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GENERAL INFORMATION

Venue

Rm. S102, Teaching Building,
Zhong-Guan-Cun Campus, UCAS
Add: No.3, Zhong Guan-cun Nan
Yi-Tiao, Haidian, Beijing, China

Registration

The registration desk will be opened at the UCAS, Zhong-Guan-Cun Campus during the following hours:
08:30-16:00, Sunday 4 November 2018
08:40-10:30, Monday 5 November 2018

Catering

Lunch

Lunch coupons are inside the package given to you when you register. You should present your coupon in order to obtain lunch.

Place: 4th Floor, Wuke Restaurant

Morning and Afternoon Tea Breaks

Tea breaks during the workshop will be served outside Rm. S102, Teaching Building

Nearby Cafes and Restaurants

There are numerous cafes and restaurants near Kavli ITS. Have fun with Chinese food and language!

The Kavli ITS Workshop on Diluted Magnetic Semiconductors: Challenges and Opportunities

4-5 November 2018, Beijing, China

S102, Teaching Building, Zhong-Guan-Cun Campus, UCAS

No. 3, Zhong Guan-cun Nan Yi-Tiao, Haidian, Beijing

PROGRAM

4 November (Sunday)

8:30-16:00 Registration

08:50-09:00 Opening **Fu-Chun Zhang**, Kavli ITS, UCAS

Sunday Session A

Chair:	**Sadamichi Maekawa**, RIKEN/ Kavli ITS, UCAS
09:00-09:25	**Masaaki Tanaka**, Univ. of Tokyo New n-type and p-type Fe-doped III-V ferromagnetic semiconductors with high Tc
09:25-09:50	**Atsushi Fujimori**, Univ. of Tokyo Impurity bands and inhomogeneous magnetism in diluted ferromagnetic semiconductors
09:50-10:15	**Pham Nam Hai**, Tokyo Inst. Tech. Spin-dependent transport phenomena in Fe-doped ferromagnetic semiconductor-based spin devices
10:15-10:40	**Igor Zutic**, Univ. of NY, Buffalo What can we do with dilute magnetic semiconductors?

10:40-11:00 Photo & Tea Break

Sunday Session B

Chair:	**Chang Qin Jin**, IOP, CAS
11:00-11:25	**Yasutomo J. Uemura**, Columbia Univ. Muon Spin Relaxation (MuSR) Studies of Magnetic Semiconductors
11:25-11:50	**Jian Hua Zhao**, Inst. of Semi., CAS Robust manipulation of magnetic properties in magnetic semiconductor (Ga,Mn)As
11:50-12:15	**Xin Hui Zhang**, Inst. of Semi., CAS Ultrafast excitation and dynamics of collective spins in ferromagnetic (Ga,Mn)As mediated by photoexcited carriers
12:15-12:40	**Xiao Hong Xu**, Shanxi Normal Univ. Magnetic and transport properties of n-p co-doped oxide semiconductors

12:40-14:00 Lunch Break

Sunday Session C

Chair: **Yasutomo J. Uemura**, Columbia Univ.

14:00-14:25 **Chang Qin Jin**, IOP, CAS
New Diluted Magnetic Semiconductors with Independent Spin & Charge Doping: from Materials to Properties toward Multiple Heterojunctions

14:25-14:50 **Xing Jiang Zhou**, IOP, CAS
ARPES on Electronic Structure of Diluted Magnetic Semiconductor $(Ba_{1-x}K_x)(Zn_{1-y}Mn_y)_2As_2$

14:50-15:15 **Xiang Gang Qiu**, IOP, CAS
Doping dependence of optical and magnetic properties of diluted magnetic semiconductor $(Ba_{1-x}K_x)(Zn_{1-y}Mn_y)_2As_2$

15:15-15:40 **Zheng Deng**, IOP, CAS
High pressure effects on new generation diluted magnetic semiconductors with decoupled charge and spin doping

15:40-16:10 Tea Break

Sunday Session D

Chair: **Jian Hua Zhao,** Inst. of Semi., CAS

16:10-16:35 **Yong Qing Li**, IOP, CAS
Anomalous Hall effect in Mn-doped topological insulators

16:35-17:00 **Li Xin Cao**, IOP, CAS
Thin films of diluted magnetic semiconductor $(Ba_{1-x}K_x)(Zn_{1-y}Mn_y)_2As_2$

17:00-17:25 **Fan Long Ning**, Zhejiang Univ.
The Synthesis, NMR and μSR investigation of bulk form diluted ferromagnetic semiconductors with decoupled charge and spin doping

5 November (Monday)

8:40-10:30 Registration

Monday Session A

Chair: **Igor Zutic**, Univ. of NY, Buffalo

09:00-09:25 **Xiao Hu**, NIMS
Topological Orbitronics in Superstructured Graphene

09:25-09:50 **Akbar Jafari**, Sharif Univ. of Tech.
Majorana fermions disappear one-by-one

09:50-10:15 **Nejat Bulut**, Izmir Inst. of Tech.
Role of the impurity bound states in bioinorganic molecules

10:15-10:35 Tea Break

Monday Session B

Chair: **Xiao Hu**, NIMS

10:35-11:00 **Chang-Beom Eom**, Univ. of Wisconsin- Madison
Epitaxial thin films and artificially engineered superlattices of $BaFe_2As_2$ pnictide (a Skype presentation)

11:00-11:25 **Guo Qiang Zhao**, Columbia Univ. & IOP, CAS
Single Crystal Synthesis, High Pressure Research and Spin Polarization Measurements of “BZA” Based Diluted Magnetic Semiconductor

11:25-11:50 **Bo Gu**, Kavli ITS, UCAS
Diluted magnetic semiconductors: Role of band gaps

11:50-12:00 Closing **Sadamichi Maekawa**, RIKEN/ Kavli ITS, UCAS

12:00-13:30 Lunch

ABSTRACT CONTENTS

New n-type and p-type Fe-doped III-V ferromagnetic semiconductors with high T_C

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Ferromagnetic semiconductors (FMSs) have been intensively studied for decades, since they have novel functionalities that cannot be achieved with conventional metallic materials, such as the ability to control magnetism by electrical gating or light irradiation [1-3]. Prototype FMSs such as (Ga,Mn)As, however, are always p-type, making it difficult to be used in real spin devices. Here, we demonstrate that by introducing Fe into InAs, it is possible to fabricate a new n-type electron-induced FMS with the ability to control ferromagnetism by both Fe and independent carrier doping. The studied $(In_{1-x},Fe_x)As$ layers were grown by low-temperature molecular beam epitaxy on semi-insulating GaAs substrates. Electron carriers in these layers are generated by independent chemical doping of donors. The ferromagnetism was investigated by magnetic circular dichroism (MCD), superconducting quantum interference device (SQUID), and anomalous Hall effect (AHE) measurements. With increasing the electron concentration (n = 1.8×10^{18} cm^{-3} to 2.7×10^{19} cm^{-3}) and Fe concentration (x = 5 - 8%), the MCD intensity shows strong enhancement at optical critical-point energies of InAs, indicating that the band structure of (In,Fe)As is spin-split due to *sp*-*d* exchange interaction between the localized *d* states of Fe and the electron sea. SQUID and AHE measurements are also consistent with the MCD results. The Hall and Seebeck effects confirm the n-type conductivity of our (In,Fe)As samples. The electron effective mass is estimated to be as small as 0.03-0.175m_0, depending on the electron concentration. These results reveal that the electrons are in the InAs conduction band rather than in the impurity band, allowing us to use the conventional mean-field Zener model of carrier-induced ferromagnetism [4]. This band picture is different from that of (Ga,Mn)As [5][6]. Our results open the way to implement novel spin-devices such as spin light-emitting diodes or spin field-effect transistors, as well as help understand the mechanism of carrier-mediated ferromagnetism in FMSs [7-14].

Furthermore, we have found new phenomena in (In,Fe)As and its quantum heterostructures: Novel crystalline anisotropic magnetoresistance with two fold and eight fold symmetry [7], and control of ferromagnetism by strain, quantum confinement, gate electric field and wave-function engineering in quantum heterostructures with a (In,Fe)As quantum well [10-12]. Very recently, we have found very intriguing phenomena; sudden restoration of the band ordering associated with the ferromagnetic phase transition in the prototypical ferromagnetic semiconductor (Ga,Mn)As [15], and control of the bias-voltage dependence of tunneling anisotropic magneto-resistance using quantization in (Ga,Mn)As quantum wells [16]. Also, we have successfully grown new narrow-gap p-type III-V-based FMS (Ga,Fe)Sb and n-type III-V-based FMS (In,Fe)Sb with Curie temperatures higher than room temperature (T_C > 300K) [17-19]. Combining different n-type and p-type FMSs with high T_C will lead to new spin-related functionalities and devices.

We thank Drs. S. Ohya, I. Muneta, M. Kobayashi, S. Sakamoto, and A. Fujimori. This work was partly supported by Grants-in-Aid for Scientific Research, CREST of JST, and Spintronics Research Network of Japan (Spin-RNJ).

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Impurity bands and inhomogeneous magnetism in diluted ferromagnetic semiconductors

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In diluted ferromagnetic semiconductors, impurity bands are formed in systems with strong p-d hybridization [1]. The position of the Fermi level is located within the impurity band [2,3], below the valence-band maximum (VBM) [4], or above the conduction-band minimum (CBM) [5] depending on the type and the amount of doped carriers, as revealed by a series of ARPES studies.

In addition to the random nature of the substitution of magnetic ions, the density of the magnetic ions may not be homogeneous, leading to complex magnetic behaviors. Analysis of M-H curves deduced from XMCD intensities reveals a mixture of superparamagnetic (SPM) and paramagnetic (PM) components above T_C [6,7]. A ferromagnetic (FM) component emerges below T_C, but the SPM and PM components survive down to the lowest temperature [8,9].

Collaboration with M. Kobayashi, Y. Takeda, S. Sakamoto, Y. X. Wan, H. Suzuki, G. Shibata, S.-i. Fujimori, K. Horiba, K. Kumigashira, V. I. Strokov, N. T. Tu, P. N. Hai, L. D. Anh, Y. K. Wakabayashi, I. Muneta, S. Ohya, M. Tanaka, S. Maekawa, B. Gu, Y. J. Uemura, K. Zhao, G. Q. Zhao, C. Q. Jin, S. Guo, and F. Ning is gratefully acknowledged.

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Spin-dependent transport phenomena in Fe-doped ferromagnetic semiconductor-based spin devices

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Ferromagnetic semiconductors (FMSs) are promising materials for future spintronic devices since they exhibit both properties of semiconductors and magnetic materials. Prototype FMSs such as (In,Mn)As or (Ga,Mn)As, however, are always p-type, making them difficult to be used in realistic spin devices. Moreover, their Curie temperature is still much lower than room temperature, and their origin of ferromagnetism is still under debate. Recently, to overcome the shortcomings of the Mn-doped FMSs, we have proposed and realized a completely new class of FMSs based on Fe-doped narrow-gap III-V semiconductors [1-7]. Since Fe atoms are in the neutral state Fe^{3+} in many III-V semiconductors, independent control of the spin and carrier characteristics is possible. This allows us to grow both n-type and p-type FMSs with unprecedented electrical and magnetic properties. With this approach, we have successfully fabricated various Fe-doped FMS-based spin devices, such as spin field effect transistors (FET) [8,9], spin diodes [10], and anomalous Hall effect sensors [11]. We observed novel spin-dependent transport phenomena in those spin devices, such as quantum size effects [12,13] and wavefunction engineering of ferromagnetism in a spin FET with an (In,Fe)As quantum wells [8], giant spin-valve effect (600%) in a p-type (Ga,Fe)Sb / n-type (In,Fe)As spin diode [10], large spin-split of the conduction band in p-type InAs/n-type (In,Fe)As Esaki diodes [14], and room-temperature ultra-high sensitivity in (In,Fe)Sb-based anomalous Hall sensors [11]. Our observation is an important step towards realization of high-performance semiconductor spin devices.

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What can we do with dilute magnetic semiconductors?

Igor Žutić

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Unlike metals, semiconductors have a carrier density that can be drastically changed by doping, electrical gates, or photoexcitations, to control their transport and optical properties. In dilute magnetic semiconductors (DMS) these changes of carrier density also enable novel opportunities to control the magnetic properties and lead to applications that are not available or ineffective with ferromagnetic metals [1]. DMS have provided the demonstrations of magnetic effects and ideas subsequently transferred to ferromagnetic metals at room temperature, for example, electric-field modulation of coercivity and magnetocrystalline anisotropy, and spin-orbit torque [2,3]. Together with the push to increase the temperature for ferromagnetic ordering in DMS [4], it is also important to increase their g-factors and improve interfacial quality of their junctions to enhance the influence of proximity effects [5,6]. These developments could enable fundamental phenomena from the competing order parameters [7] to Majorana fermions [8], as well as applications beyond magnetoresistance, such as spin lasers [9].

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Muon Spin Relaxation (MuSR) Studies of Magnetic Semiconductors

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Muon spin rotation and relaxation (MuSR) is a powerful magnetic probe which can detect the local static ordered moment size and the volume fraction of the ordered regions separately. It be applied to bulk specimens as well as thin films (thicker than 200 Angstroms) even in zero external field. We started MuSR studies of diluted magnetic semiconductor (DMS) systems in 2008, with the MBE films of (Ga,Mn)As in collaboration with Hideo Ohno. We found signature of homogeneous ferromagnetic state developing in full volume fraction in specimens with proper heat treatments [1]. After finishing this work, I attended a conference on DMS systems in Tohoku U in 2010, and attended in a talk of Thomas Junswirth [2] who proposed to replace GaAs with LiZnAs to dope Mn in isovalent (Zn,Mn) substitutions, which would allow decoupling of spin (Zn,Mn) spin doping and charge doping with Li stoichiometry.

This proposal had not been tried by materials people of DMS community who were mostly working with MBE growth which is hardly compatible with reactive Li. At that time, I had collaboration with Changqing Jin of IOP who was providing use with LeFeAs and other superconductor samples. I encouraged him to make the new DMS system proposed by Jungwirth, and within a few months the IOP group indeed succeeded in making the “111 DMS” Li(Zn,Mn)As [3]. Within two years they also made (Ba,K)(Zn,Mn)$_2$As$_2$ [4]. This “122 DMS” compound has ferromagnetic Tc up to 230 K, and can be obtained as bulk single crystals. It has the same crystal structures with superconducting (Ba,K)Fe$_2$As$_2$, antiferromagnetic BaMn$_2$As$_2$ and semiconducting BaZn2As2 with excellent lattice constant matching, as shown in the attached table. This encourages development of junction and multilayer spintronics devices.

Fanlong Ning was a postdoc with our group. I encouraged him to join in DMS studies, and he applied NMR to DMS and then synthesized the “1111 DMS” system (La,Ba)(Zn,Mn)AsO [5]. Most recently his group succeeded in making the long-awaited electron-doped DMS Ba(Zn,Co)$_2$As$_2$ [6]. In 2016, my research team was joined by Zurab Guguchia of PSI who led the projects of MuSR in transition metal di chalcogenides (TMDC). We discovered static antiferromagnetic order of 2H MoTe$_2$, 2H MoSe$_2$ [7].

In these new ferromagnetic DMS [1,3-6], MuSR confirmed static order in the full volume, and obtained the ZF relaxation rate a at T→0, proportional to the individual moment size multiplied to the moment density. The plot of a versus T_C demonstrates that the p-type (Ga,Mn)As, 111, 122, and 1111 DMS systems have the same exchange coupling constant / mechanism, while the n-type 122 DMS has much stronger exchange coupling. We tried to cleave 122 DMS crystals, but could not obtain a good material for gating / exfoliation. Epitaxial growth of thin films of 122 DMS should be a next step.

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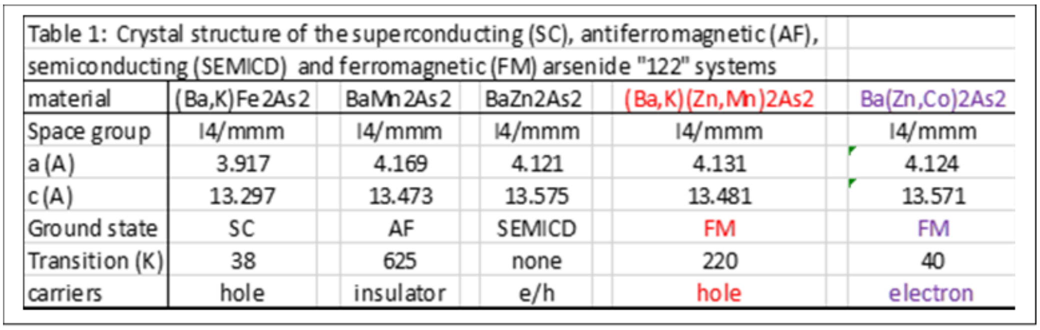

Table 1: Crystal structure of the superconducting (SC), antiferromagnetic (AF), semiconducting (SEMICD) and ferromagnetic (FM) arsenide "122" systems

material	(Ba,K)Fe2As2	BaMn2As2	BaZn2As2	(Ba,K)(Zn,Mn)2As2	Ba(Zn,Co)2As2
Space group	I4/mmm	I4/mmm	I4/mmm	I4/mmm	I4/mmm
a (A)	3.917	4.169	4.121	4.131	4.124
c (A)	13.297	13.473	13.575	13.481	13.571
Ground state	SC	AF	SEMICD	FM	FM
Transition (K)	38	625	none	220	40
carriers	hole	insulator	e/h	hole	electron

Robust manipulation of magnetic properties in magnetic semiconductor (Ga,Mn)As

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Abstract: (Ga,Mn)As with a well-accepted intrinsic ferromagnetism is a presentative material in the family of magnetic semiconductors. Through modulation of the hole density, electrical gating has been shown to alter the magnetic properties of (Ga,Mn)As films, but with limited electric-field effects on the Curie temperature ~10K and coercive force of ~10Oe [1-3]. In my talk, I will first present our recent work on modulation of magnetism in (Ga,Mn)As by electric field. We have realized a giant manipulation of the magnetism in (Ga,Mn)As ultra-thin films via electric field with the assistance of ionic liquid. The maximum modulation of the Curie temperature is up to 100K. Fowllowing that, I will mention our very recent work that we have rotated the direction of magnetization in (Ga,Mn)As film up to ~27° by organic molecules, which doubles the maximum value of 0.4 V/nm by electric field [4].

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Ultrafast excitation and dynamics of collective spins in ferromagnetic (Ga,Mn)As mediated by photoexcited carriers

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The growing interest in ultrafast manipulation of magnetization has triggered people's great attention on studying the same issue in ferromagnetic semiconductor (Ga,Mn)As, since its magnetic functionality can be manipulated by electrical or optical control of itinerant holes [1, 2]. In this work, the photoinduced magnetization dynamics with no external magnetic field applied has been studied in both as-grown and annealed ferromagnetic (Ga,Mn)As films, by combining time-resolved magneto-optical spectroscopy and ferromagnetic resonance measurement. The competing roles of laser heating and hole-induced non-thermal mechanisms responsible for laser-triggered magnetization dynamics in (Ga,Mn)As have been observed and analyzed. Our results suggest that laser heating-mediated magnetic anisotropy modulation plays major role on the magnetization precession for the as-grown sample at photoexcitation below the band edge of (Ga,Mn)As. Whereas for the regime of above band edge excitation, the non-thermal effect resulting from the photoexcited hole-mediated magnetic anisotropy modulation of the film plays major role [3, 4]. The results provide direct experimental evidence for the possibility of ultrafast nonthermal manipulation of magnetization dynamics in ferromagnetic (Ga,Mn)As by linearly polarized optical pulse excitation with no external magnetic field applied.

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Magnetic and transport properties of n-p co-doped oxide semiconductors

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Dilute magnetic oxides that exhibit ferromagnetism above room temperature have attracted considerable attention due to potential applications in spintronic devices. One of the current challenges is to incorporate transition metal ions into the lattices of oxide semiconductors while maintaining structural uniformity. We find that non-compensate n-p co-doping is a very efficient approach for achieving the substitution of transition metals in oxide lattices. We also find that the magnetization, band gap, and transport properties of the oxide semiconductors can be tuned by controlling n-p pairs. Note that n-p co-doping is also very helpful to tune the properties of topologic insulator and graphene systems.

New Diluted Magnetic Semiconductors with Independent Spin & Charge Doping: from Materials to Properties toward Multiple Heterojunctions

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We here present systematic studies on the recent discovered new type of diluted magnetic semiconductor (DMS) materials with independent spin & charge doping mechanism[1~8]. We will focus on DMS based on BaZn2As2 (refer as BZA) where carries are generated by hetero valence substitution at barium site such as monovalent K to divalent Ba while spin is introduced by isovalent substitution at zinc site such as divalent Mn for Zn. We will discuss materials synthesis, crystal growth, fabrications of binary junction with superconductors related to BZA.

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ARPES on Electronic Structure of Diluted Magnetic Semiconductor (Ba1-xKx)(Zn1-yMny)2As2

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In this talk, I will introduce our recent high resolution ARPES measurements on electronic structure of (Ba1-xKx)(Zn1-yMny)2As2 systems. The implications on the origin of magnetism will be discussed.

Doping dependence of optical and magnetic properties of diluted magnetic semiconductor $(Ba_{1-x}K_x)(Zn_{1-y}Mn_y)_2As_2$

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Diluted magnetic semiconductors have received a lot of attention because of their potential applications for spintronics devices. A lot of efforts have been devoted to raise the Curie temperature of the diluted magnetic semiconductors. $(Ba_{1-x}K_x)(Zn_{1-y}Mn_y)_2As_2$ is a new class of diluted magnetic semiconductor with isostructure to the 122 iron-based superconductors. It has been found that $(Ba_{1-x}K_x)(Zn_{1-y}Mn_y)_2As_2$ can have a curie temperature as high as 230 K. Recently we have succeeded in growing high quality single crystals of $(Ba_{1-x}K_x)(Zn_{1-y}Mn_y)_2As_2$. We have studied the optical and magnetic properties $(Ba_{1-x}K_x)(Zn_{1-y}Mn_y)_2As_2$ with different doping by Fourier transform infrared spectroscopy and magnetic torque at different temperatures and applied magnetic fields. The temperature dependence of the lattice dynamics and evolution of magnetism will be discussed.

High pressure effects on new generation diluted magnetic semiconductors with decoupled charge and spin doping

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We report our recent work on II-II-V type (Ba,K)(Zn,Mn)$_2$As$_2$, a new diluted magnetic semiconductor (DMS) which is doped with charge and spin independently. The Curie temperature (Tc) of (Ba,K)(Zn,Mn)$_2$As$_2$ (230K) is a reliable record of charge mediated ferromagnetism among all the DMS. To reach higher Tc, high pressure is used as a promising technique. With the diamond anvil cell (DAC) to generate high-pressure, high resolution synchrotron spectroscopies (diffraction, emission, absorption and dichroism) are utilized to detect evolution of crystal structure and the electronic states with pressure. We reveal that distortion of [MnAs$_4$] tetrahedra and reduction of interlayer As-As distance induced by pressure are intimately connected to electronic structure, especially the p-d hybridization, which is a key factor to affect ferromagnetism. These results provide valuable information to understand the relationship between fine crystal structure and ferromagnetism in DMS, implying higher Tc can be reached by optimizing crucial features via applying pressure.

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Anomalous Hall effect in Mn-doped topological insulators

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Mn-doping has played a very important role in the study of diluted magnetic semiconductors. However, the physics in the Mn-doped three-dimensional (3D) topological insulators has been highly controversial. For instance, there is no consensus on whether the energy gap observed in the Mn-doped Bi_2Se_3 originates from magnetic interaction. The anomalous Hall effect (AHE) has never been reported in this system despite convincing evidence of a weak ferromagnetic ordering. In this talk, we report the observation of the AHE in $(Bi,Mn)_2Se_3$ thin films and show that the sign of anomalous Hall resistances changes from positive to negative as the Mn concentration is increased. The positive and negative anomalous Hall resistances are found to coexist in the crossover regime. Such a *two-component* AHE and the sign reversal can also be obtained by electrical gating of lightly doped samples. Our results provide an important basis for understanding the puzzling interplay between the surface states, the bulk states and magnetic doping effects in 3D topological insulators.

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Thin films of diluted magnetic semiconductor $Ba_{1-x}K_x(Zn_{1-y}Mn_y)_2As_2$

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We have deposited and studied the properties of Mn-doped ZnAs-based diluted magnetic semiconductor films for the first time. Single-phased, single-oriented thin films of $Ba_{1-x}K_x(Zn_{1-y}Mn_y)_2As_2$ ($x = 0.03, 0.08$; $y = 0.15$) was deposited on Si, $SrTiO_3$, $LaAlO_3$, $(La,Sr)(Al,Ta)O_3$, and $MgAl_2O_4$ substrates, respectively. Utilizing a combined synthesis and characterization system excluding the air and further optimizing the deposition parameters, high-quality thin films could be obtained and be measured. In comparison with films of $x = 0.03$ which possess relatively higher resistivity, weaker magnetic performances, and larger energy gap, thin films of $x = 0.08$ show better electrical and magnetic performances. Strong magnetic anisotropy was found in films of $x = 0.08$ grown on $(La,Sr)(Al,Ta)O_3$ substrate with their magnetic polarization aligned almost solely on the film growth direction.

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The Synthesis, NMR and μSR Investigation of Bulk Form Diluted Ferromagnetic Semiconductors with Decoupled Charge and Spin Doping

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Our collaboration team has successfully synthesized a series of bulk form diluted ferromagnetic semiconductors (DMS) with decoupled charge and spin doping. Among them, the Curie temperature T_C of 122-type bulk form $(Ba,K)(Mn,Zn)_2As_2$ DMS has reached to 230 K [1,2]. More recently, through the doping of Co onto Zn sites in $BaZn_2As_2$, we obtained a n-type DMS with T_C as high as 45 K[3]. The availability of bulk form DMS specimens enables us to measure the bulk magnetism by volume sensitive probe μSR and site-selective probe NMR. μSR measurements confirm that the ferromagnetism is homogenous in these bulk form DMSs, and indicate that the mechanism responsible for ferromagnetic ordering in $(Ba,K)(Mn,Zn)_2As_2$ and other bulk DMSs is the same as that of (Ga,Mn)As [1,2,4,5]. On the other hand, through the measure of NMR, we successfully identified a new ^{7}Li NMR peak induced by Mn doping in $Li(Zn_{1-x}Mn_x)P$ [6] and $Li(Cd_{1-x}Mn_x)P$. We present unequivocal experimental evidences that the ferromagnetic ordering is indeed caused by randomly substituted Mn in Zn sites, instead of Mn cluster or other magnetic impurities. Through the measurement of spin-lattice relaxation rate $1/T_1$, we also established that Mn-Mn ferromagnetic interactions are not limited to the near-neighbor sites but extend over many unit cells, mostly likely due to the p-d Zener interactions.

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Topological Orbitronics in Superstructured Graphene

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Graphene provides an ideal table-top test-ground for relativistic physics due to the Dirac-type linear dispersion of the pi electrons of carbon atoms. In order to make use graphene in electronic devices, however, one needs to open an energy gap in the otherwise Dirac cones, turning the semimetal into semiconductor. Recently, we have proposed to introduce superstructures with C_{6v} crystalline symmetry into graphene and artificial graphenes [1-6]. Particularly, we reveal that triangular and honeycomb nano-hole arrays punctured in graphene yield topologically distinct states, and that in a patchworked graphene topological interface states appear and are protected by an energy gap of ~0.5 eV [7]. The unidirectional propagating states are dominated by the pseudospin, an emergent degree of freedom intimately related to the orbital angular momentum in the superstructured graphene, which can be exploited for orbitronics functionality. Using nano holes with unbalanced numbers of sites in the two sublattices of the underlying honeycomb lattice of graphene, one may generate spinful topological states, which hopefully can be developed for spintronics applications.

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Majorana fermions disappear one-by-one

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In a one-dimensional spin-chain supporting arbitrary pairs of Majorana zero modes, we study the effect of random magnetic fields. We find that by increasing the randomness, Majorana fermions disappear one-by-one which eventually results in a topologically trivial state.Thanks to the bulk-boundary correspondence, a very fast and efficient transfer matrix method captures the topological phase transitions of the model.

Role of the impurity bound states in bioinorganic molecules

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Bioinorganic molecules (BIOM's) consist of a transition-metal atom placed in an organic molecule. Examples include a wide range of molecules such as vitamin B12, hemoglobin, ruthenium-based dye molecules for solar cells, and organic light emitting diodes. By using a multi-orbital Haldane-Anderson model with Hund's coupling, we have performed density functional theory (DFT) and quantum Monte Carlo (QMC) calculations to investigate the electronic structure and correlations of various BIOM's. The DFT+QMC calculations have found that impurity bound states (IBS) exist in the electronic spectrum of the BIOM's. The IBS results from the strong electronic correlations, and plays an important role in determining the electronic and magnetic properties. In the particular case of the human adult hemoglobin (HbA), the DFT+QMC calculations show that the IBS is responsible for the well-known high-spin to low-spin transition upon O2 binding: the IBS is occupied in deoxy-HbA, while unoccupied in oxy-HbA. In fact, within this framework, the high-spin to low-spin transition is direct experimental evidence for the existence of IBS in HbA and that it is involved in the process of O2 binding. These results imply that the IBS is also important in the functioning of various other BIOM's. We suggest that, by modifying the molecular structure around the transition metal site in synthetic BIOM's, it may be possible to control the energy of IBS and, hence, the electronic structure and the functioning. This approach may lead to advances in the design of new BIOM's for the chemical, electronics and pharmaceutical industries.

Epitaxial thin films and artificially engineered superlattices of $BaFe_2As_2$ pnictide

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Since the discovery of superconductivity in iron-based materials significant progress has been made in the fabrication of high quality bulk and thin film materials to explore their intrinsic properties and evaluate novel device applications. Artificial layered pnictide superlattices offer unique opportunity towards tailoring superconducting properties and understanding the mechanisms of superconductivity by creating model structures which do not exist in nature. Recently, we have demonstrated that artificially engineered undoped Ba-122 / Co-doped Ba-122 compositionally modulated superlattices produce *ab*-aligned nanoparticle arrays by layering and self-assembled *c*-axis aligned defects that combine to produce very large J_c and H_{irr} enhancements over a wide angular range. We also report selective atomic-layer control at the heterointerface between epitaxial $BaFe_2As_2$ thin films and $SrTiO_3$ substrates by engineering surface termination of the substrates. Both DFT calculations and scanning transmission electron microscopy imaging show that the BaO layer is the first stable layer of $BaFe_2As_2$ films on TiO_2 terminated $SrTiO_3$ with an atomically sharp interface. In contrast, distorted FeO_2 is favorable on SrO-terminated $SrTiO_3$. These thermodynamic considerations between non-perovskite materials and perovskite oxides can be used to tailor and enhance the functional properties of Fe-based superconducting thin films. Success in interfacial layer control and superlattice fabrication involving pnictides will serve to spur progress in heterostructured systems exhibiting novel interfacial phenomena and device applications.

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Single Crystal Synthesis, High Pressure Research and Spin Polarization Measurements of “BZA” Based Diluted Magnetic Semiconductor

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New Diluted magnetic semiconductors (DMSs) with independent doping of spin and charge have triggered extensive research due to the fantastic physical properties and applications for spintronic devices since the discovery of Li(Zn,Mn)As[1], Li(Zn,Mn)P[2] and $(Ba,K)(Zn,Mn)_2As_2$[3-4] (BZA) bulk polycrystals. Here we report for the first time the growth of BZA single crystal with high pressure research and spin polarization measurements via Andreev reflection junction[5-10].

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Diluted magnetic semiconductors: Role of band gaps

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After the discovery of ferromagnetism in (Ga,Mn)As, diluted magnetic semiconductors (DMS) have received considerable attention owing to potential applications based on the use of both their charge and spin degrees of freedom in electronic devices. The highest Curie temperature of (Ga,Mn)As has been Tc ≈ 200 K. Owing to simultaneous doping of charge and spin induced by Mn substitution, it is difficult to individually optimize charge and spin densities. To overcome these difficulties, recently a new type of DMS $(Ba,K)(Zn,Mn)_2As_2$ was observed in experiments with Tc up to 230K [1]. Motivated by the high Tc, density functional theory calculations [2] and photoemission spectroscopy experiments [3] were conducted to understand the microscopic mechanism of ferromagnetism of p-type DMS $(Ba,K)(Zn,Mn)_2As_2$. In addition, the n-type DMS $Ba(Zn,Mn,Co)_2As_2$ was also reported in the experiment with Tc = 80 K [4]. In Mn-doped $BaZn_2As_2$, why is the ferromagnetic coupling? Why is Tc much lower in the n-type case than that in p-type case? In general, can p- and n-type DMS be realized?

Here, we propose a method to realize DMS with p- and n-type carriers by choosing host semiconductors with a narrow band gap [5, 6]. By employing a combination of the density function theory and quantum Monte Carlo simulation, we demonstrate such semiconductors using Mn-doped $BaZn_2As_2$, which has a band gap of 0.2 eV [5]. In addition, we found a new non-toxic DMS Mn-doped $BaZn_2Sb_2$, of which the Curie temperature Tc is predicted to be higher than that of Mn-doped $BaZn_2As_2$, the Tc of which was up to 230 K in the recent experiment [5]. We also predicted the DMS Cr-doped BaZn2As2 with stable ferromagnetism in p- and n-type carriers [6].

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