Reports & Summary by Discussion Leaders

EU-JAPAN Workshop on Computational Materials Design and Realization for Spintronics, Moltronics, Quantronics, Superconductivity and Topotronics

September 18-30, 2016
Peter Grünberg Institute, Jülich Research Centre, Jülich, Germany

■Organized and Sponsored by:

- **JSPS Core-to-Core Program "Computational Nano-Materials Design on Green Energy", Osaka University, Japan**
- **Center for Spintronics Research Network (CSRN), Graduate School of Engineering Science, Osaka University, Osaka, Japan**
- **Center for Spintronics Research Network (CSRN), Graduate School of Engineering, The University of Tokyo, Tokyo, Japan**
- **Center for Spintronics Research Network (CSRN), Tohoku University, Sendai, Japan**
- **Elements Strategy Initiative Center for Magnetic Materials (ESICMM), National Institute for Materials Science, Tsukuba, Japan**
- **RIKEN Center for Emergent Matter Science, Wako, Japan**
- **Peter Gruenberg Institute, Jülich Research Center, Jülich, Germany**
- **Department of Physics and Astronomy, Uppsala University, Sweden**
- **Department of Physics, Aalto University, Finland**

■Organizers:

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■Purpose of the Workshop:

Based on the discussions through the long-term workshop, we will create the new concepts and proposals for the future EU-JAPAN collaborations related to the computational materials design and realization of energy-saving, energy-creation materials and devices, such as spintronics, moltronics, quantronics, superconductivity and topotronics. Discussion leader will organize the session from 9:30-11:30 (maybe to 12:30), or, 14:00-16:00 (maybe to 17:00) per each day with the short introduction of the purpose and the goals of the session, where two or three speakers talk and keep continue the discussions through the lunch, and after the lunch or evening he can also organize a small discussion meeting in the city, if we need and available. Basically, each talk is organized with 30 min presentation and 30 min discussion (creation of new concepts and new proposal through the discussion, therefore, please keep the scheduled time). Based on the presentations and discussions, the discussion leader will prepare the repot of new proposal and summary in the wrap-up session. We will finalize the summary and new proposal on the last day and distribute it to the participants for the future collaborations.

Report on New Superconductors (Electron-Phonon Interactions and Others), 18 September, 2016 by Hiroshi Katayama-Yoshida (Osaka Univ.)

Three speakers presented the results at this session; M. I. Eremets (Max Planck Institute, Chemistry, Mintz), Ryotaro Arita (RIKEN, Tokyo) and Takahiro Ishikawa (Osaka Univ.). Eremets found superconductivity with T_C ~ 203 K in hydrogen sulfide at high pressure (~150 GPa)(see Fig.1). The superconductivity was proved by the zero resistance, Meissner effect, and isotope effect with conventional electron-phonon interactions. X-ray diffraction studies by Spring-8 confirmed predicted cubic structure (*Im-3m* H_3S) of the superconducting high-T_C phases. Arita performed fully non-empirical calculation and reported that the experimental T_C is reproduced with accuracy of 10 K by taking into account the zero-point motion and phonon anharmonicity to go beyond the Migdal approximation. Arita also reported that the possibility of magneli-phase in the low-T_C phase. Ishikawa reported that the low T_C phase of hydrogen sulfide compound, H_5S_2, using the first-principles calculation and the generic algorithm technique for crystal structure search. The H_5S_2 compound is thermodynamically stabilized at around 110 GPa. The calculated T_C for low-T_C phase is 50 – 70 K in pressure range of 100-150 GPa, which are in good agreement with the experimental data for another superconducting phase emerging in creation process of the 203 K superconducting phase. Electronic structure is characterized by the strong s-d and p-d hybridization between the broad hydrogen (H) s-, sulfer (S) p-band (~60 eV) and relatively narrow sulfer (S) 3d-band (~20 eV) under high-pressures (~150 GPa). It forms bonding and anti-bonding splitting by Fano effect, and narrow 3d non-bonding band near the pseudo-gap (see Fig. 2 (for SH_3) and 3 (for S_2H_5)).

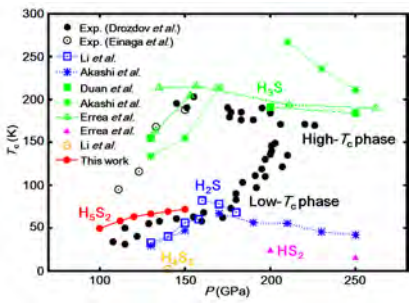

Fig. 1. (T_C vs. Pressures)

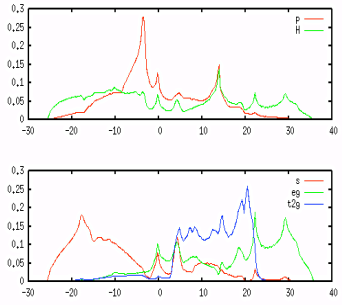

Fig.2 (DOS of SH_3)

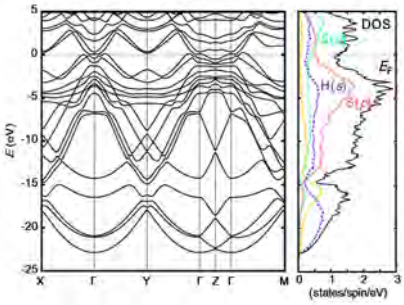

Fig. 3 (DOS of S_2H_5)

In order to increase the T_C up to room temperature, we should search for more hydrogen-rich phases such as SH_5 or another hydrogen-rich compound such as CaH_6, YH_6, ArH_2, ArH_4, CH_3 etc. We also discuss the enhancement of T_C up to 1,000K (super-High-T_C superconductors) by using the purely electronic attractive electron-electron interaction system (negative effective U_{eff}<0 system).

Report on New Methodology for Computational Materials Design I, 18 September 2016, by Tomoya Ono (Univ. Tsukuba)

Three speakers presented the results at this session; Takao Kotani (Tottori Univ., Tottori, Japan), Jussi Enkobaara (CSC, Espoo, Finland) and Rudolf Zeller (Forschungszentrum Juelich, Juelich, Germany). Kotani introduced the quasiparticle self-consistent GW (QSGW) method. As shown in Fig.1, the QSGW method can predict band gap of bulks with high degree of accuracy. The electronic structure calculation for InAs/GaSb super lattice structures was presented and the band offsets calculated by the QSGW method are in excellent agreement with the experimental results. He also calculated the impact ionization rate of 4H-SiC, which is required to determine the break down voltage of power devices. Enkobaara presented GPAW code, which is based on the real-space finite-difference (RSFD) method. He talked the scaling of GPAW code on massively parallel computers. Excellent scaling owing to the RDFD method is presented in Fig. 2 for the case of more than 30,000 processes. As an application of the GPAW code, calculation for plasmon resonance in Na nanoparticle was presented. Zeller reported KKRnano code, which is a linear scaling code and enables us to perform large scale calculation on massively parallel computers. KKRnano code achieves linear scaling calculations by introducing the cutoff for Green's function. He demonstrated the accuracy of the KKRnano code with respect to the cutoff radius and concluded that the code has a potential power for execution of accurate and large-scale electronic-structure calculations.

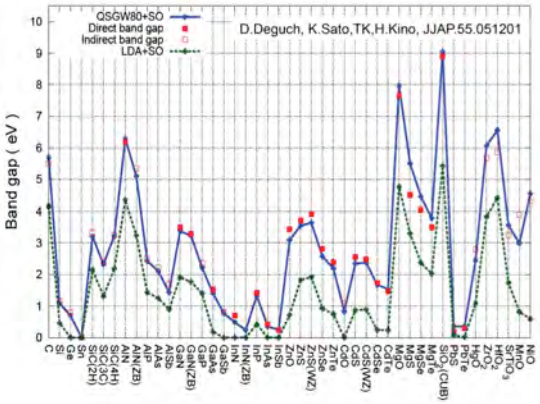

Fig. 1: Band gap calculated by QSGW.

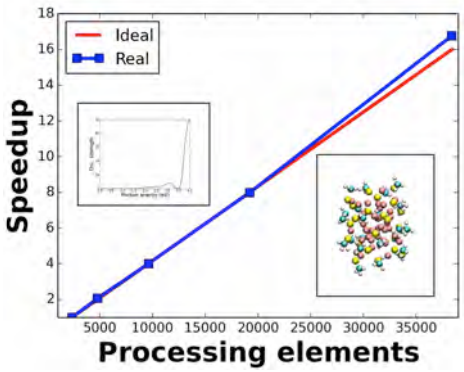

Fig. 2: Parallel scaling of GPAW.

Report on Session Topotronics I
EU-JAPAN Workshop on Computational Materials Design and Realization for Spintronics, Moltronics, Quantronics, Superconductivity and Topotronics

Tuesday 20th September 2016 by Yuriy Mokrousov (FZ Jülich)

The session Topotronics I has opened the part of the workshop, which was dedicated to the exciting developments in the field of solid state research and magnetism which are focusing on topological aspects of magnetic and electronic systems. The purpose of this session was to demonstrate the breadth of effects and phenomena, which are at the forefront of topotronics these days and in the foreseeable future.

In the 1st talk given by *Takashi Koretsune (RIKEN)* we have learned about new conceptual and computational methods to approach the fundamental Dzyaloshinskii-Moriya interaction (DMI) in complex magnets. Two new methods to access the DMI were presented, i.e. via referring to spin susceptibility, and by computing the ground state spin currents in the system. While these two methods are perfectly fitted for DMI studies in materials which exhibit a wide range of electronic structure properties, the main message that was conveyed is that the physics of the DMI is an exciting field on its own, closely related to the other fields associated with skyrmions, domain walls, spin current properties and linear response of solids to perturbations. In the light of an intensive research which is conducted both in Germany and in Japan on the physics of complex spin systems whose properties are driven by the DMI, the results presented here are of utter relevance for the future advances in this domain.

In the 2nd talk, given by *Shuichi Murakami (TIT)*, we were given a wide perspective of effect and phenomena, which occupy the minds of people working in the field of topological insulators and topological metals. As Prof. Murakami stressed in his talk, it is the properties of topological metals such as Weyl semimetals and node line semimetals, which are perhaps the most exiting direction in modern topological condensed matter. In this talk we learned that the topological metals of the latter kind are necessary ingredients in the symmetry-driven phase diagram of generic topologically non-trivial materials, and might be observable in such “trivival” metals such as Ca, Sr or Yb. The properties of the topological semimetals in terms of their robustness with respect to symmetry breaking, pressure, and edge state formation were discussed in depth, and a clear possible relation to the well-researched physics of the Rashba systems was outlined.

In the 3rd talk of the session, presented by *Maarten Wegewijs (FZJ)*, we were made aware of the recent developments in the field of quantum pumping in open systems. While this subject is perhaps a bit off the mainstream exploratory effort in the area of topological solids, it was breathtaking to see the first conceptual steps in the geometrical theory associated with complex gauge theories and observability in open systems – similar steps where undertaken in the 1980s with respect to closed systems, with remarkable consequences for the science-scape of modern solid state physics. The key message of the talk was establishing that it is the gauge freedom

associated with observables rather than with the quantum states (as opposed to closed systems) that is the key to our understanding of geometrical pumping in open systems of various nature.

Future Perspectives: The future perspectives which stem from our session are manifold: (i) extending our understanding of spin currents as the foundation for the properties of chiral magnetic systems, (ii) re-evaluating our understanding of the topological metal phases in the electronic structure of common materials with the purpose of utilizing their unique properties for discovery of novel effects and phenomena, and (iii) making further steps towards a unified topological theory of quantum pumping of generic systems strongly out of equilibrium, which served a key role in our understanding of such phenomena as quantum Hall effects and quantum spin Hall effect in closed systems.

Report on Session Topotronics II

EU-JAPAN Workshop on Computational Materials Design and Realization for Spintronics, Moltronics, Quantronics, Superconductivity and Topotronics

Tuesday 20th September 2016
by Stefan Blügel (FZ Jülich)

The session Topotronics reflects in part of the topological revolution that is currently taking place in condensed matter, with the real-space topology of magnetic structures playing a leading role in the field of chiral magnetic skyrmions and non-coplanar magnets discussed in session Spintronics II and Topotronics I and in momentum space discussed in the sessions Topotronics I+II.

In the session Topotronics II, we focused first through two contributions at the signature of topology in the electronic structure, first by an experimental contribution given by Dr. Lucasz Plucinski (PGI-6, FZ-Juelich) entitled *Band structure engineering of 3D topological insulators* followed by a theoretical contribution of Irene Aguilera (PGI-1, FZ-Juelich) entitled *Surfaces and interfaces of topological insulators -- What can we learn from relativistic many-body calculations?*

Lucasz Plucinski introduced ARPES as the most important experimental tool to decipher experimentally the topological signatures of the electronic structure such as Dirac cones and their position with respect to the Fermi level. He focused on three-dimensional topological insulators (3D TI), which are narrow band gap semi-conductors. He looked among others at the consequences of the stoichiometry of the binary 3D TIs layered compounds such as Bi_2Te_3 and Bi_2Se_3 and at Bi_2Te_3/Bi_2Se_3 heterostructures whose chemical potential is controlled.

Irene Aguilera performed world-wide probably the most accurate calculations of the band gap of the bulk phases of TI testing and analyzing carefully how the spin-orbit interaction (SOI) is added to GW self-energy as implemented into the FLEUR code and what are the influences on the bandgap and the band dispersion of these small-band gap semiconductors, for which calculations with small bandgap errors are desirable. She compared one-shot GW+SOI with (quasi-particle) QSGW+SOI for various systems ARPES and PPE. She applied the methods for example to Bi_2Te_3 and Bi_2Se_3 but also to Bi. She made several prediction, in particular the Bi maybe a TI in terms of films. Sofar the Jülich made SPEX code (FLEUR-code +GW +SOC) is despite paralleliz-ation only able to calculate a max of 20 to 30 atoms. This is insufficient to study surfaces. Therefore, a method was introduced extrapolating from the bulk band structure to the surface one using Wannier functions.

Philipp Rüßmann, was the third speaker of the session. He investigated the Quasi-particle interference images as measured by scanning tunneling microscopy which result from the scattering of surface states at impurities or other imperfections. He investigated for the topological surface states of Bi_2Se_3 the scattering propability $P_{kk'}$ for non-magnetic and magnetic impurities using the Jülich based Korringa-Kohn-

Rostoker Greenfunction (KKR-GF) method. He found that the backscattering probability changes drastically when the impurity is magnetic. He found that long-ranged and very focused quasi-particle interference states occur if Mn impurity are clustering to increase the magnetic scattering potential.

Future perspective:

Methods: The development of methods such as the SPEX code or the KKR-GF method is extremely labor intensive. We currently plan to continue with the development of these methods as long as the funding permits this. The development of the methods will be mostly in the direction of parallelization and stability to become part of automated workflows in the context of Materials Design.

Topology in Electronic Structure: I believe that the topological revolution will continue for the next 10 years. More and more topological properties in the momentum and real space and time domain of fermions and bosons will be discovered. Since topology leads to quantization, realizations in materials combinations for devices is an important issue and thus also the investigation of the electronic structure by ARPES and GW+SOC will continue. More important became concepts of virtual materials design to find the material with right properties.

Report on spintronics I sessions, 21 September by Hisazumi Akai (The University of Tokyo)

The session spintronics I was dedicated for presentations of works about semiconductor spintronics and as well as magnetic tunneling junctions. Three speakers, Masaaki Tanaka (The University of Tokyo), Fumihiro Matsukura (Tohoku University), and Yoshio Miura (Kyoto Institute of Technology), presented the results at this session. The mechanisms of ferromagnetism of diluted semiconductors have been discussed for long time since the discovery of its prototype materials (In, Mn)As and (Ga, Ma)As. Since it is clear that the systems are anyway magnetic, the main interest lies in how the ferromagnetic arrangement of the magnetic structure can lower the band energy. Until now, two mechanisms have been proposed, p-d exchange (p-d hybridization) and double-exchange. Although those are two limiting cases of essentially the same physics, namely the total band broadening expected for ferromagnetic alignment of magnetic moment, the electronic structure sometime looks differently.

Tanaka recently succeeded in fabricating (In, Fe)As with n-type (Be interstitials) doping. They found that with enough amount n-type doping, the system exhibited stable ferromagnetism. The electronic structure of the system is considerably different from those of (Ga, Mn)As and (In, Mn)As that show hole mediated ferromagnetism.

Matsukura performed ARPES experiment on (Ga, Mn)As and found that the Fermi level was located at the top of the valence band, namely no impurity band was formed in the band gap. This seems to indicate that the d-states originate from Mn majority spin is located relatively at the lower energy region of the valence band, corresponding more to the p-d exchange cases of realization of ferromagnetism than the double-exchange case.

Miura discussed the Gilbert damping constant of LLG equation. Using linear response theory, calculating torque-torque correlation functions, he obtained the Gilbert damping constant in CoFeB/MgO/CoFeB trilayer systems. One of the important conclusions is that the Gilbert damping constant at the Fe/MgO interface is strongly affected by an applied electric field, opening up the possibility of field controlled magnetic devices.

Report on session “Spintronics III (Magnetization control by electric field) ”

Thursday Morning, 22th September 2016

Yoshio Miura (Kyoto Institute of Technology)

In this session, three speakers presented topics on the electric field control of magnetization, S. Miwa(Osaka University), K. Nakamura(Mie University) and B. Dupe’ (University of Kiel). First, Dr. Miwa talked on voltage control of interfacial magnetic anisotropy at metal | dielectric interface. In his talk, he introduced the voltage controlled magnetic anisotropy (VCMA) in Fe/MgO-based magnetic tunnel junction (MTJs) with perpendicular magnetization as a promising method of magnetization reversal with ultralow power consumption. In this method, large voltage changes of the perpendicular magnetic anisotropy (PMA) of ferromagnetic layer at the interface of MTJs are required. He pointed out that monatomic Pt layer makes the dominant contributions to the PMA and VCMA. He also found that a voltage change of the magnetic dipole moment, originating from spin-flip excitation between the majority and minority spin-bands, dominates the VCMA. From these results, he proposed the general guide line for the large VCMA effect. Second, Dr. Nakamura talked on modification of symmetric and asymmetric exchange stiffness in transition-metal thin films by external electric field. In this talk, he first showed the screening charge density by the electric(E)-field and discussed the importance of *p-d* hybridization at surfaces and interfaces. He studied the electrical control of the Curie temperature and the Dzyaloshinskii-Moriya interaction (DMI) of Co films on Pt(111) by using the full-potential linearized augmented plane wave method. His results predicted that the change of the screening charge density by an E-field induces to the modification of the magnon dispersion, leading to the E-field dependence of the exchange stiffness. Furthermore, he pointed out that the E-field introduces an asymmetry of the modification with respect to the magnetization rotations in clockwise and counterclockwise ways. He concluded that the symmetry behavior of magnetization rotation by the E-field qualitatively agrees with the experimental results. Then, Dr. Dupe’ talked on direct and indirect magnetoelectric effects at surfaces. He first discussed magnetic skyrmions in ultra-thin transition metal films using first principles calculations. He demonstrated that the properties of magnetic skyrmions at transition metal interfaces such as their diameter and their stability can be tuned by the structure and composition of the interface. Then, he reported the effect of an E-field on the magnetic interactions of several Fe layers on Ir(111). He pointed out that as the Fe thickness increases, the direct magnetoelectric effect decreases and only an indirect magnetoelectric effect involving strain relaxation can occur.

Report on Spintronics IV (Spinodal Nanotechnology and Others), 22 September, 2016 by H. Katayama-Yoshida (Osaka Univ.) and Stefan Blügel (FZ Jülich)

Three speakers presented the results at this session; H. Katayama-Yoshida (Osaka Univ.), Alberta Bonanni (Johannes Kepler Univ., Linz) and Shinji Kuroda (Univ. of Tsukuba).

Based on *ab initio* electronic calculations and multi-scale simulations comparing with the experimental verifications of nano-scale super-structures of Konbu-Phase and Dairiseki-Phase in transition metal-doped semiconductors, Katayama-Yoshida pointed out that the spinodal nano-decomposition can be generalized as a new class of bottom-up nanotechnology with an outstanding potential in various fields and applications, such as nano-spintronics applications in diluted magnetic semiconductors by colossal magnetic and electric responses, high efficiency thermoelectric-power materials, nano-catalysis formation by spinodal nano-decomposition ($LaFePdO_3$, $LaFePtO_3$), and high-efficiency photovoltaic solar-cells ($CuInGa(SSe)_2$, $(MA)PbI_3$, $CsSnI_3$, etc.) with nano-superstructures, etc..

Bonanni gave an overview on how, through a comprehensive protocol of epitaxial growth, co-doping and advanced characterization, it has been allowed to unravel and now to d control the structural magnetic and optical properties of a number of modulated systems embedded in GaN or $Al_xGa_{1-x}N$, and including , self-assembled Fe_xN nano-crystals with magnetic response dictated by the stoichiometry and Mn-Mg_k complexes optically active in the mid-infrared . The functionalities of III-nitrides have been extended to the generation of pure spin current in bilayers Py/*n*-GaN:Si – at room temperature and through spin pumping. It was reported, that for *n*-GaN:Si a spin Hall angle θ_{SH}=3.03Å~10^{-3}has been found, exceeding by one order of magnitude those reported for other semiconductors, pointing at III-nitrides as efficient spin current generators. Furthermore, the electrical control of magnetization in (Ga,Mn)N was presented. It has been proven, that the magneto-electric coupling is driven by the inverse piezoelectric effect that stretches the witzite elementary cell along the *c*-axis and, thus, affects the magnitude of the magnetic anisotropy. This work bridges piezoelectricity of wurtzite semiconductors and the electrical control of magnetization in hybrid and composite magnetic structures with piezoelectric components.

Kuroda reported recent experiments on the phase separation and correlated magnetic properties in II-VI magnetic semiconductor (Zn,Fe)Te. They have grown thin films of $Zn_{1-x}Fe_xTe$ by MBE with Fe compositions up to x = 0.25. Under the growth with an excess supply of Te flux (Te-rich growth), the grown films exhibit paramagnetic behaviors in the whole range of Fe composition studied. On the other hand, the films grown with an excess supply of Zn flux (Zn-rich growth) exhibit ferromagnetism and the transition temperature exceeds room temperature above x =0.06. The TEM observation for the film containing a high Fe composition of x ~ 0.2 revealed that Fe-aggregated regions of nano-scale columnar shape are formed along the growth direction. In order to identify the material of Fe-aggregated regions, they have performed structural characterization at the atomic scale using TEM and XAFS.

Based on the discussions, we reached the conclusion that the spinodal nano-decomposition in inhomogeneous systems and a new fabrication method of ultra-high-density nano-superstructures by self-organization, such as quantum-dot and quantum nano-wire, using the two-dimensional or three-dimensional spinodal nano-decomposition in self-organization, and for a colossal magnetic and electronic response controlled by electric field or photonic excitation. The session emphasized again the technological importance and potential of chemically and structurally

inhomogeneous solids. Understanding the electronic properties of these inhomogenieties on the nanoscale is an important task for the international ab-initio community that will be taken up by us in the future investigating in the development of the ab-initio code KKRnano. We concluded that the spinodal nano-decomposition could be generalized as a new class of bottom-up nanotechnology with an outstanding potential in various fields and applications. To realize these, we will apply EU-JAPAN collaboration program on spinodal nanotechnology based on the discussion and the conclusion from the EU-JAPAN Workshop in Jülich Research Center.

Session: Moltronics

Discussion leader: Biplab Sanyal, Uppsala University, Sweden

The session started with an overview talk by Heiko Wende from University of Duisburg-Essen. He demonstrated the state-of-the-art scenario of spinterfaces with organic-inorganic hybrids by exploring the interaction between magnetic molecules and metallic surfaces, both from experimental and theoretical points of view. Results on organometallic 3d transition metal and 4f rare-earth centered porphyrines and phthalocyanines were shown, obtained by element-specific x-ray magnetic circular dichroism experiments and density functional calculations. Heike Herper of Uppsala University showed theoretical studies on the effects of ligands and adlayers on the electronic structure and magnetic properties of freestanding molecules as well as molecules adsorbed on surfaces. Critical discussions on the effects of electron correlation were made. Nico Atodiresei from Jülich extended these ideas to small organic molecules adsorbed on surfaces to modify the properties of substrates, e.g., exchange interaction among the surface magnetic atoms etc. The importance of the right choice of van der Waals interaction for describing weakly physisorbed systems was extensively discussed.

T. Ohto from Osaka University showed results obtained from first-principles calculations of electronic transport in molecular junctions via non-equilibrium Green function technique. The development of a methodology to study the effect of vibration in transport properties by taking into account electron-phonon interaction to describe features in inelastic electron tunneling spectroscopy was shown. Finally, S. Tsukamoto from Jülich discussed the development of an efficient method to calculate electron transport based on real-space finite-difference formalism, which is suitable for treating a large number of atoms in ab initio transport calculations. This gives the possibility of taking into consideration, e.g., realistic STM tip geometries along with complicated surface constructions. Results on STM simulations were shown.

Sanyal and Ohto discussed about future collaborations, e.g., in studying spin-dependent electron transport through organometallics, exploring geometries of molecules and junctions under non-equilibrium conditions etc. General discussions on proper descriptions of electronic structure of rare-earth centered molecules were made from the point of view of hybridization with ligands, strong spin-orbit coupling etc.

Report on spintronics V and VI sessions, 26 September by Olle Eriksson (Uppsala University)

Five speakers presented the results at this session; Julen Ibanez Azpiroz (Juelich), Jonathan Chico Carpio (Uppsala University) and Nikolai Kiselev (Juelich) before lunch, and Olle Eriksson (Uppsala University) and Konstantinos Koumporas (Uppsala University). The topics covered concerned I general the coupling of ab-initio electronic structure theory to atomistic spin-dynamics simulations. This focus was e.g. on calculations of response functions for single atom systems (3d and 4d elements) on a substrate (e.g. Ag substrate), where primarily direct evaluations of the response function (frequency dependent susceptibility) was discussed. Here it was suggested that a direct comparison to experimental values would be beneficial, and potentially frequency dependent field measurements could achieve this. A large fraction of this session was devoted to magnetic states with non-trivial toplogy. Examples of this are the skyrmions, toplogical bobber and chiral solitons. Various ways to use these objects in technology was discussed, in parallel to methodological aspects of these materials. The discussion around the magnetic bobber turned out to be particularly fruitful and interesting, not least since the experimental discovery of skyrmion states of the bulk e.g. MnSi and FeCo-Si systems was questioned or at least discussed.

The possibility to control magnetic objects by external means was discussed, both for topological objects like solitons and skyrmions, but also for more ‘innocent’ objects like domain walls. Temperature control of domain wall motion was demonstrated from atomistic spin-dynamics simulations, and phenomena like walker breakdown were discussed. Furthermore, it was described how atomistic spin-dynamics simulations can be used to describe all-thermal switching of magnetization dynamics and the simulations and observations are in agreement. However, a general problem for evaluating exchange parameters at finite temperature was discussed and highlighted as a needed methodological development.

The dynamics of topologically non-trivial objects was in particular discussed in this session, where current induced motion was reported for several skyrmion systems. The inertia of these moving objects was also analyzed, and compared to objects of classical mechanics. Several new materials classes that potential can host skyrmions was anlaysed, and in particular it was shown that certain Heusler alloys are good candidates.

Report on spintronics VII sessions, 27 September by Hisazumi Akai (The University of Tokyo)

The session spintronics VII was dedicated for spintronics of rather broad aspect, including metallic, semiconductor, and topological spintronics. Three speakers, Yatsuki Oda (Forschungszentrum Jülich), presented the results of their recent work.

Oda presented the results of recent DFT calculations on the electric field effects on the magnetic anisotropy of magnetic tunnel junctions. He found an asymmetric behavior in the simulated magnetization-demagnetization curves under an electric field, concluding that a field control of magnetic anisotropy might be possible in this system.

Until now, two mechanisms have been proposed, p-d exchange (p-d hybeidization) and double-exchange. Although those are two limiting cases of essentially the same physics, namely the total band broadening expected for ferromagnetic alignment of magnetic moment, the electronic structure sometime looks differently. Sato performed various super-cell calculation on (Ga, Mn)As and concluded that in this system, Mn cluster can exist stably and, in this case, the Fermi level lies at near the top of the valence band. This result seems consistent with recent various experimental observations.

dos Santos Dias gave a talk about resent activities of his group on topological orbital magnetic moment, namely the orbital magnetic moment that may exist without the spin-orbit coupling. The point is that if scalar chirality in three local magnetic moments exist in non-centrosymmetric system, e.g. Fe_3 trimers on the surface of Cu(111), an orbital current circulating these local moments will appear. He showed this fact through first-principles electronic structure calulations.

Report on "New Methodology for Computational Materials Design II" Tuesday 27th September 2016 by Daniel Wortmann (FZ Jülich)

In this session thee speakers presented their work on new approaches for Material design: I. Hamada (NIMS, Tsukuba), K. Rushchanskii (FZ-Jülich) and T. Nishimatsu (U. Tohou). In the first presentation I. Hamada stressed the importance of approaches beyond standard LDA/GGA DFT to achieve accuracy in total energy calculations. After shortly introducing the WEST code for GW calculations of large systems he then focused on calculations employing non-local correlation functionals to account for the van-der Waals interaction. Here he reported on a new functional he introduced and demonstrated its performance by the investigation of several test-sets of molecules, bulk materials and complex compounds. He also pointed out that the desired accuracy can only be reached if the pseudo-potentials are chosen carefully and consistently. In the second talk K. Rushchanskii introduced his work on multiferroics. He showed that $GaFeO_3$ in different composition ranges of Ga and Fe as well as Fe_2O_3 in its ϵ-phase can be multiferroic and investigated in detail the possible structural changes necessary for switching the ferroelectric polarization. For this purpose many structural relaxations have been performed as determined by a genetic algorithm. This approach was reported to be very effective in the determination of possible crystal structures and different crystal phases. In particular the in-build generation of structures following an estimate of the phonon-spectrum and the soft phonon modes has proven to limit the effort of sampling significantly. In the last presentation of the session T. Nishimatsu also reported on simulations of ferroelectric materials. His focus was the simulation of ferrorelectric polarization and its domain structures on large scale. Here he applied molecular dynamics using a model Hamiltonian which was constructed with parameters obtained from ab-initio calculations. Together with an efficient treatment of the calculation of the coulomb term his mapping allowed to evaluate the time evolution of the polarization.

Report on Permanent Magnet Materials (Session: Spintronics VIII)

28th September 2016 by Tatsuki Oda (Kanazawa Univ.)

Four speakers presented the results at this session; Hisazumi Akai (Tokyo Univ.), Alexander Edström (Uppsala Univ.), Takashi Miyake (The National Institute of Advanced Industrial Science and Technology), Yoshihiro Gohda (Tokyo Institute of Technology). In this session, we discussed stronger permanent magnets. In a strategy of the project, people has to discuss the topics of how to maximize the magnetic energy drawn from the B-H hysteresis curve, and also how to find (design) a new material of permanent magnet and how to improve properties. We actively discussed the mechanism of having a stronger magnetic property from the electronic structure theory, theory of computational material science, theory for impurities, ligand field theory, etc. The target materials consist of almost Fe or Co. They are alloying with the other supporting elements; element of f-states, 1st low elements, and 5d series of elements. Akai presented the results of electronic structures and the exchange coupling constants in the rare-earth magnets ($SmCo_5$, $Nd_2Fe_{14}B$, and $Sm_2Fe_{17}N_3$), after the brief introduction of the background on such research project. His points discussed are as follows; what is the role of the f-states in the rare-earth element for the large magnetic anisotropy, the localized atomic orbital of f-states, and the importance of itinerant nature of them as well as those of exchange interactions among Fe atomic magnetic moments and between Fe and Nd ones. As one of the conclusions, the "Cobaltization" on Fe electronic structure for minority spin states, whose concept was expressed philosophically by Kanamori, causes the novel electronic structure in the magnets associated with enhancement of the magnetic anisotropy originated from the large spin-orbit coupling on the rare-earth atom. Edström presented the new results on magnetic anisotropy and discussed the impurity effects of 5d transition metal elements in the FeCoB alloy with using CPA approximation. In his result, 3d magnetic alloy can get the benefit of the large spin-orbit coupling through the orbital hybridization with 5d elements. He also discussed the experimental result on the case of $(Fe_{1-x}Co_x)_2B$, resulting in a support of the computational results and, the new material of such as $Fe_2Ta_{1-x}W_x$. Miyake presented the results of $NdFe_{12}N$, $NdFe_{11}TiX$ (X=B, C, N, O, F). He found a new permanent magnetic material $NdFe_{12}N_x$ in the collaboration with the experimental group. The material, obtained on the substrate, shows a large magnetization and a larger anisotropy field at the high temperatures, compared with those of $NdFe_{14}B$. He discussed the role of N element on the Fermi level in conjunction with Cobaltization. Gohda presented the results of the electronics structures and MAEs in the interface of grain boundary models for the real magnet of $NdFe_{14}B$. He discussed the role of impurity atoms (Cu and so on).

Report on spintronics VIII sessions, 28 September by Hisazumi Akai (The University of Tokyo)

The session spintronics VIII was dedicated to review recent efforts to reveal the mechanism of appearance of the strong coercivity in rare-earth permanent magnets and to develop new permanent magnet materials. Four speakers, Hisazumi Akai (The University of Tokyo), Alexander Edström (Uppsala University), Takashi Miyake (AIST and NIMS), and Yoshihiro Gohda (Tokyo Institute of Technology) presented the results of their recent work.

Akai first explained the essential ingredients that are need for a ferromagnetic material to be a permanent magnet. Then, he discussed the role of Sm f-state in exhibiting uniaxial magnetic anisotropy in $Sm_2Fe_{17}N_3$. The importance of chemical bonding between Sm f-states and N p-states in addition to the electro-static effects caused by the existence of N was pointed out.

Edström discussed the possibility of obtaining magnetic anisotropy without relying on rare-earth elements. He showed the results of recent first-principles calculation on $(Fe_{1-x}Co_x)_2B$ system. The overall agreements with experiments are reasonable for magnetization. However, he pointed out, the magnetic anisotropy showed some qualitative disagreement with experiments in the vicinity of Co_2B, implying more sophisticated ways of calculations using the full-potential treatment and DMFT might be needed.

Miyake showed the results of the recent theoretical work of his group on newly synthesized permanent magnetic materials $NdFe_{12}N$, which shows comparable or even better performance compare to the so far known best permanent magnet $Nd_2Fe_{14}B$. He discussed the role of N in this system and showed a systematics seen when N was replaced for other metalloid, B, C, etc., explaining the result in terms of the hybridization between Fe d- and metalloid p-states. The temperature dependence of the magnetic properties was also discussed.

Gohda presented the first-principles calculation on $Nd_2Fe_{14}B/NdO_x$ interface, which simulated the grain boundary formed between $Nd_2Fe_{14}B$ grains in NdFeB permanent magnets. He concluded that the in-plane magnetic anisotropy that occured at $Nd_2Fe_{14}B$ surfaces was largely reduced by the existence of NdO_x at the interface. This would suppress the nucleation of domain walls or pin the domain wall motion, contributing to the coercivity.

Report on Large inhomogeneous Systems (High Entropy Alloys and Phase Change Memories), 28. September 2016
by Peter H. Dederichs

The session was concerned with DFT applications to two very large and complex inhomogeneous systems, which represent a challenge for DFT applications, but which are also of strong interests for applications.

The first presentation by Tetsuya Fukushima were centered at the understanding of High Entropy Alloys (HEA). These recently discovered alloys consist of many different components of similar high concentration and are energetically favoured by the disorder entropy. This leads to a lowering of the Gibbs free energy, due to the increase of the disorder entropy with the number of disordered components. In his calculations for the disordered CrFeCoNi system on a fcc lattice Fukushima used the KKRnano code for a supercell of about 1300 atoms and in particular calculated the local moments of the components and compared with CPA results. As second example the considered the doping of the phase change material $Ge_2Sb_2Te_5$ with transition metals atoms. The idea is that the local moments of these metals atom might be controlled by an magnetic field possibly yielding interesting information about the crystal and amorphous phase of GST materials.

The presentation of Riccardo Mazzarello focussed on the physics and in particular on the structural and electronic properties of the phase change material $Ge_2Sb_2Te_5$. These materials show at high temperatures a very fast and completely reversible transition between the crystalline and the amorphous phases. Due to the strong difference of the optical properties and the resistivity between both phases these GST materials are used as rewritable optical devices and electronic non-volatile random access memories. Based on ab-initio molecular dynamics methods Mazzarello first discusses the electronic structure of crystalline GST. Contrary to normal semiconductors the valence band maximum of these materials consists of antibonding states resulting from the hybridization of Ge-s with the Te-p states leading in a rather small formation energy of Ge-vacancies. Then, he discussed metal-insulator transitions in crystalline GST, which are driven by vacancy disorder. In the last part of his talk, Mazzarello focused on "interfacial" phase change materials consisting of layers of GeTe, GeSbTe and Sb_2Te_3. While these new PCMs are used already in applications, he discussed in detail the structural switching process and the possible transition between two topological distinct phases. He also discusses that ab-initio MD methods combined with enhanced sampling methods can investigate time-scales being not accessible by plain ab-initio MD methods.

Report on Materials Exploration
30 September, 2016 moderated by Tamio Oguchi (Osaka University)

Three speakers presented some topics in this session: Hiroyoshi Momida (Osaka University), Tomoki Yamashita (National Institute for Materials Science, Tsukuba), and Hitoshi Fujii (National Institute for Materials Science, Tsukuba).

Momida talked on his recent study on materials exploration for high-temperature piezoelectric applications. Perovskite oxide materials such as Pb-Zn-Ti-O show high piezoelectric coefficients though their applications at high temperatures are very much limited because of relatively low Curie temperature. On the other hand, some of wultzite materials such as AlN has high Curie temperature but low piezoelectric performance. Momida investigates the electronic mechanism of large enhancement of piezoelectric constant in Sc doped wultzite AlN and find the lattice constant ratio c/a as the key parameter in the piezoelectric response, that can be a good descriptor for further exploration.

Yamashita developed structure search method starting from random set-up of structure for a given composition of elements. In the case of a system with a relatively small number (roughly up to 20) of atoms in unit cell, it is found that a combination of the random generation of structure and the structure optimization by first-principles calculations is quite efficient to obtain the equilibrium structure of intermetallic compounds. However, the configurational space becomes vast for a system beyond that cell size and further methods are needed to accelerate the structure search. In this context, Yamashita demonstrates that space-group classification and Bayesian optimization might be good techniques for the acceleration of structure search.

Fujii performed machine learning for the spin magnetic moments of 3d transition-metal alloys, the so-called Slater-Pauling (SP) curve, by using the LASSO (least absolute shrinkage and selection operator) method with several descriptors taken from atomic and pure elemental solid data including both experimental database and KKR-CPA calculation results. He finds that the SP curve is well reproduced by considering the third-order dependence of the alloy concentration. It is also suggested that the physical meaning of the descriptors selected by LASSO should be investigated. This type of approach may be quite useful and promising for exploring the system that has large targeted concrete magnetic properties for ternary and multinary alloy systems.

Report on the Session of Nano-fabrication & Crystal Growth, 30 September, 2016 by Tetsuya FUKUSHIMA (Osaka Univ.)

Two speakers presented the results at this session; A. Masago (Osaka Univ.) and H. Shinya (Osaka Univ.). Masago reported the investigation of electronic and magnetic properties of Eu-doped GaN, on the basis of *ab initio* electronic structure calculation and multi-scale simulations of the crystal growth. Magnetic exchange interaction between Eu atoms calculated by magnetic-force theorem is mainly short-ranged Zener's double exchange interaction, and a weak-long-ranged Zener's *p-d* exchange interaction also coexists. Based on the multi-scale simulations of 2D and 3D crystal growth using the calculated chemical-pair interactions, Masago demonstrated that the self-organized nano-superstructures (Konbu-Phase in 2D and Dairiseki-Phase in 3D) induced by the spinodal decompositions can be fabricated in Eu doped GaN. System becomes super-paramagnetic with high-blocking temperature, and a large hysteresis loop appears in the magnetization when the external magnetic field is applied (M-H curves). These nano-superstructures are controllable by the crystal growth conditions, so that the hysteresis loop in M-H curves appear, depending on these nanostructures. Moreover, the nano-superstructures are suitable for high light-emission.

Shinya reported the computational nano-materials design and general design-rules for high-efficient thermoelectric power materials in $(GeTe)_x(AgSbTe_2)_{1-x}$. Shinya predicted the stable structures by the cluster expansion method, and found that the structural stability is attributed to the formation of the Ag-Te-Sb chain structure. Shinya also found that the Te-5p anti-bonding states are dominant at the valence band maximum (VBM) by the Sb-5s and Te-5p hybridization. Due to the inherent instability by the anti-bonding coupling, $AgSbTe_2$ produces vacancy-ordered phase by the self-regeneration of defect complexes $[2V_{Ag}+Sb_{Ag}]$ in the Ag-poor and Sb-rich crystal growth conditions. These mutation phases and the grain boundaries might work as the phonon scattering center and decrease the lattice thermal conductivity in $AgSbTe_2$. Additionally, the calculations of the mixing energy clearly show that the defect complexes $[2V_{Ag}+Sb_{Ag}]$ in $AgSbTe_2$ spontaneously gather together, so that the vacancy-rich region also works as the scattering center. Thus, one can synthesize the $AgSbTe_2$ with high thermoelectric efficiency by constructing nano-structures of the mutation phase, changing the Ag and Sb vapor pressures. These design rules can be generalized to other thermoelectric materials, which have anti-bonding character at the VBM.

Based on the above two-talks, we can conclude that (1) the spinodal nano-decomposition is the general nano-fabrication method in the bottom-up nanotechnology using the self-organized nano-fabrication method in the thermal non-equilibrium conditions, and (2) the self-regeneration mechanism caused by the low-formation energies of metallic-vacancies and metallic-anti-site defects could be generalized for the formation of ordered vacancy phases by phonon-scattering or electron and hole accumulation.

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A. Advanced Research Networks

Computational Nano-Materials Design
on Green Energy

EU-JAPAN Workshop on Computational Nano-Materials Design and Realization for Spintronics, Moltronics, Quantronics, Superconductivity and Topotronics

Peter Grünberg Institute, Jülich Research Centre, Jülich, Germany, September 18th – 30th, 2016

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Scope of The Workshop

(1) Spintronics,
(2) Moltronics,
(3) Quantronics,
(4) Superconductivity,
(5) Topotronics

Scope of The Workshop

■Discussion leader will organize the session with the short introduction of the purpose and the goals of the session, where two or three speakers talk and keep continue the discussions through the lunch.

■Basically, each talk is organized with 30 min presentation and 30 min discussion, therefore, please keep the scheduled time.

■Based on the presentations and discussions, the discussion leader will prepare the repot of new proposal and summary in the wrap-up session. ➡ March 21~22, 2017 Summary Workshop in Osaka.

■We will finalize the summary and new proposal on the last day and distribute it to the participants for the preparation of the future collaborations.

New Proposal (2017~2021FY)

■Swedish & Japan (JSPS) : Energy Saving & Creation
Oguchi – Sanyal (already submitted in September)

■US & Japan (JSPS, NEDO, JST) : Catalysis
Morikawa – Norskov

■Swedish & Japan (JSPS): Moltronics
Ohto- Sanyal

■Austria & Japan (JSPS) : Semiconductor Spintronics
Sato – Bonanni

■Germany & Japan (JSPS, JST) : HPC
Ono – Stefan Bluegel

and More.