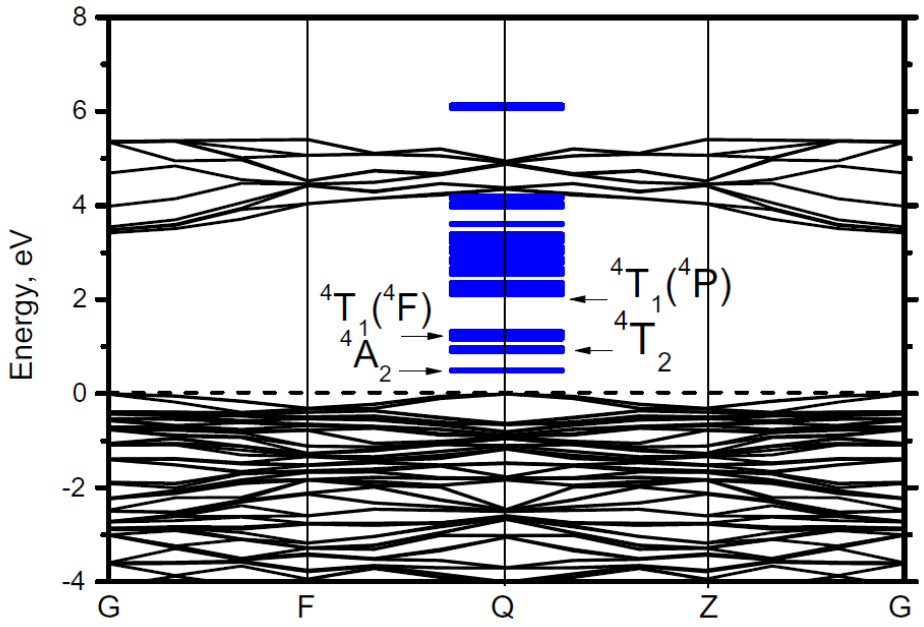

FIG. 1. Energy level scheme of $ZnAl_2S_4:Co^{2+}$ [1].

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Topological insulators: magnetism, strong electron correlation and ferroelectricity

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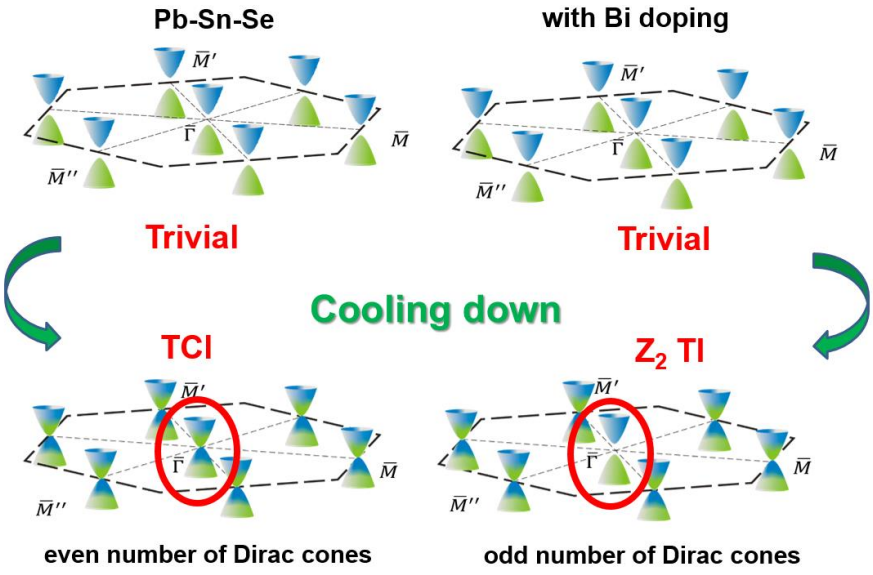
Topological matter is of high current interest as the bestowal of the Nobel prizes 2016 shows. Generally, a topological insulator features a metallic surface protected by time-reversal symmetry and an isulating bulk. We start from the first prediction of spin-orbit coupled topological systems for the example of graphene and discuss the properties of three-dimensional topological insulators through their signatures in spin- and angle-resolved photoelectron spectroscopy. We discuss the magnetic functionalization of topological insulators and the conditions for the creation of magnetic band gaps by impurities as they are a necessary condition for the quantum anomalous Hall effect. Topological insulators are a pure band structure effect, however, electron correlation would add interesting aspects. SmB_6 has meanwhile been established as the first correlated topological insulator and the first topological Kondo insulator. We show, however, that the existing ARPES evidence does not support topological surface states and that the surface metallicity of SmB_6 has a simple, topologically trivial origin. So-called topological crystalline insulators are more vulnerable systems where surface states are protected by mirror symmetries only instead of time-reversal symmetry. We show that the system $Pb_{1-x}Sn_xSe$ can be driven by doping into a topological quantum phase transition from mirror- to time-reversal symmetry protection.



Ultrafast Spin Dynamics in CoFeB/MgO/CoFeB Magnetic Tunnel Junctions

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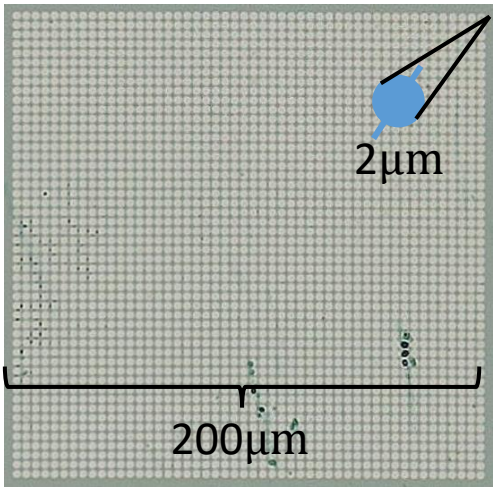
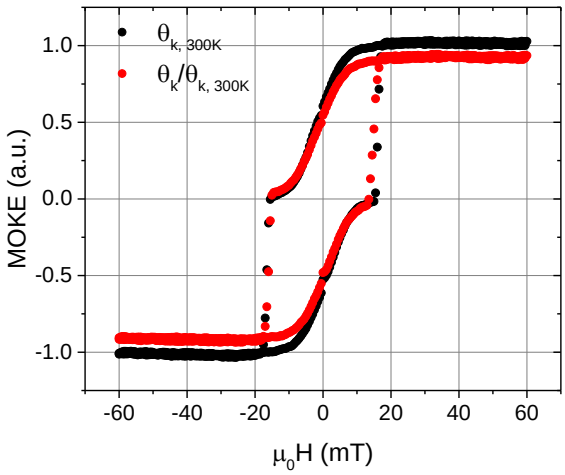
CoFeB films with layer thicknesses between 0.8nm and 1.3nm show an out-of-plane magnetic anisotropy (PMA). Choosing films with two different thicknesses within this range, separating those with a crystalline MgO barrier and patterning them into micrometer sized circles, creates magnetic tunnel junctions (MTJ), the so called pseudo spin valves. Due to different thickness, both layers have different anisotropy strength leading to different coercive fields. This sample layout allows to set two different configurations. One in parallel and the other in antiparallel magnetization of both layers.
In 2013 He et al. [1] have shown, that the laser excitation of magnetization dynamics in such layered f can induce an exchange of spins through the MgO barrier. We extend those measurements to samples with patterned circular structures with diameters from 1 µm to 5 µm and observe both processes in individual MTJs. Due to the small sizes and a crystalline structure, the exchange of spins through the MgO barrier takes place by coherent tunneling. The dynamics are probed using both, the Kerr rotation and ellipticity. Because the stacks are thinner than the penetration depth of the laser light, each component provides the information at different depths of the layer stack [2]. Thus we observe the dynamics from both magnetic layers individually, gaining insight into the processes inside, which stem from spin-flip scattering and from spin-polarized transport. Both, the spin dynamics and the spin transport depend on the properties of the magnetic electrodes and the tunnel barrier.





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Ultrafast Laser Pulse Switching the Magnetization of FePt Nanoparticles Deterministically for Data Storage Application

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FePt granular medium is a special material of interest for application in magnetic data storage. Writing on these nanoparticular medium with optical angular momentum was reported[1] although the mechanism remained unclear. In our work[2] we study experimentally and theoretically the all optical switching of FePt and show that the magnetization switching is a stochastic process. A complete multiscale model was developed which allowed us to optimize the number of laser shots needed to switch the magnetization of high anisotropy FePt nanoparticles. We have predicted that only angular momentum induced by Inverse Faraday Effect (IFE) can do the deterministic switching with only one pulse by choosing the desired circular polarization of the laser output. Our latest experiments prove that that there is a strong dependence of IFE on the photon energy and also prove that it is indeed possible to switch the magnetization deterministically using one laser pulse.

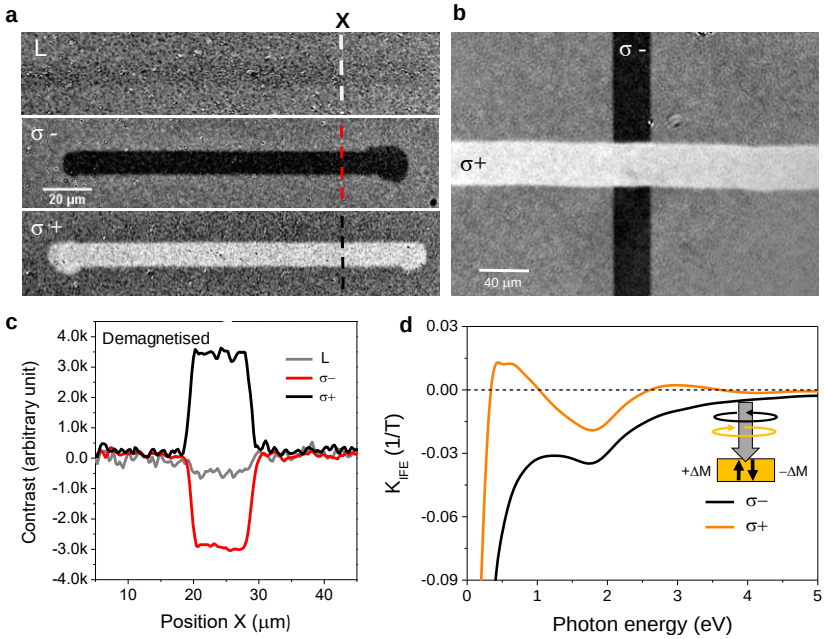

Figure 1. (a) Magneto optical contrast images, starting with a demagnetised sample one obtains opposite contrasts for switching with right and left circular polarizations of laser. (b) Overwriting is possible with contrast reverses independent of the initial state of magnetization. (c) contrast profiles along the line (X) in (a) for the 3 polarization states and (d) the dependence of IFE on photon energy giving us indication of the optimum photon energy for all-optical switching.

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Spintronic Emitters of Ultrashort Terahertz Pulses

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Sub-picosecond terahertz (THz) electromagnetic pulses are a powerful tool to probe and even control numerous low-energy modes of condensed matter [1]. Examples include phonons, excitons, free electrons and Cooper pairs. To date, the generation of THz pulses with a spectrum covering the full THz window from 1 to 30 THz is still challenging and requires miilijoule-class femtosecond lasers.

Here, we employ a new emitter concept based on recently discovered spintronic effects. By using nanojoule optical pulses from a standard femtosecond laser oscillator, we launch spin transport from a ferromagnetic (e.g. iron) into a heavy-metal thin film (e.g. platinum). The inverse spin Hall effect deflects spin-up and spin-down electrons in opposite directions, thereby resulting in a transverse charge current burst that acts as a source of a THz pulse [2]. Optimization of the spintronic thin-film structure has led to new, efficient and scalable emitters of THz pulses that fully cover the range from 1 to 30 THz without gap [3]. By upscaling of the emitter area and the pump-pulse energy, we are able to generate THz pulses with peak fields as large as 0.3 MV/cm.

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Active and Passive Control of Dissipation in Light-Induced Coherent Ultrafast Dynamics

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In this talk I will speak about light-induced coherent dynamical processes in the spin- and in the lattice system. Regarding the latter, I will show how the elastic response of metallic nano-cavities can be tailored by tuning the interplay with an underlying phononic superlattice. In particular, we optically address a resonance mode in a Tungsten thin film, grown on top of a periodic MgO/ZrO_2 multilayer. Setting up a simple theoretical model, we can explain our findings by the coupling of the resonance in the Tungsten layer to an evanescent surface mode in the superlattice. To demonstrate a potential benefit of our findings beyond characterization of elastic properties of multilayer samples, we show by micromagnetic simulation how a similar structure can be utilized for magneto-elastic excitation of exchange-dominated spin waves.
In the second part of the talk I will elucidate how spin currents can affect light-induced magnetization dynamics, as a more active way to compensate dynamic losses. Here, we investigate a simple trilayer system, consisting of 8 nm β-Tantalum, 5 nm CoFeB, capped by 3 nm Ruthenium. Due to the spin Hall effect, the Ta layer generates a transverse spin current when a lateral charge current passes through the strip. We monitor changes of the dynamics by means of time-resolved all-optical pump-probe spectroscopy. We find an impact on the nanosecond Gilbert damping, as well as on ultrashort processes.

Regarding both projects, we acknowledge financial support by the DFG within CRC 1073.

Modelling THz Spin Dynamics

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Understanding the dynamics of a spin system that can be triggered by laser light is one of the most interesting and promising branches of modern magnetism. The first observation of an ultrafast, laser-induced magnetisation dynamics was the demagnetisation dynamics of ferromagnetic transition metals [1]. Optical frequencies were used and the spin dynamics followed from the heating of the electronic system. A rapid heating process alone can even trigger magnetization switching in certain ferrimagnets on sub-picosecond time scales - a promising discovery for future data storage applications [2]. Additional opto-magnetic effects like the inverse Faraday effect or a circular magnetic dichroism allow for an exploitation of their helicity-dependence to control the result of the switching process [3].
In comparison the THz-range of laser pulses has been less investigated and this talk summarizes our recent findings regarding the spin dynamics triggered by ultra-short laser pulses in the THz regime. In insulating antiferromagnets, heating is less relevant, while the time dependent B-field component of the light can excite the spin system resonantly [4]. Using analytical calculations as well as computer simulations we show that antiferromagnets can even be switched on a time scale of picoseconds using THz laser pulses only [5]. This all-optically triggered switching mechanism rests on the coordinated dynamics of the two interacting sub-lattices with an inertial character. We calculate the resonance frequencies in the non-linear regime, the orbits, and estimate the field strength required for switching analytically. Furthermore, we demonstrate that ferrimagnets can be switched similarly at their compensation point.
For ferromagnetic metals the situation is different. While the THz magnetic field component provides a direct route to coherently control the magnetization where the observed off-resonantly excited spin precession is phase-locked to the THz magnetic field, at strong THz fields, the coherent spin dynamics become convoluted with an ultrafast incoherent magnetic quenching due to the heating [6]. This demagnetization takes place upon a single shot exposure time. We find that, although the spins precess in response to the THz magnetic field, magnetization switching cannot be reached.

Acknowledgment: This work is supported by the Center for Applied Photonics at the University of Konstanz.

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Development of Functional Dielectric Materials in Silicates and Aluminates

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Development of eco-friendly materials have recently been attracted keen attention due to growing environmental concerns. Our group focuses on designing novel functional dielectric oxides, which are mainly composed of silicate and aluminate polyhedra of excellent environmental affinity and rich natural abundance. Though the silicates and the aluminates possess fine refractoriness and strong corrosion resistance, there have been few reports on electronic functionalities for them. Here I show two functional oxides that have developed recently in our group: ferroelectric stuffed zeolites and reduced $LaAlO_3$ with a photo-dielectric effect.

Ferroelectric stuffed zeolites:

A stuffed aluminate sodalite, $A_8[Al_{12}O_{24}](XO_4)_2$, belongs to the stuffed zeolites family with a sodalite-type framework of $[Al_{12}O_{24}]$. Ferroelectricity of the stuffed zeolites family was first reported in $Sr_8[Al_{12}O_{24}](CrO_4)_2$.[1] Since $Sr_8[Al_{12}O_{24}](CrO_4)_2$ is partially composed of the toxic hexavalent chromium, we have explored the ferroelectric stuffed aluminate sodalite without chromium. In the present study, the ferroelectricity in $A_8[Al_{12}O_{24}](XO_4)_2$ (A = Ca, Sr and X = Mo, W) is demonstrated by dielectric and pyroelectric measurements.[2,3] Systematic investigations with first-principles calculations and structural analyses using synchrotron x-ray diffraction clarify a mechanism of ferroelectricity in the stuffed aluminate sodalites.

Reduced $LaAlO_3$ with a photo-dielectric effect:

Dielectric materials are ubiquitously applied in electronics as capacitors, frequency filters, and so on. An optical control of dielectric response is thus expected to provide a new route to the development of innovative photo-electronic devices. A change of dielectric permittivity due to photo-irradiation (photo-dielectric effect: PDE) has been reported to date in several sulfides and oxides.[4,5] Almost all PDE are, however, recognized as an extrinsic effect due to the photoconduction, which fatally deteriorate an insulating property of the material. In the present study, an intrinsic PDE has been demonstrated in reduced $LaAlO_3$ with dielectric measurements under the photo-irradiation.[6] An origin of the intrinsic PDE is suggested to be dielectric response of strongly localized photo-excited carriers trapped in non-dispersive in-gap states due to oxygen-vacancies.

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Strain Disorder: A New Degree of Freedom to Control Structurally Dissimilar Magnetic Phase Separation in $La_{5/8-y}Pr_yCa_{3/8}MnO_3$ Epitaxial Thin Films

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Understanding of micrometer sized phase separation in $La_{5/8-y}Pr_yCa_{3/8}MnO_3$ (LPCMO) has been debated. Some researcher believed that strain interaction between structurally dissimilar magnetically contrasting phases shapes the larger sized phase separation. Present study reveals that the length-scale of phase separation in $La_{5/8-y}Pr_yCa_{3/8}MnO_3$ thin films can be controlled by strain disorder invoked during the growth and relaxation process of the thin films. Strain disorder provides an additional degree of freedom to tune colossal magnetoresistance.

Reciprocal space mapping of thin films demonstrates coherent epitaxial growth of the films and also evidenced that strain relaxation mechanism during thin film growth resulted in inhomogeneous distribution of lattice strain termed as '*Strain Disorder*'. Presence of '*Strain Disorder*' stabilizes ferromagnetic phase while coherent uniform strain stabilizes antiferromagnetic phase. Raman spectroscopy confirms the coexistence of charge-ordered-insulating and ferromagnetic-metallic phases which are structurally dissimilar and possess $P2_{1/m}$ and R-3C like symmetries, respectively; therefore the larger sized lengthscale of phase separation is found to be highly correlated with strain field inhomogeneities.

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Ab-Initio Multiplet Calculations for X-ray Absorption Spectroscopy: Application to Cathode Materials

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Lithium transition metal (TM) oxides have been extensively studied as cathode materials of lithium ion batteries. Characterization of the TM ions in the cathodes during the charge/discharge cycles is crucial for designing and developing new cathode materials. Recently, soft X-ray absorption spectroscopy (XAS) observing TM $L_{2,3}$-edges, which monitors the TM 2p→3d electric dipole transition, re-attracts the attentions for this purpose. The method is advantageous in the sense that the changes of 3d electronic structure of TM ions during the lithium insertion/extraction can be directly observed. On the other hand, the interpretation of observed spectra is not straightforward. The TM-$L_{2,3}$ XAS shows widely spreading multiplet structures which are originating from the strong electronic interaction between 2p core-hole and 3d electrons. Conventional electronic structure programs for solids based on the density functional theory cannot reproduce the spectra. For the quantitative simulation of those complicated spectra, I have developed the *ab-initio* configuration interaction (CI) method using relativistic molecular orbitals for calculating TM-$L_{2,3}$ spectra [1]. The method has succeeded to quantitatively reproduce TM-$L_{2,3}$ XAS of 3d TM oxides with various oxidation states and local coordination [2].

The *ab-initio* CI method was applied to provide the theoretical fingerprints for TM-$L_{2,3}$ XAS of cathode materials lithium ion batteries [3]. The obtained theoretical spectra should be useful for the analysis of experimental spectra. The oxidation states, spin states, and local atomic structures of TM ions can be determined using those theoretical fingerprints. Fig. 1 shows the theoretical Ni-$L_{2,3}$ XAS of Li_xNiO_2 calculated with different oxidation states and spin states. In this case, Ni ions are 3+, low-spin state in $LiNiO_2$, and oxidized into 4+, low-spin state by Li-extraction. Other results of typical cathode materials, including layered rocksalt and olivine type structures will be shown in the presentation.

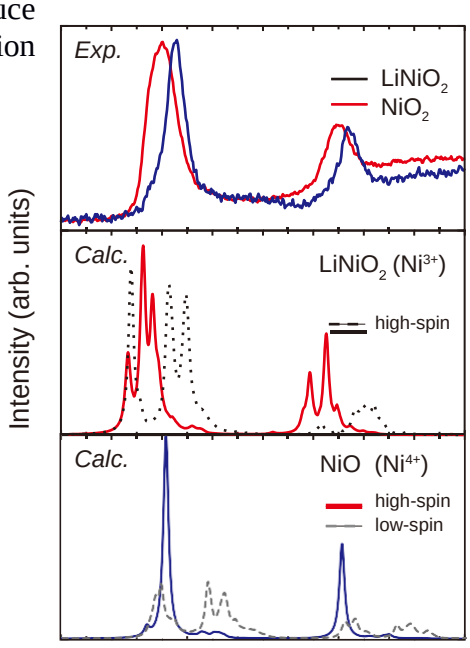

Fig. 1 Experimental and theoretical Ni-$L_{2,3}$ XAS of Li_xNiO_2

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Magnetic Field-Induced Synthesis of Mn-Based Ferromagnetic Alloys

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In this presentation, we will present our recent results of the magnetic field effects on the synthesizing Mn-based ferromagnetic materials. It was found that equilibrium diagrams of Bi-Mn binary system is controlled by applying magnetic fields using a high-field differential thermal analysis [1-3]. The peritectic temperature of MnBi increased by 82 K with applying magnetic field of 45 T [1]. Then, we found that the magnetic field dramatically enhanced the formation of ferromagnetic MnBi from bismuth and manganese during a solid-state reaction sintering [4]. In addition, the c-axis of a hexagonal structure of MnBi was oriented parallel to the magnetic field direction.

Magnetic field changes a metastable ferromagnetic phase into a stable ferromagnetic phase. For example, it has been known that ferromagnetic t-phase MnAl is metastable. t-phase MnAl with a CuAu-type tetragonal structure is a ferromagnetic alloy with a large magnetic moment (M_S = 144 emu/g), high Curie temperature (T_C = 655 K) and large uniaxial anisotropy [5-7]. However, the synthesis of the t-phase is accompanied by the appearance of non-ferromagnetic equilibrium phases because the t-phase is non-equilibrium phase. Therefore, it is difficult to obtain the bulk t-phase MnAl. In this study, in-field heat treatment for MnAl alloys was carried out in magnetic fields up to 15 T to clarify the magnetic field effects on synthesis of the bulk t-phase MnAl. The results clearly show that the in-field heat treatment enhanced the crystallization of ferromagnetic t-phase MnAl [9].

We concluded that the origin of these magnetic field effects on synthesis of the ferromagnetic MnBi and t-phase MnAl is mainly the gain of the Zeeman energy (Magnetic energy).

Acknowledgments:

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First-Principles Study on the Magnetic Anisotropy of Ga-Added Nd-Fe-B Magnets

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Nd-Fe-B magnets are known as the strongest magnets and are installed various kinds of applications for example, vehicles, mobile phones, electric tools, etc. However, the coercivity is quite small at high temperatures and the reason is still unveiled. There are several experimental studies showing that the coercivity of Nd-Fe-B magnets is improved after the Ga addition [1, 2]. Nevertheless, the mechanism of the coercivity improvement due to the added Ga is not clear from the experimental sides. In these Ga-added magnets, the existence of $Nd_6Fe_{13}Ga$ with tetragonal structure around the grain boundaries is confirmed, however, the relationship between the $Nd_6Fe_{13}Ga$ existence around the main phase and the coercivity improvement remains still as an open question.

In order to understand the relationship between the existence of $Nd_6Fe_{13}Ga$ forming the interface with the main phase and the coercivity of Nd-Fe-B magnets, we performed first-principles calculations for $Nd_2Fe_{14}B/Nd_6Fe_{13}Ga$ grain-boundary-model structures as shown in Fig. 1 using a computational code OpenMX [3]. The main purpose of this study is to investigate whether $Nd_6Fe_{13}Ga$ is able to improve the magnetic anisotropy K_1 of Nd at the interface with $Nd_2Fe_{14}B$. We also calculated the formation energies of several model structures. All atomic positions and cell parameters were optimized. After the structural optimization, we can see that atomic positions of the inner region of $Nd_2Fe_{14}B$ and $Nd_6Fe_{13}Ga$ are barely changed after the structural optimization. On the other hand, the interfaces have complicated structures. We also find that the K_1 recovery of Nd at the interface of the main phase in the $Nd_2Fe_{14}B/Nd_6Fe_{13}Ga$ systems is better than that of Cu-doped Nd-Fe-B grain boundary model systems that we calculated in the previous study [4]. By analyzing the spin densities of Nd at the interface, we conclude that Nd 5*d*-electron distribution stretches to the longitudinal direction due to $Nd_6Fe_{13}Ga$, which leads to increasing K_1 of Nd.

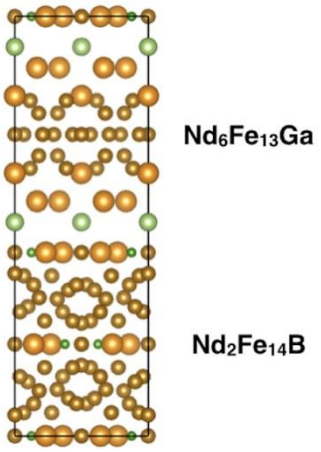

FIG.1. One of the $Nd_2Fe_{14}B/Nd_6(Fe,Ga)_{14}$ model structures.

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Dielectric Properties of $BaTiO_3$ by Molecular Dynamics Simulations Using a Shell Model

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We studied dielectric susceptibilities of $BaTiO_3$ by molecular dynamics (MD) simulations using a shell model[1]. We used a MD program developed by us[2-4]. The Nosé-Hoover chain method and the Parrinello-Rahman method were used for generating constant temperature and constant pressure (NPT) ensembles. The dielectric susceptibilities were calculated by the fluctuation formula. The anisotropies of the dielectric susceptibilities were reproduced, although they are seriously underestimated in all the phases compared to the experiments. The effects of modifying the structure on the dielectric susceptibilities will also be discussed.

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Complex Field Induced Phases in the Frustrated Quantum Spin Chain Linarite, $PbCuSO_4(OH)_2$

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Low-temperature elastic and inelastic neutron diffraction, combined with NMR studies, of the complex magnetic phases in linarite are presented for zero field and magnetic fields $B\|b$ axis [1,2] (Fig. 1). We firmly establish the magnetic exchange parameters, proving that the material represents a model system for the frustrated nearest-neighbor/next-nearest-neighbor (J_1-J_2) spin chain. A two-step spin-flop transition is observed, as well as a transition transforming a helical magnetic ground state into an unusual magnetic phase with sine-wave-modulated moments $\|B$. We discuss our findings within an effective J_1-J_2 single-chain model, with special emphasis on the role of interchain interactions, and the appearance of high-field phases containing exotic multi-magnon bound states.

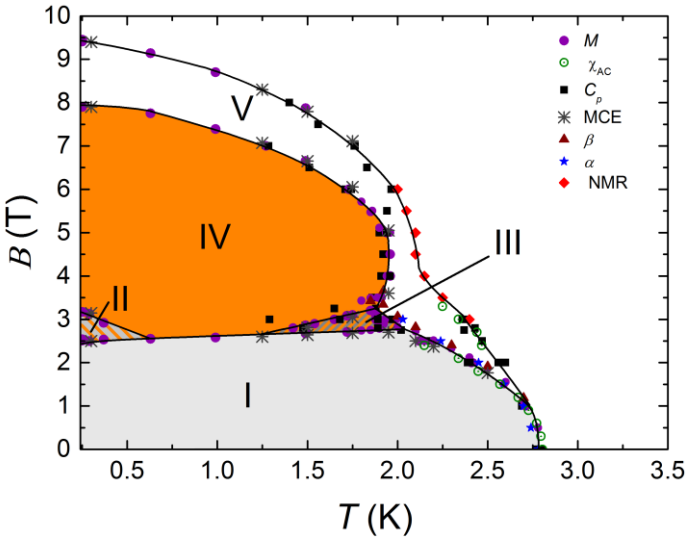

FIG. 1. The magnetic phase diagram for a magnetic field $B\|$b axis of linarite (from Ref. [1]).

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Thermoelectric Properties of Spinel Sulfide $ZnCr_2S_4$ and Electron Transport Calculation using OpenMX and BoltzTraP

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Thermoelectric (TE) conversion, a technology of mutual conversion between thermal energy and electrical energy, is attracting much attention from the viewpoint of resolving waste heat recovery difficulties. Sulfides are attracting attention as alternatives to tellurides because sulfur is an abundant and cheap group 16 element.

In this study, we investigated the TE properties of spinel sulfide $ZnCr_2S_4$ and the Ga substitution $Zn_{1-x}Ga_xCr_2S_4$ based on experimentally and theoretical calculation.

The experimental electrical resistivity ρ of $ZnCr_2S_4$ is very high as an insulator. However, the ρ of $Zn_{1-x}Ga_xCr_2S_4$ (x = 0.10, 0.25, 0.50, 0.75) decreases with increasing temperature, which is a semiconductor behavior. The sign of thermopower S of $Zn_{1-x}Ga_xCr_2S_4$ (x = 0.10, 0.25, 0.50, 0.75) is negative, and that of absolute value and slope of S decreases with increasing x.

The electronic structure of $Zn_{1-x}Ga_xCr_2S_4$ (x = 0, 0.50) was calculated using OpenMX[1] based on density functional theory (DFT). $ZnCr_2S_4$ is spinel-type structure having tetrahedral Zn and octahedral Cr sites as shown in FIG. 1. The density of states (DOS) of $Zn_{1-x}Ga_xCr_2S_4$ (x = 0, 0.50) is presented in FIG. 2. The chemical potential μ of x = 0 locates in the forbidden band, reflecting that the $ZnCr_2S_4$ is an insulator. For x = 0.50, the μ shifts to the conduction band, which denotes that the carrier concentration of $ZnCr_2S_4$ can be controlled by the Ga substitution with Zn sites.

The electron transport calculation of $ZnCr_2S_4$ and electron doped $ZnCr_2S_4$ was performed using OpenMX and BoltzTraP[2]. The sign of the calculated S is negative, and the slope and absolute value of the calculated S decreases with increasing the carrier concentration of electron. This result reproduces the experimental S-T, which indicates that the electron dope is occurred by the Ga substitution of the Zn sites.

The nominal content x dependence of the calculated ZT_{DFT} and the experimental ZT_{Exp} is indicated in FIG. 3. The Ga substitution of $ZnCr_2S_4$ enhances the ZT_{Exp}, and the suitable x is around 0.25, which is agreed with the ZT_{DFT}. These results promise that the theoretical calculation is effective for carrier tuning of the $ZnCr_2S_4$ system.

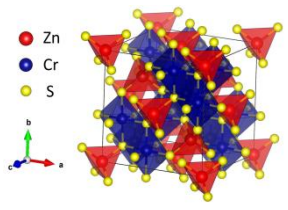

FIG. 1. Crystal structure of $ZnCr_2S_4$.

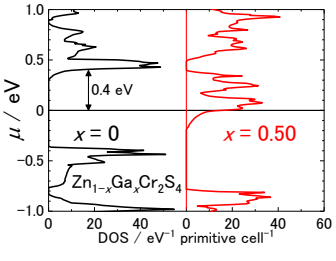

FIG. 2. Density of states for $Zn_{1-x}Ga_xCr_2S_4$ (x = 0, 0.50).

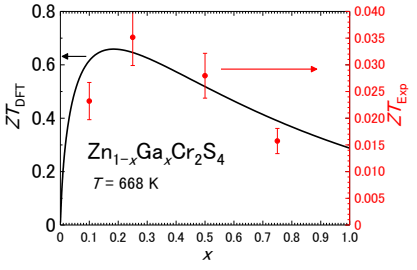

FIG. 3. Nominal content x dependence of experimental and theoretical ZT for $Zn_{1-x}Ga_xCr_2S_4$ at 668 K.

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Correlated Electrons – a Molecular Approach

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Strong electron-electron interactions are the source of intriguing phenomena such as novel types of superconductivity, multiferroicity or spin liquid behavior. In recent years, molecular solids, made up of molecular building blocks have emerged as suitable model systems for exploring these fascinating states of matter under well-controlled conditions.

Of particular interest has been the Mott metal-insulator transition, a paradigm of strong electron-electron correlations. Despite its importance for a wide range of materials, fundamental aspects of the transition are still under debate. A crucial question concerns the role of the lattice degrees of freedom in the Mott transition for real materials. By employing a novel experimental setup enabling high-resolution measurements of relative length changes to be performed as a function of continuously controlled helium-gas pressure [1], we found that the Mott transition in the organic conductor □-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl is accompanied by a highly non-linear strain–stress relation, reflecting a breakdown of Hooke's law of elasticity [2]. We assign this effect to an intimate, non-perturbative coupling of the critical electronic system to the lattice degrees of freedom. Our results are fully consistent with mean-field criticality, predicted for electrons in a compressible lattice with finite shear modulus [3]. We argue that the Mott transition for all systems amenable to pressure tuning shows the universal properties of an isostructural solid-solid transition.

As a second example, we discuss molecular materials close to a quantum phase transition, a $T = 0$ transition driven by strong quantum fluctuations. We could show, in a proof-of-principle demonstration, that this transition, although inaccessible by experiment, can be used for realizing a highly efficient magnetic cooling [4,5].

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Materials for Spin-Orbitronics

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Spintronics promises to be a paradigm shift from using the charge degree of freedom to using the spin degree of freedom. To this end three key requirements are: (i) stable spin structures for long term data retention; (ii) efficient spin manipulation for low power devices and (iii) ideally no susceptibility to stray fields as realized for antiferromagnets.
We explore different materials classes to tackle these challenges and explore the science necessary for a disruptive new technology.
To obtain ultimate stability, topological spin structures that emerge due to the Dzyaloshinskii-Moriya interaction (DMI), such as chiral domain walls and skyrmions are used. These possess a high stability and are of key importance for magnetic memories and logic devices [1,2]. We have investigated in detail the dynamics of topological spin structures, such as chiral domain walls that we can move synchronously with field pulses [3]. We determine in tailored multilayers the DMI [4], which leads to perfectly chiral spin structures.
For ultimately efficient spin manipulation, spin transfer torques are maximized by using highly spin-polarized ferromagnetic materials that we develop and we characterize the spin transport using THz spectroscopy [2]. Furthermore we use spin-orbit torques, that can transfer 10x more angular momentum than conventional spin transfer torques [4-6].
We then combine materials with strong spin-orbit torques and strong DMI where novel topologically stabilized skyrmion spin structure emerge [5]. Using spin-orbit torques we demonstrate in optimized low pinning materials for the first time that we can move a train of skyrmions in a "racetrack"-type device [1] reliably [5,6]. We find that skyrmions exhibit a skyrmion Hall effect leading to a component of the displacement perpendicular to the current flow [6]. We study the field - induced dynamics of skyrmions [7] and find that the trajectory of the skyrmion's position is accurately described by our quasi particle equation of motion. From a fit we are able to deduce the inertial mass of the skyrmion and find it to be much larger than inertia found in any other magnetic system, which can be attributed to the non-trivial topology [7].
Finally we explore spin-orbit effects in antiferromagnets, such as Mn_2Au [8].

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Increase of Pulse Laser-Induced Terahertz-Wave Intensity in Ta/CoFeB/MgO Films by Annealing Process

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Coherent terahertz (THz) wave is emitted from magnetic metal (FM) /heavy metal (HM) layer with a pulse laser shining on films (FIG. 1) [1,2]. The proposed mechanism of THz wave emission is that the ultrafast spin current across FM/HM is induced by the photon absorption then the THz electric current generates in HM by the inverse spin hall effect [1]. In this study, we investigated thickness and annealing temperature dependence of laser-induced THz wave emission in Ta/CoFeB/MgO films to gain the insight into the relationship among magnetization, crystal structure and THz wave emission intensity.

Ta(5.0)/$Co_{20}Fe_{60}B_{20}$(t_{CFB}=0~10.0)/MgO(2.0)/Ta(2.0) (thickness in nm) films were deposited on a thermally oxidized Si substrate by using ultrahigh vacuum magnetron sputtering method and were annealed at various temperature T_a in vacuum for 1 h. The THz wave emitted from the sample was detected by means of an electro-optic sampling with a 1-mm-thick (110) ZnTe crystal with a Ti: sapphire laser and regenerative amplifier. A magnetic field of 1 T was applied parallel to the film plane.

Figure 2 shows the observed peak value of THz wave emission signals as a function of annealing temperature T_a. Peak value of THz wave emission signals increased with increasing annealing temperature, and it was by a factor of 1.5 larger than that for as-deposited films. This result demonstrates that the photon-spin current conversion efficiency can be tuned by the annealing via increasing saturation magnetization and crystallization.

This work was partially supported by the Grants-in-Aid for Scientific Research B (No. 16H03846) and for Innovative areas (Nano Spin Conversion Science, No. 26103004). Y. S. thanks to G. P. spin in Tohoku University.

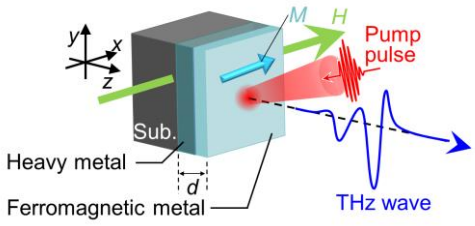

FIG. 1. Geometry of the THz emission from a magnetic metal multilayer. *H*, *M*, and *d* are an applied magnetic field, magnetization, and the total metal thickness, respectively.

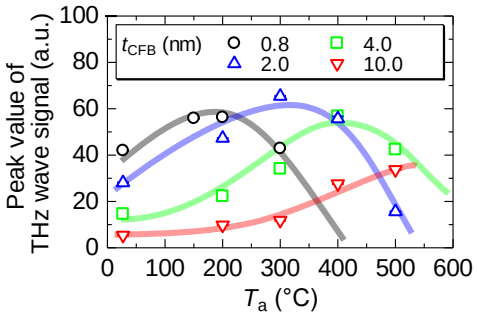

FIG. 2. Annealing temperature T_a

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Spin Absorption Effects due to Various Functional Materials

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Generation, manipulation and detection of spin currents are important issues for the developments of spintronic devices because a spin current plays an important role in spin-dependent transport and spin-transfer switching. Especially, pure spin current which is the spin current without accompanying the charge current is an attractive quantity for utilizing the spin current efficiently. Nonlocal spin valve measurements in laterally configured ferromagnetic metal (FM)/nonmagnetic metal (NM) hybrid nanostructures is a powerful means for evaluating the intriguing properties of pure spin current precisely because of its flexible electrode design. Especially, the reliable results based on the quantitative analysis is an important advantage for the diffusive pure spin current compared with the dynamical spin injection. In this presentation, we show that the spin current transport induced in a nonmagnetic metal are significantly modulated by bring the functional material into the nonmagnetic metal.

First, we show that the pure spin current induced in the nonmagnetic Cu strip is effectively absorbed into the ferromagnetic metal in contact with the Cu strip. Absorbed spin current exerts the torque on the magnetization, resulting in the switching and/or steady precessional motion of magnetization.[1] Also, the absorption rate can be modulated by the spin orientation.[2.3] It should be noted that the absorption efficiency is increases with decreasing temperature. This characteristic provides a consistent description about the unconventional feature of the temperature dependence of the nonlocal spin valve signal.

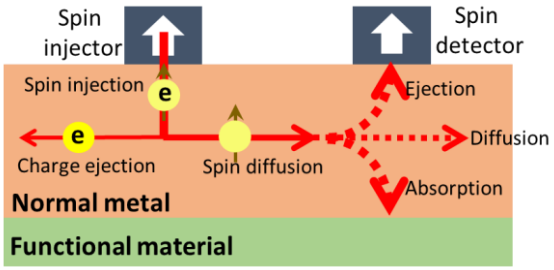

Fig. 1 Nonlocal spin injection, spin diffusion and spin absorption effect

Then, we introduce the spin absorption effect due to the Nb. When the Nb is normal conductor, the spin current is effectively absorbed because of its strong spin-orbit interaction. On the other hand, when the Nb becomes superconductor, the spin absorption is significantly suppressed because of the superconducting gap.[4] Thus, the superconductor is a perfect conductor for the charge current but is an insulator for the spin current.

We also would like to introduce the results on the spin absorption effects on other functional materials such as the anti-ferromagnetic film [5] and transition metals.

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Rocking at the Nanoscale: Controlling and Probing Optically Active Nanosytems by Nanoquakes on a Chip

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Over the past more than 20 years, surface acoustic waves (SAWs) have been applied to probe and manipulate charge, spin, magnetic and optical excitations in condensed matter, in particular semiconductor heterostructures. In this field of fundamental and applied research, these “nanoquakes on a chip” provide a particularly useful and versatile tool for massively parallel addressing a broad variety of nanosystems at radio frequencies via strong acousto-mechanical and acousto-electric couplings.

In this presentation, I highlight our recent advances in the control and probing of fundamental physical properties in electrically and optically active hybrid nanosystems. Specific examples include the contract-free measurement of (i) the transport mobilites of electrons and holes in individual semiconductor nanowires in the native material limit [1] or (ii) photoconductivity in monolayer MoS_2, the archetypical direct bandgap two-dimensional semicondurctor directly grown on $LiNbO_3$ [2].

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Evidence for Electronic Phase Separation in the Diluted Magnetic Semiconductors (Ga,Mn)As and (Ga,Mn)P

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Diluted magnetic semiconductors combine the benefits of semiconducting and magnetic materials and thus are considered as highly promising candidates for future spintronics applications. Although the archetypal compound (Ga,Mn)As has been in the focus of research for already two decades [1], the precise electronic structure and the exact mechanism of the carrier-induced long-range ferromagnetic order are still under debate. In detail, theoretical approaches range from the assumption of free charge carriers (p-d Zener model) to the opposite case of strongly localized carriers (impurity- band model). For the latter case, an intriguing theoretical concept for the origin of spontaneous magnetization is the percolation of magnetic polarons [2]. Motivated by recent results of a diverging 1/f-noise magnitude in the ferromagnetic semimetal EuB_6, where the existence of percolating nanoscale magnetic clusters has been demonstrated [3], we study the low-frequency charge carrier dynamics by resistance noise spectroscopy. Systematic electronic transport measurements were carried out on a series of thin film samples covering a large parameter space with regard to the Mn content and the use of different post-growth treatments, such as thermal annealing and He-ion irradiation, which are commonly applied in order to control the defect characteristics and thus the Curie temperature T_C.

We find a strongly enhanced noise magnitude near the corresponding Curie temperature for samples with localized charge carriers, whereas for metallic compounds with stronger Mn doping the resistance fluctuations are dominated by defect physics and no prominent features occur around T_C [4]. We discuss our results within the context of the major debate on the development of spontaneous magnetization and infer that the impurity-band picture appears to be more appropriate for (Ga,Mn)P and insulating (Ga,Mn)As, whereas the well-established p-d Zener model can be applied to metallic (Ga,Mn)As. Finally, by means of noise spectroscopy and corresponding analysis, we compare the defect landscape of various samples and discuss the effects of the utilized post-growth treatments as well as the possible formation of nanoscale clusters composed of Mn interstitial atoms with a fluctuating spin orientation.

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Theoretical Design of ZnO Nanoporous Crystalline Structures

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Nanoporous framework materials capture a great deal of research attention because of their advantages for a wide range of technology applications in the environment, sensors, shape-selective and bio-catalysis, to name just a few. Within this active research area, computational prediction and theoretical study of these materials are crucial important. We have designed a large family of ZnO nanoporous crystalline structures employing the density functional theory based methods. Our modeling scheme is based on the two approach, "bottom up" and "top down" designs, owing to the advanced nanofabrication techniques. Depending on their secondary building blocks, e.g. ZnO magic cluster cages, nanowire, nanosheet, quantum dot, our modeling crystalline can classified as cage-like hollow, hollow channel, hollow quantum dot nanoporous. For the structural stability, our calculations show that these nanoporous structures could survive in periodic systems without structural collapse, which leads to nanoporous low-density phases of ZnO. Their electronic and thermodynamical properties of the structures, e.g., band structure, free energy and simulated XRD patterns are calculated and discussed in the connection with hollow properties, i.e. shape, size and wall thickness and in the relation with their symmetry. Our results show the convergence of the nonlinear dependences of bulk modulus on hollow's thicknesses of about of larger than three layers regarding to hollow-to-bulk density ratio and the common rule for the dependences on porosity for different type of hollow topology. We also found that these ZnO hollow phases, if synthesized, would preserve the valuable properties of the ZnO materials, such as wide bandgap semiconducting, piezoelectric and optically transparent, while, at the same time, would possess novel properties as of gap engineering possibility.
Keywords: ZnO nanoporous, structure prediction, density functional theory

Memristor-Based Neural Networks

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In recent years, Memristors have attracted great interest for a variety of applications. An obvious use would be as a memory device or, more ambitiously, a reconfigurable logic device. However, the arguably most interesting implementation of memristive devices is neuromorphic computing.

Neuromorphic engineering is a relatively young research field, which was originally proposed by C. Mead in the late 80s. Neuromorphic devices and architectures are designed to emulate the style of computation of biological systems and exploit biological strategies for optimizing robustness to noise and fault tolerance, as well as maximizing compactness and minimizing power consumption. Nevertheless, the most attractive feature of biological systems is their ability to learn and adapt to new situations.

A possible realization of a memristive device is a metal-insulator-metal structure. In particular, this could be a tunnel junction. Then, a 1–3 nm thin insulator separates two metal electrodes. We can apply a bias voltage at this device and measure the corresponding current.

Utilizing the memristive properties, we looked into the use of the junction structures as artificial synapses. We observed analogs of long-term potentiation, long-term depression and spike-time dependent plasticity in these simple two terminal devices. We will explain these mechanisms and their significance in biological systems. Finally, we suggest a possible pathway of these devices towards their integration in neuromorphic systems for storing analog synaptic weights and supporting the implementation of biologically plausible learning mechanisms.

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Reservoir Computing with Spin-Torque Nano-Oscillators

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In this work, we prove that nanoscale magnetic oscillators called spin-torque nano-oscillators [1-3] can be used to emulate the oscillatory behavior of collections of neurons. We first highlight their two main assets for neuromorphic computing: their exceptional ability to synchronize and their well-controlled magnetization dynamics. We then demonstrate experimentally that a single spin-torque oscillator can realize neuromorphic tasks such as spoken digit recognition reaching state of the art performances.

For many tasks such as facial recognition, speech recognition or prediction, the brain processes information much faster and with much less power than any computer. Some models interpret the way brain process information treating the neurons as interconnected non-linear oscillators. In particular, reservoir computing is a recently introduced braininspired computing paradigm [4]. Its efficiency at dealing with complex cognitive tasks such as speech recognition or chaotic series prediction has already been demonstrated [5].

Reservoir computing can be implemented with a recurrent network (the reservoir) composed of an assembly of interconnected oscillators with fixed connections. A fast input signal, encoding the data to process, is applied to the network. The input signal modifies the frequency and amplitude of each oscillator. Different input waveforms will create different transient dynamics in the network, allowing for separation and classification. The responses of all the oscillators are recorded and recombined. This recombination corresponds to the output of the computation. When the input signal is applied to the reservoir of coupled oscillators, the initial problem (classifying the inputs) is projected non-linearly in a higher dimensional state where separation is easier. If the number of non-linear oscillators is sufficient, the projection of the initial problem in the reservoir state is linearly solvable. It is then sufficient to recombine linearly the response of the different oscillators of the reservoir in order to generate different outputs for different inputs. The optimum coefficients are determined using a training procedure, which consists in a simple linear regression. In other words the working principle of reservoir computing is to leverage non-linearity to transform the problem in another one that is easier to solve. Reservoir computing is one of the few neural network approaches demonstrated in hardware. However, existing implementations are restricted to FPGAs or optical systems, where the power consumption is high and oscillators are not nanometric [4,5].

In this context, spin-torque nano-oscillators are particularly promising building blocks for reservoir computing. They have a nanometric size and low energy consumption, they are compatible with CMOS and can be built in large quantities. In addition, these oscillators are highly non-linear and can synchronize to each other. They are therefore ideal candidates to mimic neurons [6]. Here we give the first experimental demonstration of neuromorphic computing with spin-torque nano-oscillators. We show that a single oscillator can emulate the behavior of a whole neural network. By time multiplexing the input waveform we create a temporal complexity which is the analog of the spatial complexity of a network. By exciting the oscillator with this preprocessed signal, we generate complex transient dynamics that we record and recombine. In order to have good performances in term of noise, we use vortex based spin-torque nano-oscillators with FeB free layer. The dynamics of our oscillator is controlled

through the applied dc current and magnetic field. By changing these two parameters we have tuned the oscillator operating point to optimize the neural network-like behavior. By leveraging the transient dynamics of our spin-torque vortex oscillator, we have performed several cognitive tasks. First we have tested our system with a simple pattern recognition task, which consists in discriminating sequences of sine and squares randomly disposed in the input waveform. This task is not trivial since the recognition is piecewise, which means that at each moment the system should recognize if the input value belongs to a square or a sine. We achieved a perfect recognition of sines and squares. Then we moved to speech recognition task, which is more complex (Fig1). Our input signals are recorded digits said by 5 different speakers. After recombining the transients of the oscillator response, we were able to recognize which digit was said and which speaker said it with a success rate of 99,8% [7]. Our results are comparable to the best results observed in hardware reservoir computing [4,5] and open the path to building large spintronics neural networks that exploit magnetization dynamics for computing.

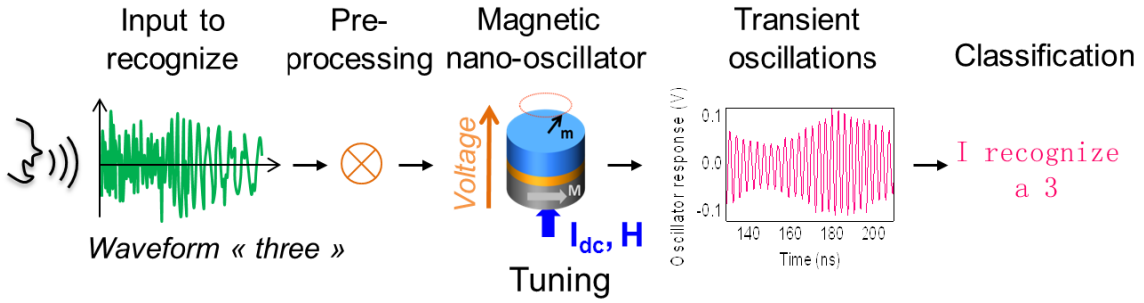

Fig. 1: Principe of speech recognition task leveraging the transient dynamic of a spin-torque nano-oscillator. The digit is recorded. The signal is then preprocessed in order to generate a temporal complexity. The dynamics of the oscillator excited by preprocessed input are transient and interdependent like responses of interconnected neurons. Combining linearly the transients, we are able to recognize the digit.

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Mutually Synchronized Spin Torque and Spin Hall Nano-Oscillators

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In this talk I will discuss our most recent advances in synchronizing both nano-contact spin torque oscillators (NC-STOs) and spin Hall nano-oscillators (SHNOs). The synchronization of NC-STOs [1-3] is mediated by propagating spin waves (SWs), which, under the influence of the local Oersted field, can form SW beams. Not only have we recently demonstrated the robust synchronization between two oscillators separated by over 1 micron, but also the driven synchronization of up to five oscillators by purposefully taking advantage of such SW beams [1]. More recently, a new breed of nanoscale magnetic oscillator, which rely on the transverse spin currents generated by the spin Hall effect, have emerged. Our particular SHNO device geometry relies on a nano-constriction [2, 3] to focus the spin currents and stabilize auto-oscillations. By carefully considering the importance of the applied field angle [4] we have demonstrated the robust synchronization of up to nine serially connected SHNOs [5]. The mutual synchronization is observed both as a strong increase in the power and coherence of the electrically measured microwave signal. The mutual synchronization is also optically probed using scanning micro-focused Brillouin light scattering microscopy (μ-BLS), providing the first direct imaging of synchronized nano-magnetic oscillators. Through tailoring of the region connecting two SHNOs, we can extend the synchronization range to 4 μm. Given the design flexibility of nano-constriction SHNOs, and their very long synchronization range, we argue that our results open up many research and application opportunities where coherent phase locking is believed to be advantageous, e.g. for energy efficient spin wave computing on the nanoscale.

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Gold-Based Magnetic Alloys: Fe-Au Thin Films by Heavy Ion Implantation

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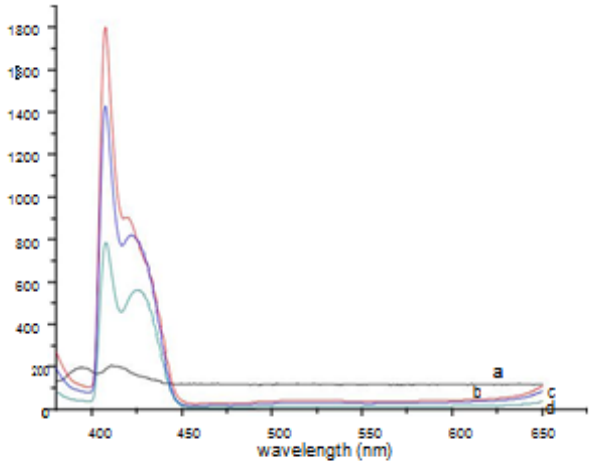
This work reports the experimental results on doped gold-iron alloy thin films which were prepared in acquired molar ratios by mean of the thermal evaporation method. The films were later bombarded with carbon heavy ion source accelerated at 1.7 MV using the linear accelerator Pelletron 5SDH-2 equipped at the VNU-Hanoi University of Science. The characterization of content shows a film was composed of 46.28 wt% iron and 52.72 wt% gold, corresponding to almost exact molecular ratio of 3:1 between iron and gold. The films possess a well defined fcc structures but with slightly modified lattice constants due to the doping contents (alias, the time of bombardment). The optical behavior of the films shows a strong absorption band in the violet region and exhibits a considerable photoluminescence with a maximum at around 415 nm. The electric conductivity of the doped films is recognizably lower than that if the un-doped films and all the films are still ferromagnetic at the temperature between 80 and 1100 K.

Keywords. Gold-Iron, carbide, nanostructure, novel materials



Photoluminescence spectra of the Fe-Au thin films

Micro-Hall Magnetometry Studies of 2D and 3D Magnetic Nanostructures

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Micro-Hall magnetometry, where the magnetization of a sample is investigated via the response of a GaAs/AlGaAs-based Hall sensor to the stray field emanating from a magnetic sample, is a versatile method that allows for studying the local magnetic induction of macro- and microscopic samples [1]. In addition, the method is particularly well suited for measuring stray fields of individual or small arrays of magnetic nanostructures in a wide range of temperatures and external magnetic fields.

In the last years, we demonstrated the capability of investigating the intrinsic properties of a single magnetic nano-element by studying individual and small clusters of Co nano-islands in a frustrated lattice (2D artificial spin-ice) fabricated by focused electron beam induced deposition (FEBID) [2]. Besides the fundamental switching processes and their thermal dynamics, we have utilized micro-Hall magnetometry to measure first-order reversal curves (FORC) [3] in order to investigate interaction effects in the dipolar-coupled arrays.

The FEBID technique is a highly flexible direct-write fabrication method which allows for excellent control in creating free-form 3D structures very much like 3D printing on the nanometer scale [4,5]. Very recently, in a collaborative effort, we have succeeded in measuring the stray fields of 2 x 2 arrays of 3D ferromagnetic CoFe nano-cubes and -trees at various temperatures and magnetic field angles. Taking information from microstructure analysis into account, micromagnetic and macro-spin simulations have been performed that allow us to deduce the spatial magnetization profiles in the structures and analyze their switching behavior. Our findings pave the way for future work on 3D artificial spin-ice which is but one example of various other possible application fields of 3D magnetic FEBID structures on the single-element and array basis.

The work has been done at the Institute of Physics, Goethe-University Frankfurt, in collaboration with Merlin Pohlit, Mohanad Al Mamoori and Jonathan Pieper (micro-Hall measurements), and Lukas Keller, Dr. Fabrizio Porrati and Prof. Michael Huth (FEBID).

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Ultrafast STM Driven by THz Fields

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State-of-the-art scanning tunneling microscopy (STM) is capable of steady-state imaging, spectroscopy, and manipulation of molecules with atomic resolution [1]. Pictures of individual molecular orbitals can even be captured in real space by selective tunneling through a specific electronic state. Still STM on the molecular level has lacked the ultrafast temporal resolution that would provide access to molecular motion and chemical reactions on their intrinsic length and time scales. However, the recent invention of terahertz (THz) STM, which utilizes coherent THz control to achieve femtosecond temporal resolution in an STM, has introduced new possibilities [2-5].

Here, we build on the concept of ultrafast THz-STM and demonstrate, for the first time, ultrafast imaging of a single molecular orbital [3]. We enter an unprecedented tunneling regime where the oscillating electric field of a THz pulse removes a single electron from a single molecular orbital of one molecule within a time window faster than an oscillation cycle of the THz wave [3]. Two ultrafast THz- STM snapshot images are shown in Fig. 1: the highest occupied molecular orbital (HOMO) of a pentacene molecule (Fig. 1a) and the lowest unoccupied molecular orbitals (LUMOs) of three nearby pentacene molecules (Fig. 1b).

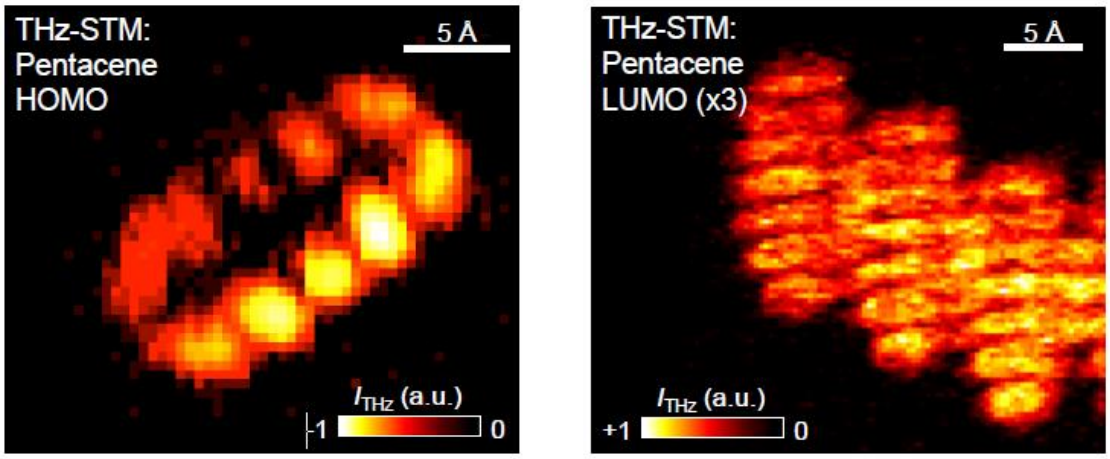

FIG. 1. Femtosecond snapshot images of pentacene molecular orbitals resolved by ultrafast state-selective THz-STM. (a) Highest occupied molecular orbital (HOMO) of a pentacene molecule. (b) Lowest unoccupied molecular orbital of three pentacene molecules, with a fourth just off the image to the right. I_{THz} is the average THz-induced current across the STM tunnel junction, where positive numbers correspond to electron flow from the tip, through the molecule, to the substrate

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Nanoscale Magnetic Imaging Using High-Harmonic Radiation

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Magnetic arrangements and their dynamics span a wide range of length- and time-scale down to few nanometers in space and sub-100-femtosecond in time. Magneto-optical mapping using high-harmonic radiation is very appealing due to the nanometric wavelength and femtosecond temporal accuracy. Here, we demonstrate the first magnetic imaging using high harmonics. We implement coherent diffractive imaging enhanced by Fourier transform holography to reach 60 nm resolution, which is comparable to recent achievements at large scale facilities even at larger field of view and limited only by diffraction [2]. The enhancement mechanism for high spatial resolution relies on the interference of weak magnetic signal with strong reference waves containing fine features. This approach provides a unique possibility for spatially resolved studies of ultrafast magnetization dynamics with the spatial resolution down to few nanometers and unprecedented temporal resolution down to few femtoseconds and even attoseconds.

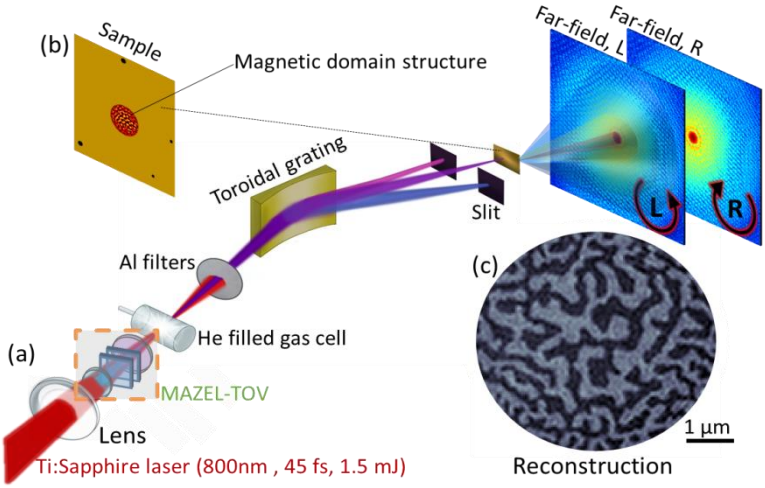

FIG. 1. (a) Schematic of the experimental setup and results. Circularly polarized high harmonics are generated in a He filled gas cell. A toroidal diffraction grating isolates and refocuses 38th harmonic onto the sample (b). Holographic far-field diffraction patterns are recorded for left- and right-hand circularly polarized harmonic. The sample is a Co/Pd multilayer stack exhibiting perpendicular magnetic anisotropy, where an additional 180nm thick gold film serves as a holographic mask. (c) Worm-like domains with out-of-plane magnetization are reconstructed with 60 nm spatial resolution using holographically enhanced coherent diffractive imaging.

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Ultrafast Spin Dynamics Probed By Fs Lasers

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In my presentation I will discuss the current state of understanding of ultrafast spin dynamics, specifically ultrafast magnetization dynamics in metallic ferromagnets. I will highlight the two major competing ideas behind femtomagnetism, Elliot-Yafet scattering [1] and spin transport [2] and discuss selected experiments using the time-revolved magnetooptical Kerr-effect in both the visible regime and using high harmonics [3,4]. After this introduction to the field in general, I will present some of our recent results on femtosecond spin dynamics, where we directly follow the evolution of the electronic band structure of the ferromagnet Co after a femtosecond optical excitation using time-, spin- and angle-resolved photoemission spectroscopy in an IR-pump extreme ultraviolet probe scheme. Here, we want to elucidate whether ultrafast demagnetization, i.e., the ferromagnetic to paramagnetic phase transition, is driven by a collapse of the exchange splitting or by collective excitations, a question, which is yet unanswered. We find that collective excitations seem to be responsible for the loss in magnetization in Co thin films on a Cu substrate via the signature of band-mirroring after laser excitation [5].

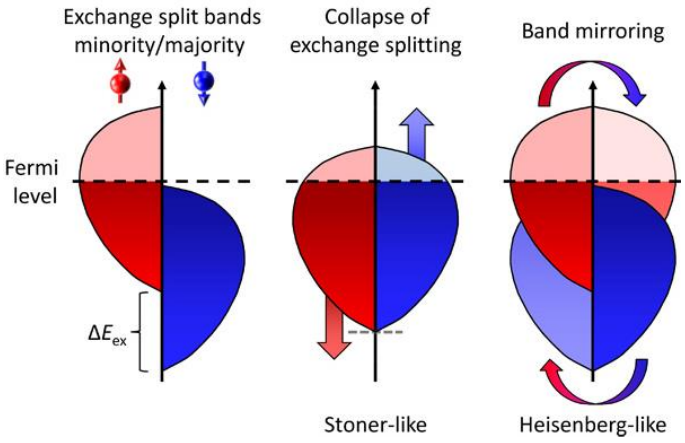

FIG. 1. The two possible microscopic processes responsible for a loss in magnetization after a femtosecond optical stimulus. From Ref. [5]

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InAs Nanowire-Based Devices for Applications in Quantum Information Technology

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InAs nanowires are not only interesting as building blocks for future nanoelectronic device applications they are also very promising candidates for realizing circuits for quantum information processing. Here, two major directions can be identified. First, InAs nanowires can be employed to create Majorana fermions for robust topological quantum computing. One essential prerequisite is the verification of spin helical transport. In quantum point contacts based on InAs nanowires we achieved ballistic transport with quantized conductance (cf. Fig. 1). At the last step a dip feature is observed which is attributed to the presence of helical states [1]. The emergence of this dip feature is explained in the framework of exchange interactions. As a second option InAs nanowires are also interesting for gate-controlled Josephson junctions in transmon qubits. In order to optimize the junction performance, the InAs nanowire is covered in-situ by a superconducting Al or Nb shell. These junctions are subsequently integrated in a superconducting resonator circuit.

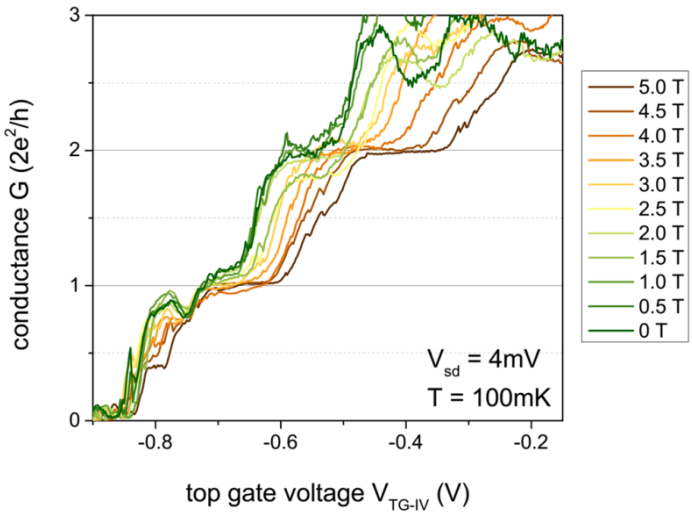

FIG. 1. Quantized conductance of an InAs nanowire at various magnetic fields measured at a temperature of 100 mK. At the first step at $2e^2/h$ a dip feature is observed which is attributed to helical transport.

Work done in collaboration with: D. Grützmacher, Y. Günel, N. Güsken, S. Heedt, M. Lepsa, T. Rieger, J. Schubert, S. Trellenkamp, P. Zellekens (all Jülich), N. Traverso Ziani, F. Crepin, B. Trauzettel (University of Würzburg), F. W. Prost (University Duisburg-Essen), M. Weides, S. Schlör (KIT Karlsruhe).

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1D and 2D hybrid Materials for Nanoelectronics

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Atomically thin materials in 1D and 2D are attracting much interest since reduction of dimensionality strongly modifies their properties and provides a playground to revisit physical phenomena at the nanoscale. The possibility to exfoliate lamellar materials down to the single layer has provided a wealth of 2D materials with a wide range of physical properties. This talk will show that, though individually promising, the intrinsic nature of low dimensional materials along with the vast range of the available properties make it even more stimulating to couple these materials together [1].

Hybrid materials will be discussed in terms of new functionalities. Accent will be put on application of hybrids to nanoelectronic devices. In particular, graphene and nanotubes exhibit outstanding electrical properties and have already been implemented into quantum devices. We have shown that hybrids allow to realize optoelectronic devices with tailor-made light response from room temperature down to the single electron memory regime. In this case tunneling turns out to be light sensitive [2]. Moreover, using normal-superconducting 2D hybrids allowed us to design tunable superconducting devices at the macroscale [3]. From these studies we show the realization of advanced materials with specific functions.

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Electrochemical Deposited ZnO/Magnetic-Metal Hybrid Core/Shell Nanowires for Spintronic Device Application

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ZnO nanowires (NWs) are well-known promising functional nanomaterials for various applications. Furthermore, it is expected that hybrid structures with ZnO and other functional materials will improve the functionalities. Especially, ZnO/magnetic-metal hybrid structures can be useful for spintronic device applications [1]. We investigated ZnO NW synthesis on patterned Si, GaAs, and InP using electrochemical deposition method, which is a low-energy and low-cost process, and obtained good position and orientation controllability [2]. In this paper, we report on ZnO/magnetic-metal hybrid core/shell NWs synthesized by electrochemical deposition method.

The method is schematically shown in Fig. 1. The deposition was carried out using a potentiostat system with Ag/AgCl reference and Pt counter electrodes, and p-Si(111) substrates as working electrodes. For ZnO NW synthesis, a mixture solution of 0.025 M zinc nitrate hexahydrate ($Zn(NO_3)_2 \cdot 6H_2O$) and 0.025 M hexamethylenetetramine ($C_6H_{12}N_4$) was used as the electrolyte. The deposition temperature, time and applied potential were 90 °C, 2 hours and -0.8 V, respectively. For coating of magnetic-metal shells, 0.025 M cobalt (II) acetate ($(CH_3COO)_2Co$) or 0.025 M nickel (II) acetate tetrahydrate ($(CH_3COO)_2Ni \cdot 4H_2O$) solutions was used as the electrolyte. The deposition temperature, and applied potential were 70 °C and -1 V, respectively.

For characterization, we performed scanning electron microscopy (SEM), energy dispersive X-ray (EDX), Raman scattering, X-ray diffraction (XRD), and magnetization measurements using super-conducting quantum interference device magnetometer (SQUID). We confirmed magnetic-metal deposition on hexagonal ZnO NWs by SEM-EDX, Raman scattering, and XRD. We also confirmed ferromagnetic responsea from the NWs at room temperature by SQUID.

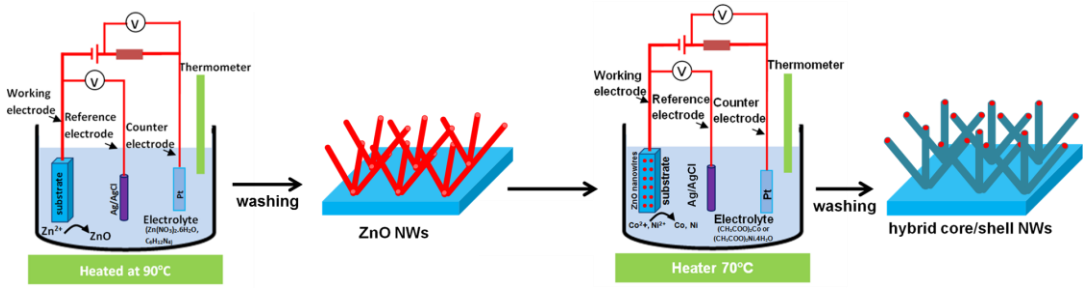

Fig. 1. Schematic illustration of electrochemical deposition method of ZnO/magnetic-metal hybrid core/sell NWs.

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Phase-Locked Dynamic Wide-Field Magneto-Optical Microscopy

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The dynamic imaging of magnetic domains or spin textures in magnetic materials is a prerequisite for understanding the underlying mechanisms of magnetization processes in magnetic systems. Phase-locked, time-, and component-resolved wide-field magneto-optical Kerr effect microscopy offers unique possibilities for the imaging of magnetization dynamics down to the picosecond time-scale. In addition to the imaging of resonant domain wall oscillations and precessional effects, we demonstrate, as an example, the direct imaging of low-damped plane as well as overlapping propagating spin waves. Spin waves are generated in the proximity of domain walls and due to non-uniform internal demagnetization fields in magnetic thin film structures. The findings are of significance for the general understanding of structural and configurational magnetic boundaries for the creation, the propagation, and elimination of spin waves.

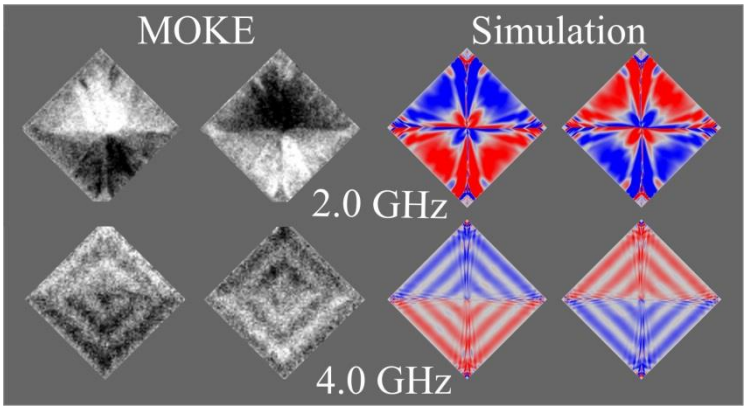

FIG. 1. Edge mediated spin waves in a tilted Landau structure and corresponding modelled spin wave distribution.

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Advanced Spectroscopy Methods: Magnetic Dichroism in Transmission Electron Microscopy

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Novel magnetic functionalities that go along with the properties of nanoscopically small magnetic materials, so-called nanomagnets, are usually brought about by their size and their surfaces or interfaces, e.g., to a substrate or matrix material. Hence, in order to gain a solid understanding of the magnetic properties of nanomagnets, structural characterization with up to atomic resolution of the material of interest is mandatory.

While magnetic properties are usually measured from ensembles of nanomagnets (e.g., from a piece of a hard disk sample), structural peculiarities or modifications of the atomic configuration in particular at surfaces or interfaces occur on a statistical basis and *vary* among such an ensemble. Hence, a comparison of magnetic ensemble properties with microscopic structure information is only of limited value in order to derive reliable structure-property relations for this kind of nanomaterials. Rather, high resolution, i.e., *local* structural characterization needs to be paired up with *local* magnetic measurements on *identical* materials entities. While atomic resolution structural characterization can be traditionally provided for by (aberration-corrected) high-resolution transmission electron microscopy (TEM), recent developments in TEM-based magnetic measurements may even pave the way towards determining structure *and* magnetic properties on identical nano objects.

The present talk will address the potential of a local, TEM-based correlation of structure and magnetic properties. It will be shown as an example, how the understanding of technologically relevant prototype media for the next generation's heat-assisted magnetic recording systems (HAMR) or of nanocomposite thin films of multiferroics can be significantly improved following this concept [1,2]. Along this way, electron energy loss magnetic chiral dichroism (EMCD) and its potential for quantitative local magnetic measurements will be introduced and its current limitations will be discussed [3]. The general possibility of measuring magnetic properties with up to atomic resolution as provided by combining EMCD with the use of electron vortex beams will by highlighted [4] and the persistent challenges will be discussed.

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Ultrafast Nanoscale Dynamics
Probed by Time-Resolved Transmission Electron Microscopy

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Ultrafast transmission electron microscopy (UTEM) is a promising technique which provides access to ultrafast dynamics on nanometer length scales [1]. In UTEM, a pulsed electron beam with sub-picosecond bunch duration is utilized to stroboscopically probe optically triggered processes. Dynamics in structural, electronic and spin degrees of freedom are generally accessible in UTEM by utilizing the versatile imaging and diffraction capabilities of state-of-the-art electron microscopes. However, up to now, the broad applicability of UTEM was limited by the coherence properties of available pulsed electron sources.
In the Göttingen UTEM project, we developed nanoscale laser-driven photocathodes, which allow for the generation of electron pulses with largely improved coherence properties. With this approach, we achieve, at the sample position, electron focal spot sizes down to below one nanometer and pulse durations of about 200 fs [2].
High-coherence ultrafast electron probes now enable the investigation of fast processes in nanostructured systems and at interfaces. I will present first applications, including the coherent phase modulation of free-electron states in optical near-fields [3], which provides a novel approach for plasmon imaging, electron-light interferometry [4], and the optically- induced structuring of electron pulses into attosecond electron pulse trains [5].
Furthermore, an overview on our current developments will be given, with a focus on ultrafast nanoscale mapping of strain tensor fields [6] and nanoscale magnetic processes [7].

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Influence of Cu Addition on Precipitation and Growth Behavior of MnS in Silicon Steel: Experimental Observation and KWN Modeling

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It is well known that MnS can affect various properties of steels. For example, their mechanical properties, corrosion resistance and magnetic properties can be changed by MnS precipitation. Thus, many researchers have investigated the precipitation and growth behavior of MnS in steels. However, the influence of Cu addition has not yet been investigated in detail even though Cu addition is known as a way to improve the magnetic property of silicon steels[1]. In this study, MnS precipitation and growth behavior has been investigated with and without Cu addition and been analyzed by using Kampmann and Wagner Numerical (KWN) model[2].

Silicon steel, whose composition was Fe-2.88Si-0.1Mn-*x*Cu (*x*=0, 0.25), was hot-rolled at 1100°C before solution-treatment at 1350°C for 30 min. The solution-treated specimens were precipitation-treated at 1000°C for 0.3, 0.6, 1.2, 9, 18, 36 and 72 ks to investigate precipitation and growth of MnS. MnS particles were observed by SEM and TEM to quantify the size distribution and its temporal evolution of MnS particles. The growth behavior of average size of MnS could not be explained only by diffusion limited growth and Ostwald ripening theory. Thus, KWN model was adopted to analyze the temporal evolution.

Secondary Electron (SE) images of precipitation-treated specimens are shown in FIG. 1. The white precipitates were found to be MnS from Energy Dispersive X-ray spectrometry (EDX). As the annealing time became longer, MnS particles became larger and its number density became smaller, which suggest Ostwald ripening occurs. The temporal evolution of average size of MnS had a plateau region, which cannot be explained only by diffusion limited growth or Ostwald ripening theory. KWN model successfully reproduced the precipitation and growth behavior of MnS including the plateau region. Cu addition reduced the growth rate at Ostwald ripening stage. This is possibly due to the decrease in interfacial energy by the segregation of Cu at the interface between MnS and ferrite matrix. Scanning Transmission Electron Microscope (STEM)-EDX analysis, experimentally confirmed the segregation.

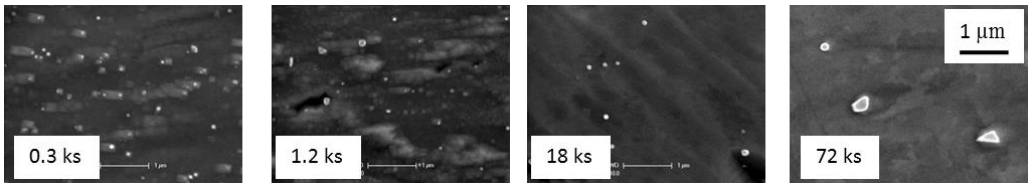

FIG. 1. SE images of the specimen without Cu addition after precipitation-treatment.

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First-Principles Calculations on Point Defects in Semiconductors

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Point defects and impurities are ubiquitous in semiconductors and are undeniably relevant to any kinds of their properties such as photovoltaics, photocatalysts, and electronic devices. Therefore, knowledge and precise control of defects is inherently key to the smart design of semiconductors with superior performance. Nowadays, accurate predictions of the point-defect properties in semiconductors are plausible using first-principles calculations.

In my talk, I would like to review our recent theoretical work on point defects. First, I discuss technical details on first-principles calculations of point defects. I especially focus on the problem of spurious electrostatic energies caused by periodic-boundary condition. Recently I and our colleagues have proposed a general scheme to remove such spurious electrostatic interactions from the defect formation energies in a wide variety of compounds [1]. The corrective capability was systematically assessed for 17 defects in 10 materials (Fig. 1). The defect formation energies in diverse materials are excellently corrected within errors of less than 0.2 eV for small supercells containing around 100 atoms. I then briefly introduce several applications for oxides, nitrides, sulfides, and phosphides compounds [2-5].

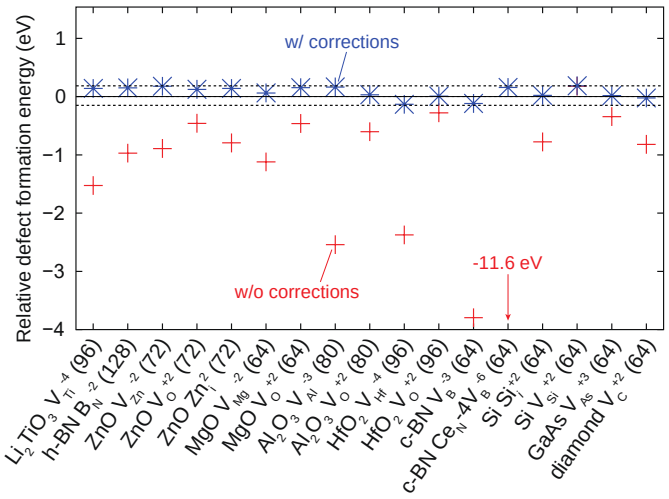

Fig. 1. Defect formation energies estimated using supercells containing around 100 atoms with respect to the extrapolated energies to the infinite interdefect distance limit. The numbers of atoms before introducing defects are shown in brackets.

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Ca Substitution Effect and Relation Between the Dielectric Relation Time and Piezoelectric Property of $Ba_{1-x}Ca_xTiO_3$ (BCTx) and $BaZr_{0.2}Ti_{0.8}O_3$-$Ba_{1-x}Ca_xTiO_3$ (BZT-BCTx)

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In this paper we report the influence of Ca substitution on the electrical and properties of both $Ba_{1-x}Ca_xTiO_3$ (BCTx) with x =0.0-0.3 and $BaZr_{0.2}Ti_{0.8}O_3$-$Ba_{1-x}Ca_xTiO_3$ (BZT-BCTx) compounds fabricated by solid state reaction method. The study was focused on the influence of Ca substitution on AC conduction and piezoelectric properties of the BCTx and BZT-BCTx. The obtained results have shown that the single polaron hopping-conduction is dominated in the AC conduction of the BZT-BCTx. In contrary the localized reorientation polarization is dominated in the BCTx and fitted well with the frequency exponent parameter higher than 1.5. Regarding to the dielectric and piezoelectric behaviors it was shown that the d_{33} and k_p parameters increased in dependence of Ca concentration while inversely the dielectric relaxation time decreased. The d_{33} and k_p reached the maximal value while the relaxation time decreased to the minimal value when the substituted Ca concentration increases to 14.8 at %. The relation between the dielectric relaxation time and piezoelectric property of the materials was discussed in detail and it was supposed to be related with the morphology phase boundary (MPB) that appeared around 14.8 at% of Ca concentration.

Keywords: substitution effect, AC conduction, dielectric relaxation time, Lead free piezoelectrics, .

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Abstracts Poster

Experimental Study on Backgroung Signal in Lateral Spin Valve

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The lateral spin valve device is flexible and useful for measurement of spin signal. There should be no background signal in this device, but it has been observed. This causes are considered for this. We considered that it is caused by thermoelectric effect at nonmagnetic / ferromagnetic interface. As a result, we succeeded in reducing the background signal.
The structure of the device used in this experiment is a lateral spin valve that have three ferromagnetic wires. The ferromagnetic and the nonmagnetic wire are made of NiFe and Cu. We show a spin signal using two ferromagnetic wires in FIG. 1(a). It shows that this spin signal contains 16.8 mΩ background signal. Next, we show a spin signal using three ferromagnetic wires in FIG. 1(b). In this measurement, two ferromagnetic wires are used for the spin generation terminal. As you can see, the background is suppressed
0.07 mΩ. It is because the heat generation and the heat absorption due to the Peltier effect canceled each other out at the two spin generation terminal interfaces. I will refer to these details on the day.

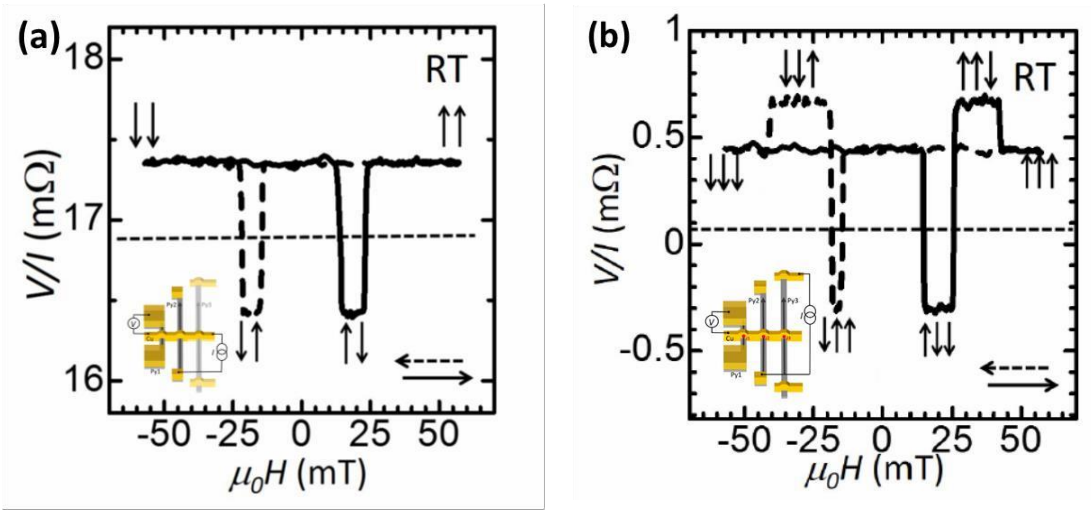

FIG. 1. Field dependence of the nonlocal signal measured at room temperature.

Heat Transport in GMR Nanowires: Evidence for Thermal Magneto Resistance

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The interplay between spin and heat transport has received a lot of recent attention, thus creating a new field of spin-caloritronics. In this abstract, we study the thermal transport in a Ferromagnet(FM)/Nonmagnet(NM)/Ferromagnet trilayer nanowire, which is essentially the basis of a conventional Giant MagnetoResistance(GMR) device. We fabricated a nanoscale temperature sensing device using a GMR nanowire. It has Pt nanowires perpendicular to the GMR nanowire, which act as both heating elements and as temperature sensors based on Seebeck effect, similar to the method used by Bakker et al[1]. We use a lock-in measurement technique to measure only the second harmonic, which eliminates the possibility of spurious voltages[2]. We finally show that thermal transport also shows a magnetoresistance similar to that of electrical GMR.

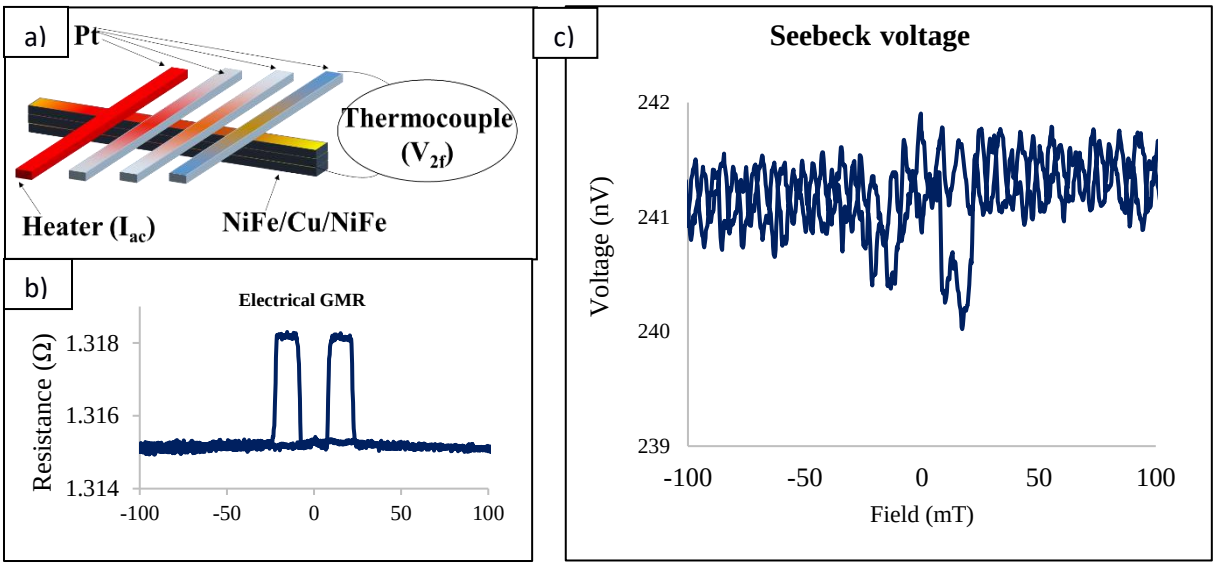

Fig. 1 (a) Schematic of the device. The horizontal strip is a trilayer of NiFe(20nm)/Cu(10nm)/NiFe(10nm (b) Conventional electrical GMR for comparison showing switching. (c) Seebeck voltage generated at the thermocouple showing magnetoresistance.

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Photocatalytic Ability Of G-C_3n_4nanosheets Loaded Ag Clusters To Use As Catalyst In Degradation Of Rhodamine B

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Abstract. g-C_3N_4 nanosheets loaded Ag clusters have been synthesized and systematically investigated by powder X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy(TEM)**,** X-ray photoelectron spectroscopy (XPS), Fourier transform infrared spectroscopy (FTIR), UV–vis absorption and photoluminescence (PL). Ag clusters are successfully loaded on the surface of g–C_3N_4, which was proofed by HRTEM images and XPS survey. The photocatalytic activities of as-synthesized photocatalysts were carried out by the degradation of Rhodamine B under Xenon lamp irradiation. UV–vis absorption spectra showed a decrease of the band gap energy as loading Ag clusters to g–C_3N_4 which agrees well with the measured PL spectra. Additionally, the FTIR spectra and XRD pattern reveal that the loading of Ag cluster affects on the crystal structure of g-C_3N_4. The photocatalytic RhB degradation experiments indicated that g-C3N4 nanosheet loaded Ag cluster with different molar concentration of Ag^+ in starting solutions made an extraordinary effect on photocatalytic activity. It was demonstrated that g–C_3N_4 loaded Ag cluster with Ag concentration of 0.01M in starting solution exhibited the highest photocatalytic efficiency which decomposed 100 % RhB after 60 minutes under Xenon lamp irradiation, almost 4 times that of pure g–C_3N_4.

Keywords: photocatalysis, g-C_3N_4 nanosheet, Ag cluster

Influence of Annealing Temperature on Physical Properties and Photocatalytic Ability of g-C_3N_4 Nanosheets Synthesized through Urea Polymerization in Air

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Abstract. The effect of heating temperature on structural, morphology, vibrational, optical properties and photocatalytic ability of g-C_3N_4nanosheets synthesized from urea in air were investigated in detail by using x-ray diffraction (XRD) analysis, scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), Brunauer–Emmett–Teller (BET), Fourier transform infrared spectroscopy (FTIR), UV–vis absorption, and photoluminescence (PL) measurements. It was found that the preparation temperature strongly influenced on structure and physical properties of g-C_3N_4. g-C_3N_4 nanosheets with some degree of disorders in crystal structure were formed at 450 ^oC in 2.0 h, however disorders disappeared after the heating temperature increased to 600 ^oC. The photocatalytic activity of synthesized g–C_3N_4 nanosheets was evaluated by photocatalytic degradation of Rhodamine B (RhB) aqueous solution under simulated sunlight radiation. Samples calcinated at 550 °C exhibited good photocatalytic ability, decomposed 90 % rhodamine B after 3h of xenon lamp exposure.

Keywords: *nanosheets, photocatalytic, RhB, preparation temperature*

Weak localization of magnons in chiral magnets

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In the studies of transport of particles and waves it is known that there are different transport regimes. Under ideal conditions, like in vacuum or a perfect crystal, transport will be ballistic. However, in reality one has usually to deal with some kind of imperfections that induce disorder in the system. If this disorder is strong enough, the transport will become diffusive. As Anderson showed back in 1958 in case of phase coherent transport disorder can also lead to completely suppressed transport, known as Anderson localization [1].
In the framework of a classical spin model the effect of disorder on magnonic transport is studied utilizing the Landau-Lifshitz-Gilbert equation. Numerical in-vestigations of spin waves in momentum space show the existence of coherent back-scattering (CBS) [2], a weak localization phenomenon, that is a precursor for Anderson localization, in 2D. In addition, a system with weak Dzyaloshinskii-Moriya interaction is investigated, which gives the opportunity to study CBS in a system owning a dis-persion with broken inversion symmetry. This leads to a backscattering peak not located at the $-\mathbf{k}_0$ position anymore, where $\mathbf{k}_0$ is the initial wave vector. The CBS peak position $\mathbf{k}_{CBS}$ is slightly shifted with respect to $-\mathbf{k}_0$ and the shift is direct related to the strength of the Dzyaloshinskii-Moriya interaction [3]. An application of this result might be the quantification of this interaction, once if the backscattering peak is measured.

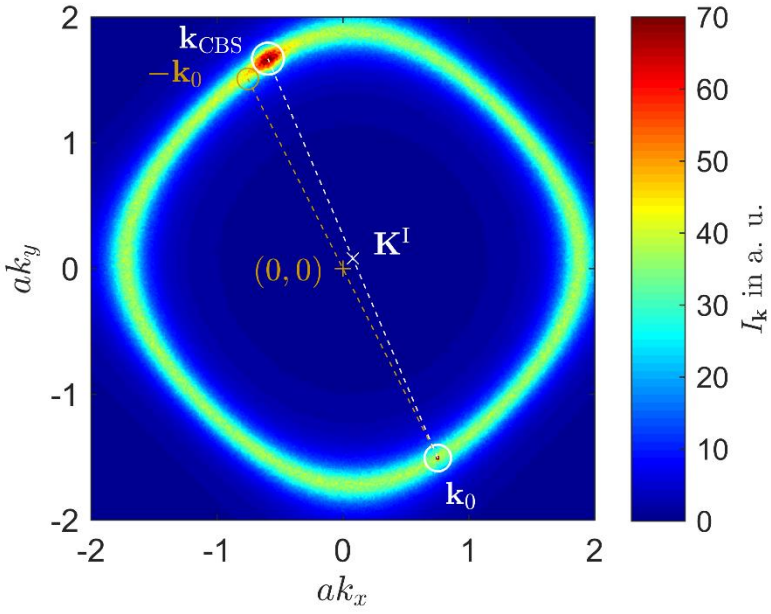

Fig. 1: Spin-wave intensity in momentum space in a disordered system. The CBS peak is not at the $-\mathbf{k}_0$ position as usual, but shifted because of the shifted dispersion relation due to the Dzyalo-shinskii-Moriya interaction.

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Electronic Structure of Cu-Doped Hydroxyapatite/β-Tricalcium Phosphate Composite

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Calcium phosphate based ceramics have been extensively developed as an artificial bone material, so-called bioceramics, which are widely used for dental and medical applications such as osteoporosis treatment. In particular, hydroxyapatite (HAp: $Ca_{10}(PO_4)_6(OH)_2$) and β-tricalcium phosphate (β-TCP: β-$Ca_3(PO_4)_2$) have been widely investigated and recently effectiveness of their composite was reported [1]. In addition, it was reported that the ability of ossification can be improved by doping of mineral element in the calcium phosphates, e.g., Zn in β-TCP [2]. Although there are a lot of studies on such doping effects by various kinds of dopants, there are few reports on that by Cu doping. Hence, influence of Cu-doping in calcium phosphate has not been well understood yet. It was also reported that Cu ions play crucial role to form natural bone in our human body and lack of Cu ions may cause osteoporosis [3].
In this study, Cu-doped HAp/β-TCP composites were synthesized with conventional solid state reaction method changing a ratio of HAp/β-TCP. Crystal structure of the synthesized samples was characterized with the powder X-ray diffraction (XRD) technique. In order to investigate the substitution mechanism of doped Cu ions in HAp/β-TCP composites, firstly X-ray absorption near-edge structure (XANES) measurements at Cu K-edge were carried out at BL-12C in KEK-PF in the transmission mode. Observed Cu-K XANES spectra are shown in Fig. 1, which suggests that valence state of doped Cu ions is 1+. For further understandings of the substitution mechanism of Cu ions, the first-principles calculations within a density functional theory were also performed. Calculated formation energy to substitute at Ca site in HAp is lower than that in β-TCP, which indicates Cu ions are likely to substitute in HAp. Finally, the electronic structure of Cu-doped HAp and β-TCP were examined using the above substituted models to understand change in bone formation rate due to Cu-doping.

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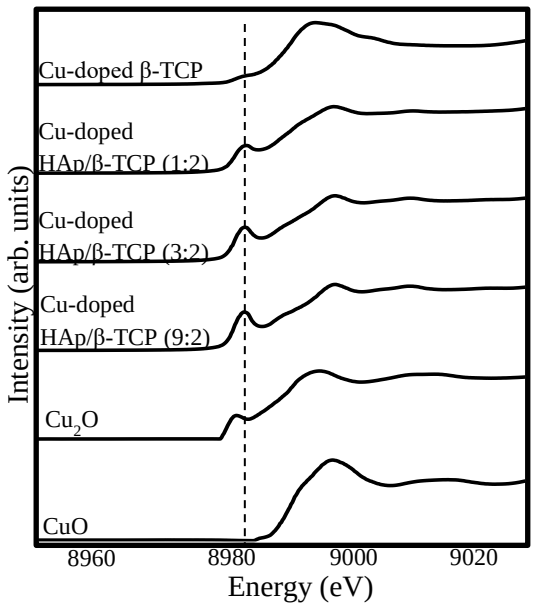

FIG.1 Cu-K XANES spectra of Cu-doped HAp/β-TCP composites and Cu oxides.

EXAFS Debye-Waller Factors of Transition Metals Under High Pressure

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The anharmonic correlated Debye model [1] has been developed to study the pressure effects on the extended X-ray absorption fine structure (EXAFS) Debye-Waller factors of transition metals. Within the Debye model, we derive the pressure-dependent analytical expressions of the effective spring constant, correlated Debye frequency and temperature. Combing with the anharmonic correlated Debye model, the EXAFS Debye–Waller factor under pressure can be investigated. For numerical calculations, the interatomic potential between two intermediate atoms is described by the second-moment approximation to the tight-binding model and its parameters were determined from first-principles calculations [2]. Our results of EXAFS Debye-Waller factors and anharmonic effective potentials for transition metals are compared with those of experiments showing the good and reasonable agreements. We have shown in detail that the anharmonicity contributions of the thermal vibration of atoms are important to EXAFS cumulants at high temperature and the values of EXAFS Debye-Waller factors become smaller with the increasing of pressure.

Keywords: Debye-Waller factor, Transition metals, EXAFS, Debye model, Pressure

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Phenalenyl-Cu for Organic Magnetic Tunnel Junctions (MTJ)

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Phenalenyl (PLY) based molecules are promising candidates for spintronic applications. Attempts to use open shell PLY molecules have been unsuccessful due to their instability. Mandal and co-workers took a new route for PLY-based molecules with a closed shell ground state. For example, zinc methyl phenalenyl (ZMP) shows a magneto-resistance of 20% even near room temperature [1].

Motivated by these results, we are investigating a new closed shell molecule, PLY with a Copper complex, for its spintronics suitability. Ferromagnet/PLY-Cu/ferromagnet heterostructure devices are fabricated by deposition through an in-situ mask with different angles under UHV conditions. These devices are characterized by atomic-force microscopy (AFM), scanning electron microscopy (SEM) and Fourier transform infrared spectroscopy (FTIR). For a certain range of PLY-Cu thicknesses the IV-curves are non-linear (see figure 1(a)), suggesting tunnelling controlled transport. In addition, magneto-optical Kerr effect (MOKE) measurements shows increase of coercive field, when the PLY-Cu layer is present.

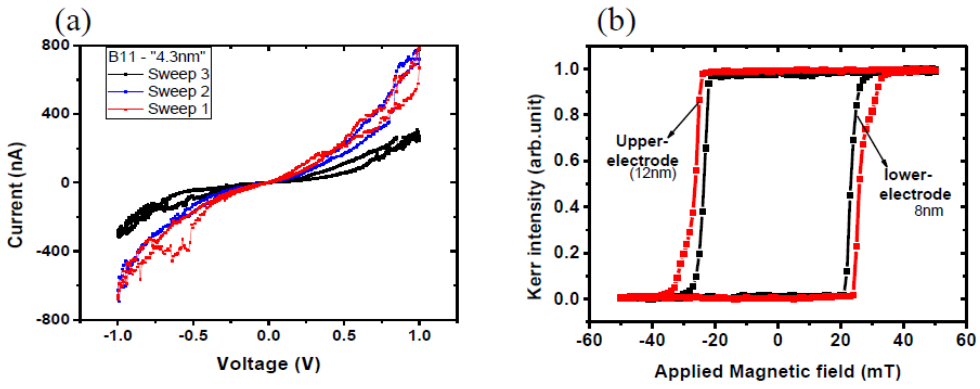

FIG. 1. (a) I-V curve at 300K.

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Laser Induced Photocurrents in a FM/TI-Heterostructure Analyzed by 2D Maps for VIS

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Topological Insulators (TI) open up a new route to influence the transport of charge and spin in a surface film via spin-momentum locking [1,2]. It has been demonstrated experimentally [2] that illumination by circularly polarized light can result in excitation of a helicity-dependent photocurrent. We report our recent results on laser induced photocurrents with a Ferromagnet (FM) added to the surface of the TI, which is aligned by an external magnetic field. The resulting photocurrents have been studied by 2D photocurrent maps for different polarizations of the magnetic field and for VIS laser excitation.

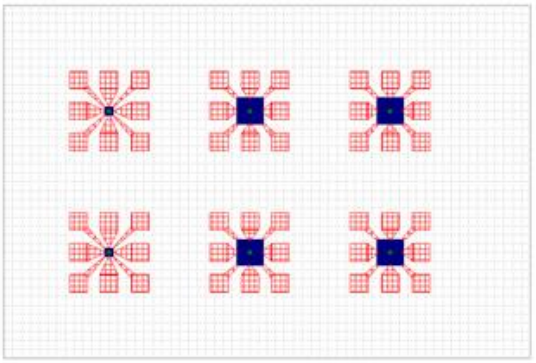

Fig. 1: Scheme of FM/TI-hetero-structure

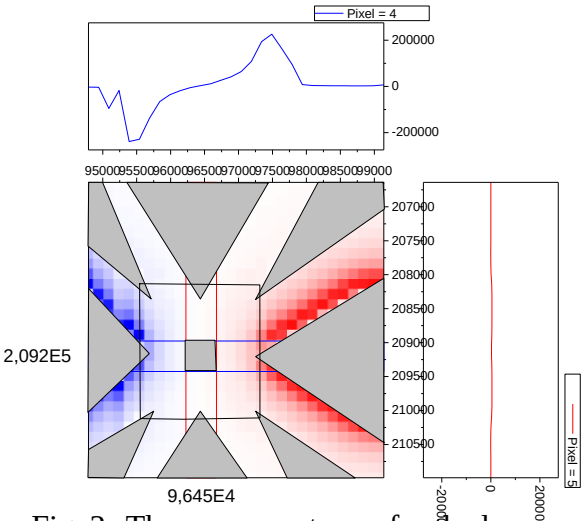

Fig. 2: Thermocurrent map for the laser induction

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Fabricating a Microlense to Build a THz Emitter

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THz radiation has become increasingly important for quality control of food or medicine [1,2]. Since most plastic products are transparent to THz radiation, it is possible to verify the ingredients of medicine by detecting their absorption lines even when the medicine is plastic-wrapped [1]. To lower costs and simplify analysis small and cheap THz Spectrometers are needed.

To achieve this, we are building a THz emitter in the order of micrometer, which is also easy to reproduce. In the emitter, THz radiation is generated through irradiation of a magnetic heterostructure made out of a ferromagnetic thin film and a non-magnetic cap layer with a femtosecond laser pulse. The laser pulse generates a transient spin current, which produces THz radiation of up to 20 THz through the inverse spin hall effect [3]. The femtosecond laser pulse is guided through an optical fiber and focused on the magnetic heterostructure by a microlense. Microlenses written directly on an optical fiber can be fabricated with a 3D printer and have the advantage that lenses with a curvature radius of less than 150µm can be fabricated [4,5].

In this Poster we focus on the fabrication of the microlenses and the impact of the writing parameters. For writing the microlenses we used a 3D printer (photonic professional GT, nanoscribe) with a resolution of 100nm. All lenses were written on a glass substrate. For the first microlenses we used the negative-tone photoresist IP-Dip. Fig. 1 shows a lens written with IP-Dip. The surface is rough because the different layers written by the 3D printer are visible. For the following, we used IP-S instead of IP-Dip to increase the smoothness of the surfaces. Furthermore, we changed the design from a biconvex lens to a hemisphere to exclude any scattering by the holders for the biconvex lens. For the hemisphere, no holders were needed to connect the lens and the glass substrate since the plane surface of the hemisphere is in touch with the substrate.

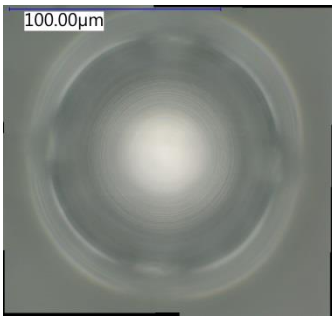

Fig.1 Picture of a microlense taken by a microscope written with IP-Dip as resist.

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Thermovoltage Generation by Inhomogeneous Laser Heating of Magnetic Tunnel Junctions

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We investigated the tunnel magneto-Seebeck (TMS) effect in magnetic tunnel junctions (MTJs) consisting of CoFeB electrodes with in-plane magnetic anisotropy and a separating MgO layer. Our method for temperature gradient generation across the MTJs layer stack is laser heating. This configuration enables a controlled temperature variation over micrometer length scales. In fact, we are creating different heat distributions across one single tunnel junction and investigate the resulting thermovoltages and the corresponding TMS effect. Additional longitudinal temperature gradients lead to thermal effects e.g. the planar Nernst effect, which influence the thermovoltage signal observable in a voltage difference depending on the magnetization direction. For this study, we recorded two-dimensional maps of voltages generated by heating in dependence of the laser spot position and the corresponding calculated TMS values. The voltages change in value and sign, from large positive values when heating the MTJ directly in the center to small values when heating the junction on the edges and even small negative values when heating the sample away from the junction. Those zero crossings lead to very high calculated TMS ratios. Our systematic analysis shows, that the distribution of the temperature gradient is essential, to achieve high voltage signals and reasonable resulting TMS ratios.

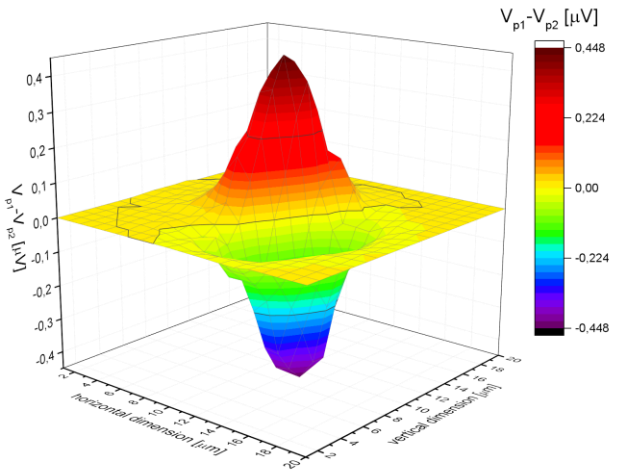

FIG. 1. Voltage change for the parallel magnetization states depending on the magnetization direction on a MTJ.

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Simulation of Nanoscale Femtosecond Acoustics in Phononic Superlattices

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We present our numerical technique for simulation of light-induced elastic and thermal dynamics in nanoscale superlattices and multilayers. In particular we present results for a multilayer made of two insulators (magnesium oxide and zirconia), which is capped by a tungsten layer, featuring a lateral thickness gradient. We show that this structure allows to optically detect band gaps in the spectrum of elastic waves of the multilayer. Perfect agreement between experiments, analytic theory and the numerical finite differences time domain calculations discussed here enables us to proceed further in exploring the spectroscopic possibilities and limitations of this experimental approach. In addition we present micromagnetic simulations suggesting that magnetoelastic coupling can be used to efficiently generate high frequency spin waves in such structures. We acknowledge financial support by the DFG within the CRC 1073 'Atomic scale control of energy conversion'.

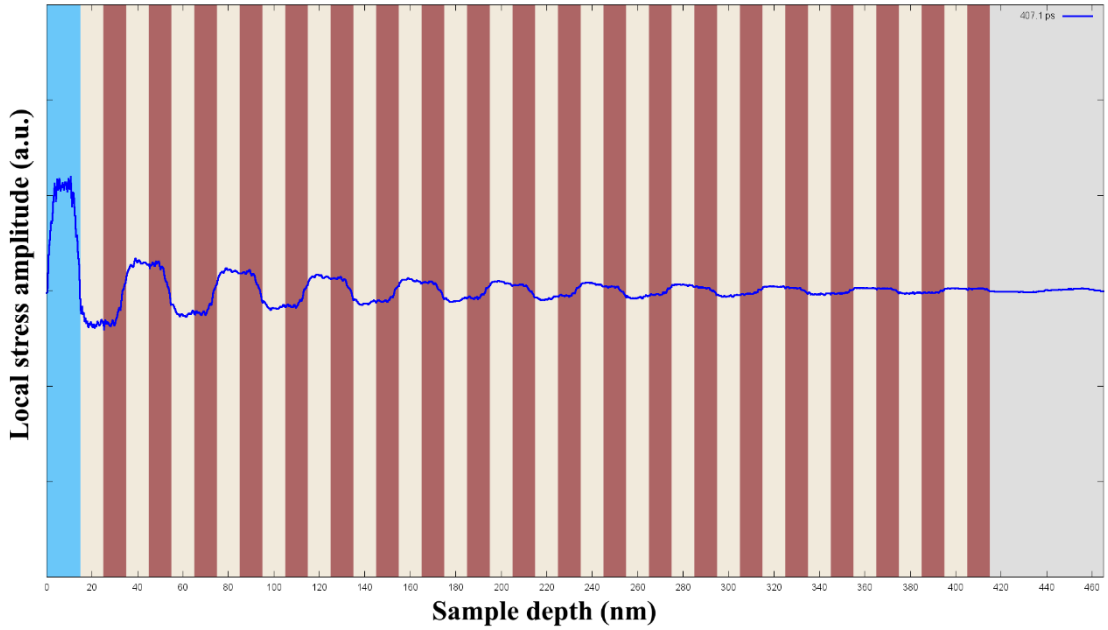

FIG. 1. Simulation of an elastic surface wave in a tungsten capped MgO/ZrO_2 bilayers superlattice.

Determining the Spotsize of a Microlense to Build a THz Emitter

Nina Meyer[1], Finn-F. Lietzow[1] Jakob Walowski[1], Christian Denker[1], Markus Münzenberg[1]

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THz radiation has become increasingly important for quality control of food or medicine [1,2]. Since most plastic products are transparent to THz radiation, it is possible to verify the ingredients of medicine by detecting their absorption lines even when the medicine is plastic-wrapped [1]. To lower costs and simplify analysis small and cheap THz Spectrometers are needed.
To achieve this, we are building a THz emitter in the order of micrometer, which is also easy to reproduce. In the emitter, THz radiation is generated through irradiation of a magnetic heterostructure made out of a ferromagnetic thin film and a non-magnetic cap layer with a femtosecond laser pulse. The laser pulse generates a transient spin current, which produces THz radiation of up to 20 THz through the inverse spin hall effect [3]. The femtosecond laser pulse is guided through an optical fiber and is focused on the magnetic heterostructure by a microlense. Microlenses written directly on an optical fiber can be fabricated with a 3D printer and have the advantage that lenses with a curvature radius of less than 150µm can be fabricated [4,5].
In this poster we show measurements to determine the spotsize of a femtosecond laser λ=1560nm after passing through the microlense. For the measurements micorlenses with a curvature radius of 300µm were written on a glass substrate with and without a circular aperture with a radius of 200µm and a thickness of 50nm. The lenses were fabricated with a 3D printer (photonic professional GT, nanoscribe). To verify that the lenses focus the laserspot, we used a CMOS sensor (The image source) to take a picture of the laser spot contrary to the propagation direction of the laser beam. We changed the distance between the CMOS sensor and the microlens from nearer to farer than the focus length and toke a picture of the laser beam at each position. From the pictures we extracted the spotsize of the laser beam. For a hemisphere with a radius of 300µm we measured a spotsize smaller than 20µm in the focus length.

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Metal-Insulator Transition with Structural Distortion in a Layered Perovskite $La_3Ni_2O_7$: A First-Principles Study

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Perovskite-related oxides have been intensely studied since they exhibit diverse and fascinating phenomena such as ferromagnetism, ferroelectricity, piezoelectricity, superconductivity, and so on. These properties are closely correlated with structural distortions: rotation, tilting, and deformation of the oxygen-coordinated octahedra [1]. Therefore, it is of great importance to explore structural distortions that modify and stabilize the high-symmetry parent structures and, thereby provide novel functionalities. In this study, we focus on an n=2 Ruddlesden-Popper phase $La_3Ni_2O_7$, which has similarities to the cuprate high-temperature superconductors from the viewpoints of atomic and electronic structures. We performed first-principles calculations in order to explore the biaxial-strain dependence of ground-state structures, and investigated their electronic structures.

Our first-principles calculations were carried out using the VASP code [2] and PBEsol functional [3] with a Hubbard U correction for the Ni-3d states [4]. Phonon calculations for exploring stable structures were carried out using the PHONOPY code [5].

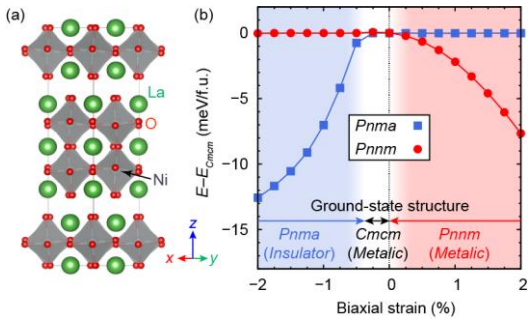

FIG. 1. (a) Crystal structure of $La_3Ni_2O_7$ (*Cmcm*).

Figure 1 (a) shows the crystal structure of $La_3Ni_2O_7$ with a *Cmcm* space group and (b) shows the total energies of relevant structures, which are normalized by the energy of the *Cmcm* structure. Under compressive strain, we found an unstable phonon mode that deforms the NiO_6 octahedra and causes a metal-insulator transition; the energy levels of the Ni d_{x2-y2} states are lifted up due to compression of the octahedra, leading to opening of the band gap. The metal-insulator transition is likely to be related to the charge-density wave instability at the Brillouin zone boundary coupled with the periodic deformation of the octahedra.

This work was supported by the MEXT Elements Strategy Initiative to Form Core Research Center.

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Crystal Structure and Soft Phonon Mode in Improper Ferroelectric $BaAl_2O_4$

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The crystal structure of the stuffed tridymite-type oxide $BaAl_2O_4$ consists of corner-shared AlO_4 tetrahedra network and one-dimensional arrays of Ba ions in channels along the [001] direction [1]. $BaAl_2O_4$ undergoes an improper ferroelectric structural phase transition at T_C = 451.4 K. Structural phase transitions are often accompanied by phonon mode softening. When approaching T_C from above, the frequency of a single phonon mode decreases normally and eve1ntually reaches 0 on T_C, the atomic displacement corresponding to the phonon mode occurs. However, in the case of $BaAl_2O_4$, the thermal diffuse scattering measurements revealed that the two phonon modes at K-point and M-point showed mode softening, and only the M-point mode was frozen below T_C [2]. In this study, we performed the single-crystal synchrotron radiation X-ray diffraction experiments to find out the crystal structures of both soft-modes in the crystal structural fluctuation of the high-temperature phase.

Figure 1 shows the paraelectric average structure of $BaAl_2O_4$ (space-group $P6_322$). Three kinds of unit cells which correspond to the high-temperature fundamental structure, the low-temperature supercell structure (M-point mode), and K-point mode structure respectively, are indicated. There exists the network of Al_2O_7 units formed by two AlO_4 tetrahedra combined by one oxygen ion named O(1) on the three-fold axis. The high-temperature structure analysis revealed that one Al_2O_7 unit had several orientations and the O(1) ion occupied the on-centered and three off-centered sites. If only the off-centered O(1) sites were selected, the K-point mode structure (space group $P6_3$) would be consisted, but actually both sites were selected to realize the M-point mode structure (space group $P6_3$) in the low-temperature phase. The potential energy of these structures calculated was almost same. Thus two competing mode softening were observed in $BaAl_2O_4$ in the vicinity of T_C.

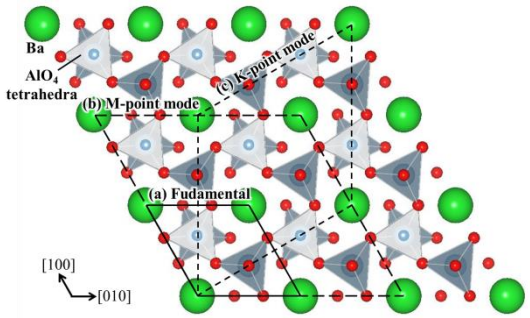

FIG. 1. Paraelectric structure of $BaAl_2O_4$. Three kinds of unit cells are summarized. (a) Fundamental (high-temperature phase. $a \times b \times c$). (b) M-point mode (low-temperature phase. $2a \times 2b \times c$). (c) K-point mode (not frozen. $\sqrt{3}a \times \sqrt{3}b \times c$).

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Fe-Embedded g-C_3N_4: Effective Catalyst for Rhodamine B Decomposition

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Herein, high-performance Fe-doped C_3N_4 photocatalysts synthesized by a facile and cost effective heat stirring method were characterized systematically using powder X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), diffusion reflectance UV-vis spectroscopy (DRS) and photoluminescence (PL) techniques. The corporation of Fe into g-C_3N_4 crystal lattice was confirmed by XPS, DRS, and PL results which showed that Fe existed primarily in the 3+ oxidation state. Absorption edge shifted slightly to the long wavelength along with the increase of absorbance in visible region. The reduction of PL intensity with increasing of Fe content revealed the decline of the recombination rate of electron-hole pairs. The results revealed that photodegradation rate of RhB proceeded much rapidly with the presence of Fe-doped g-C_3N_4 samples compared to pure g-C_3N_4 sample. 7mol% Fe-doped g-C_3N_4 (CNF7) exhibited the strongest photocatalytic performance, which could degrade almost 100% RhB after 40 minutes of Xenon lamp exposure. Samples arranged in the decrease order of photocatalytic performance were CNF7>CNF6>CNF5>CNF10>CNF8>CNF3>g-C_3N_4 which could be well explained base on electron-hole pair recombination rate showed in PL result.

Keywords: *Fe-embedded g-C_3N_4, photocatalytic, recombination rate, electron-hole pair*

Electronic structure of topological point- and line-node semimetals

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Discovery of topological insulators (TIs) has triggered a search for new types of topological materials based on discrete symmetries of crystal. Topological semimetals are recently becoming a leading platform for realizing such novel topological matter. In contrast to conventional semimetals with a finite band overlap between valence band (VB) and conduction band (CB), topological semimetals are categorized by the band contacting nature between the VB and CB in the Brillouin zone; point-contact (Dirac/Weyl semimetals) or line contact (line-node semimetals; LNSMs). In this presentation, we show our recent ARPES results on the candidates of such topological semimetals; NbP of Weyl semimetal [1] and HfSiS of LNSMs [2]. NbP is a non-centrosymmetric polar crystal which has two different cleavage planes along [001] terminated with Nb or P. We revealed a drastic difference in the Fermi-surface topology between the two surfaces of NbP, whereas the Fermi arcs on both surfaces are likely terminated at the surface projection of the same bulk Weyl nodes [1]. For HfSiS, We found a quasi-two-dimensional Fermi surface hosting bulk nodal lines (Fig. 1a) . Most notably, we discovered an unexpected Dirac-like dispersion extending one-dimensionally in *k* space – the Dirac-node arc – near the bulk node at the zone diagonal as schematically depicted in Fig. 1b [2]. These novel Dirac states reside on the surface and could be related to hybridizations of bulk states, but currently we have no explanation for its origin. This discovery poses an intriguing challenge to the theoretical understanding of line-node semimetals.

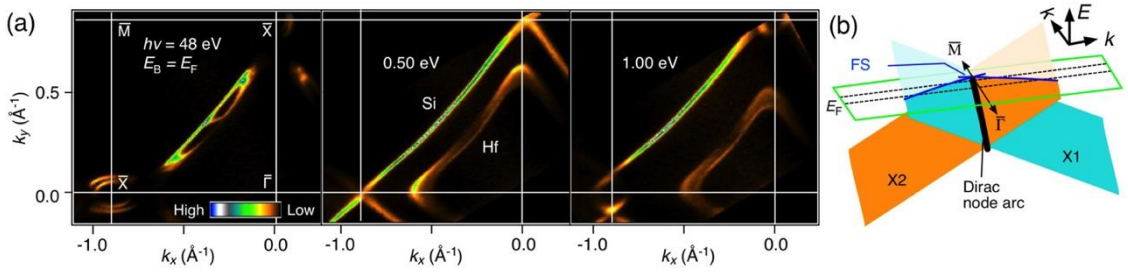

FIG. 1(a) ARPES-intensity mapping as a function of 2D wave vector for various binding energies. (b) Schematic band dispersion in 3D E-*k* space for the new surface state. The black line at crossing line of X1 and X2 surface bands shows the Dirac-node arc.

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Three-Dimensional Twinning of GaAs Nanowires on Hydrogen-Silsesquioxane Covered GaAs(001) Using Molecular Beam Epitaxy

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We report on anomalous growth behaviors of inclined GaAs nanowires (NWs) self-catalyzed on GaAs(001). The NWs were grown on hydrogen-silsesquioxane (HSQ) covered substrate using molecular beam epitaxy (MBE). Usually, epitaxial growth of <111>B NWs on (001) along [1-10] in plane-view is prominently observed; however, we yieled a remarkable number of NWs along [110] in addition to the <111>B NWs as shown in Fig. 1a. In side-views as shown in Figs. 1b and 1c, we found two inclined angles of 35º and 74º from (001) plane in both [110] and [1-10] zones. The inclined angle of 35º in [110] and [1-10] zones correspond to <111>B and <111>A, respectively, with keeping epitaxial relation to the original GaAs(001) substrate. The NWs with the inclined angle of 74º in [110] and [1-10] zones seems similar to <111>A and <111>B NWs with the inclined angle of 35º, respectively, as shown in Figs. 1d and 1e. In morphological point of view, the <111>B NWs show almost symmetric and clear hexagonal, and asymmetric and blunt ones seem <111>A NWs. The inclined angle of 74º can be explained by the 1st order three-dimensional twinning due to 60º rotation along <111> axes [1]. Transmission electron microscope observations reveal high density of twinning in the <111>B NWs and less in the <111>A NWs that is in accordance with the Au-catalyzed GaAs NWs in metal-organic vapor phase epitaxy [2].

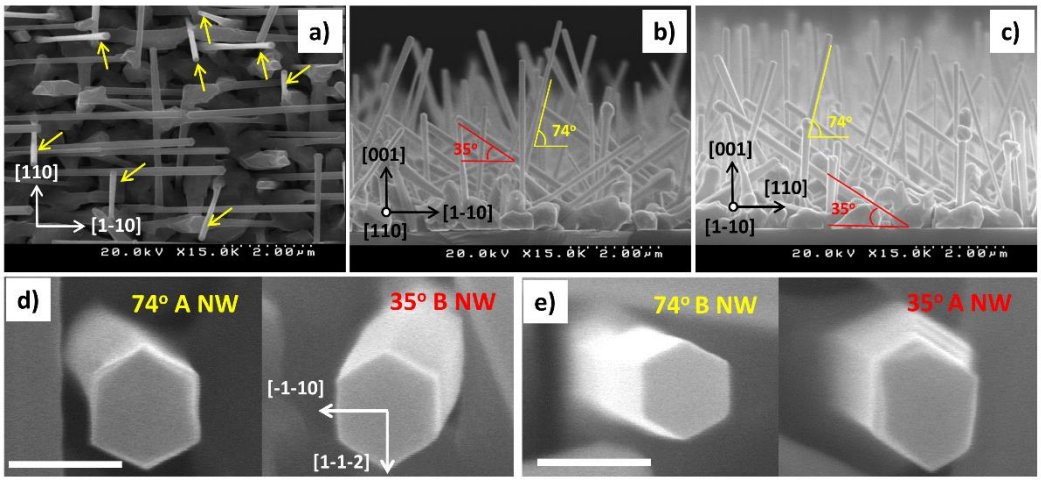

Figure 1. Scanning electron microscope images of GaAs NWs grown on HSQ-covered GaAs(001) substrate. a) plane-view, b) side-views in [110] zone and c) in [1-10] zone, d) morphology of inclined NW tops observed in [110] zone, and e) in [1-10] zone.

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Electronic Properties of Noncentrosymmetric Superconductor Th_7Ni_3

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Investigations of superconducting materials possessing noncentrosymmetric crystal structure are highly attractive subjects in materials science today. In these materials, the electrons are influenced by antisymmetric spin-orbit coupling (ASOC), which emerges due to electric field gradient associated with lacking a center inversion. When ASOC is strong enough, there is possibility of mixed singlet and triplet states. The new form of pairing can give rise to unusual temperature, field dependences of the superconducting parameters. As the first, noncentrosymmetric heavy-fermion superconductor $CePt_3Si$ revealed unconventional Cooper pairing [1]. Recently, our interest has focused on superconductors crystallizing in the hexagonal Th_7Fe_3-type structure (space group $P6_3mmc$) [2-4]. The investigated Th_7Fe_3 and Th_7Co_3 compounds do not exhibit heavy fermion properties at all, thus any exotic property of superconductivity is presumably not due to electron correlation effect. In fact, our experimental data have evidenced anisotropic superconducting gap in Th_7Co_3 [2] and two-gap superconductivity in Th_7Fe_3 [4]. In this contribution, we present the results of first-principles calculations of electronic band structure (EBS), density of states (DOS), electron localization function (ELF), charge density and Fermi surfaces (FS) for Th_7Ni_3. We performed the calculations using all-electron full-potential linearized augmented-plane-wave Elk code [5], utilizing both scalar relativistic (SR) and fully-relativistic (FR) approximations. Some of the FR data are shown in Fig. 1. We discuss the data in terms of ASOC effect, contributions of 3d-, 6d-electrons to DOS and anisotropic properties of ELF and FS. We also compare electronic properties of Th_7Ni_3 to those of Th_7Fe_3 [3] and Th_7Co_3 [2].

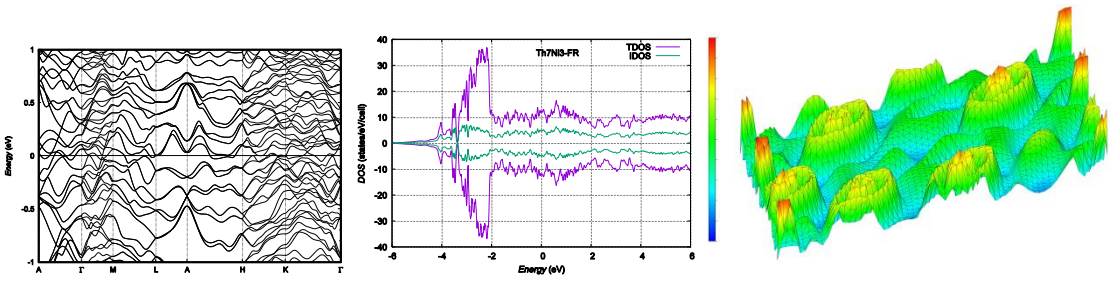

Fig. 1. EBS, DOS and (110)-surface ELF of Th_7Ni_3 obtained by utilizing fully relativistic LSDA.

Acknowledgements: This work was supported by the National Science Centre in Poland (grant No. 2016/21/B/ST3/01366).

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Enhancement of the Sensitivity of Magnetic Field Sensor Based on Anisotropic Magetoresistance Effect in NiFe thin Films

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The sensitivity magnetic sensors have become essential for applications in many fields such as biomedicine, computer memories, geophysics and etc. It is known that the sensitivity of magnetic anisotropy sensor depends on current density as well as the rotation of the magnetic moments corresponded to the external magnetic field. In this study, we fabricated and investigated a number of different configurations of resistor bar in the Wheatone bridge sensor. The samples were made in magnetic field pins with varying intensity from 0 to 900 Oe. Furthermore, different shapes of resistor, as in circle, rectangle, ellipse, were fabricated with the film thickness of 15 nm. The analyzed results indicated that the rotation of the magnetic moments occurs rapidly and sharp in the small magnetic field (0 - 3 Oe) with samples fabricated in the high magnetic field pinned. The strong magnetic anisotropy was also observed in the rectangular configuration. In addition, the sensors have been optimized for measuring small magnetic field.

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Electronic Structure of Mn-doped Oxide Phosphor Materials

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Most of the current phosphor materials are prepared by doping dilute amount of rare-earth or transition metal ions, which act as emission center, in matrix materials. Among such phosphors, rare-earth doped oxides show good properties such as high luminescence and high stability for long term use, etc. However, due to the limitation of the rare-earth elements in the earth, rare-earth free phosphor materials have been strongly demanding, and therefore such materials have been extensively investigated these years. Although there are wide varieties of dopants for such rare-earth free phosphors, Mn^{4+} doped phosphor materials, which show red emission, are one of the most attractive materials. In order to design new phosphors doped with Mn ions, it is essential to know the local environment of the doped Mn ions in an atomic scale and the electronic structures of Mn-doped materials. Although such local environment analysis is mandatory, such analysis have been often skipped due to a difficulty of such analysis for dilute dopants. We have developed an analytical method to determine such local environment of dilute dopant using X-ray absorption near-edge structure (XANES) measurements and the first-principles calculations within a density functional theory, which enabled us to determine local environment of various kinds of dilute dopants in functional materials [1, 2]. In the current study, local environment analysis of Mn ions doped in some oxides and the electronic structure calculations for such materials have been carried out.

All the samples were fabricated with the conventional solid-state reaction method changing the concentration of Mn ions and/or matrix oxides, $CaTiO_3$, $SrTiO_3$, Mg_2TiO_4 and Mg_2SnO_4. Crystal structures of the synthesized materials were characterized with powder X-ray diffraction. Mn K- and L- XANES spectra were observed at BL01B of SPring-8 in transmission mode and BL4B in UVSOR in total electron yield mode, respectively. Theoretical XANES spectra to be compared with the experimental ones were prepared with the WIEN2k package [3]. The electronic structure of the Mn-doped materials were investigated with modified Becke-Johnson potential [4], which was recently developed electron-electron correlation functional and is accurate for the band-gap estimation of the wide variety of semiconductors.

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History of the meeting

In April 2009, the Leibniz Prize recipient and vice president of the Deutsche Forschungsgemeinschaft (DFG, the German Science Foundation) Prof. Dr. Konrad Samwer from Georg-August Universität in Göttingen gave the first DFG "Leibniz Lecture" in Hanoi, Vietnam. During his visit to Vietnam National University, he proposed the idea of organizing a bilateral German-Vietnamese seminar on Materials Sciences, which would bring the scientists from the two countries together for a closer collaboration in the development of modern science in South-East Asia.

The first German-Vietnamese Workshop on Frontiers in Materials Sciences (Hanoi, October 20–22, 2010) and Second Joint German-Vietnamese Symposium on Frontiers in Materials Sciences (Frankfurt, October 6–9, 2011) were the next fruitful steps along this line. At that time, the organizers decided to extend the bilateral meetings to a larger scale of an International Symposium on Frontiers in Materials Sciences (IS FMS), which would certainly be more beneficial not only for the Vietnamese and German scientists, but also for the scientists from other countries. Following that in 2013, the *1st International Symposium on Frontiers in Materials Science* (IS FMS) has been organized in Hanoi, Vietnam, Nov. 17–19, 2013, under the initiatives of the Deutsche Forschungsgemeinschaft (DFG, the German Science Foundation) and the National Foundation for Science and Technology Development of Vietnam (NAFOSTED). As it provided a new and effective communication platform for selected research groups in fast emerging fields, the symposium gained immediate attention and was successful with participants coming from all over the world. The *2nd* IS FMS was held in the middle of the autumn of 2015 (Nov. 19–21) at Waseda University, Tokyo, Japan, with a focus on magnetism and nanostructured magnetic materials, functional materials, theoretical and computational materials science, and nanoscale materials characterization. After the 3rd meeting in Hanoi in 2016, Greifswald will host in 2017 the 4th FMS international symposium.

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