# Research Group for Condensed Matter Theory

Group Leader: Michiyasu Mori

Electric power generation and storage are indispensable for our lives. Although the nuclear power plant produces a huge amount of energy, the most part is dissipated away by the heat flow. To enhance its efficiency, the thermoelectric material is one of plausible candidates. We study such functional materials emerging from the electrons internal degrees of freedom (spin, charge and orbital) by combining various numerical methods and quantum field theory. Our results on spin Seebeck effect and giant spin-Hall effect must play a role to develop new thermoelectric material and device.

### Theory of spin Seebeck effect in ferromagnetic insulators

Electric power generation by a temperature gradient (Seebeck effect) is one of important issues in condensed matter physics, since such a thermoelectric device possesses several appealing features necessary for future technologies. However, most of thermoelectric devices adopt conductors, and thereby its low efficiency due to the energy loss by conduction electrons scattering prevents the thermoelectric devices from practical applications.

Using a prototypical magnet ($LaY_2Fe_5O_{12}$), Saitoh and co-workers experimentally established a new principle that spin-current generation by a temperature gradient, so-called spin Seebeck effect, occurs in an insulating magnet even in the absence of conduction electrons [1] (See Fig.1). They established another principle that a spin current flowing in a magnetic insulator can be converted into the electricity [2]. By these two principles, the insulator-based thermoelectric devices can be realized. Electric voltage generation from heat flow in an insulator is a new principle of thermoelectric device, and has never been considered so far.

We investigate a gigantic enhancement of the spin Seebeck effect in a prototypical magnet $LaY_2Fe_5O_{12}$ at low temperatures [3]. Our theoretical analysis sheds light on the important role of phonons; the spin Seebeck effect is enormously enhanced by nonequilibrium phonons that drag the low-lying spin excitations. We further argue that this scenario gives a clue to understand the observation of the spin Seebeck effect that is unaccompanied by a global spin current, and predict that the substrate condition affects the observed signal.

In addition, we formulate a linear response theory of the spin Seebeck effect [4]. Our approach focuses on the collective magnetic excitation of spins, i.e., magnons. We show that the linear-response formulation provides us with a qualitative as well as quantitative understanding of the spin Seebeck effect observed in the magnetic insulator.

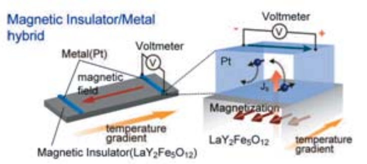


Fig. 1 Spin Seebeck effect in the magnetic insulator ($LaY_2Fe_5O_{12}$).

### Giant spin Hall effect (SHE) of Au films with Pt impurities

The SHE indispensable for the spin-electronics and the spin Seebeck effect is induced by the spin-orbit interaction (SOI). We study the SOI of an Fe impurity in Au host metal by quantum Monte Carlo (QMC) simulation of a realistic multiorbital Anderson impurity model [5]. We show that the SOI is strongly renormalized by the quantum spin fluctuation. Based on this mechanism, we can explain why the gigantic SHE in Au with Fe impurities was observed in recent experiments, while it is not visible in the anomalous Hall effect. In addition, we show that the SOI is strongly renormalized by the Coulomb correlation $U$. Based on this picture, we can explain past discrepancies in the calculated orbital angular momenta for an Fe impurity in an Au host.

In addition, we show theoretically a novel route to obtain giant room temperature SHE using surface-assisted skew scattering [6,7]. By a combined approach of density functional theory and the QMC method, we have studied the SHE due to a Pt impurity in different Au hosts. We show that the spin Hall angle could become larger than 0.1 on the Au (111) surface, and decreases by about a half on the Au (001) surface, while it is small in bulk Au. The QMC results show that the SOI of the Pt impurity on the Au (001) and Au (111) surfaces is enhanced, because the Pt 5d levels are lifted to the Fermi level due to the valence fluctuations. In addition, there are two SOI channels on the Au (111) surface, while only one for Pt either on the Au (001) surface or in bulk Au.

### Enhanced pairing correlations near oxygen dopants in cuprate superconduct

Recent experiments on Bi-based cuprate superconductors have revealed an unexpected enhancement of the pairing correlations near the interstitial oxygen dopant ions. In this study, we propose a possible mechanism -- based on local screening effects -- by which the oxygen dopants do modify the electronic parameters within the $CuO_2$ planes and strongly increase the superexchange coupling $J$ [8]. This enhances the spin pairing effects locally and may explain the observed spatial variations of the density of states and the pairing gap. The effect is of an entirely dynamical nature and thus goes beyond the band structure calculations. Apart from the STM experiments, there is an interesting possibility to test our theory by the resonant inelastic x-ray scattering; it monitors the high-energy spin excitations, and a broad distribution of $J$ values predicted here can be directly observed.

### References

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# Research Group for Molecular Spintronics

Group Leader: Seiji Sakai

Spintronics is an emerging technology taking advantage of the dual freedom of both charge and spin degrees. Since the discovery of the giant magnetoresistance effect in 1988, spintronics has been developed based on inorganic substances like metals and semiconductors. Recent studies have started to shed light on the spintronic application of organic molecules (OMs) and nanocarbons (NCs), in which the spins of conduction electrons can be preserved for a long time and distance. We call this new field “Molecular spintroncis”. In molecular spintronics, the efficient control of the spin transport process (e.g., spin-injection, modulation, detection and accumulation) in OMs and NCs by using magnetic heterostructures is of special importance to realize spintronic applications taking advantages of the potential for spin transport media. Our group aims at establishing the advantages of OMs and NCs as innovative spintronic materials by developing novel systems for spin operations based on the hybrid structures of OMs/NCs and magnetic transition metals and by employing advanced spectroscopic techniques on the electronic and spin structures in such systems.

### Finding of difference in interactions with ferromagnetic metals between single-layer and multilayer graphene

Understanding chemical interactions and electronic structures at the graphene/magnetic metal interfaces is of special importance in designing spin opeartion sources for graphene-based spintronic devices. The influence of the interface formation with ferromagnetic metals on the vibrational properties of graphene was investigated by using confocal micro-Raman spectroscopy [1,2]. Micro-Raman measurements on the micrometer-scale patterned graphene/ferromagnetic metal heterostructures [Fig. 1(a)], which are consisting of patterned regions of the graphenes with various layers number covered with and without metals on the same graphene sheet, enables us to examine the interactions at the graphene/ferromagnetic metal interface as a function of the graphene layers number. From the dependences of the peaks shifts of the Raman bands (e.g., the G band) on the graphene layers number [Fig. 1(b)], it is revealed that the interfacial interactions with ferromagnetic metal are dramatically different between single-layer graphene (SLG) and multilayer graphene (MLG): In the MLG/ferromagnetic metal heterostructures, the Raman bands show a gradual shift in the peak position depdending on the layers number, which are reasonably attributed to electron doping from the ferromagnetic metal to a few graphene layers from the interfaces. Meanwhile, the SLG/ferromagnetic metal heterostructures show a different band-shift feature as in Fig.1, suggesting that there exist strong covalent interactions between SLG and the ferromagnetic metal. The present study would provide important information for improving the performance (e.g., the spin-injection efficiency and interfacial resistance) of graphene-based spintronic devices.

### Elucidation of very high spin polarization at fullerene-transition metal compound/ferromagnetic metal interface

The tunneling magnetoresistance (TMR) effect of granular fullerene-cobalt ($C_{60}$-Co) films [3-5] was studied in the current-perpendicular-to-plane geometry to elucidate the spin-dependent tunneling process bringing about a remarkably high magnetoresistance as compared to the expectations from the conventional theory. The occurrence of cooperative tunneling (so-called cotunneling) through a few to several Co nanoparticles is confirmed from the current-voltage characteristics in the Coulomb blockade regime. Analysis based on the cotunneling model considering the magnitudes of the zero-bias magnetoresistance ratios ($\Delta R/R_{max}$ = 90% at low temperatures) reveals that the spin polarization ($P$) of tunneling electrons generated at the $C_{60}$-Co compound/Co interface is remarkably high ($P$ = 80%) compared to that in Co crystal ($P$ = 37%). The present study suggests that the spin polarization of conduction electrons can be tuned with a proper design of the OM-/NC-transition metal hybrid structures, unlimited by the spin polarization in ferromagnetic metals and also overcoming the problems of interfacial degradation.

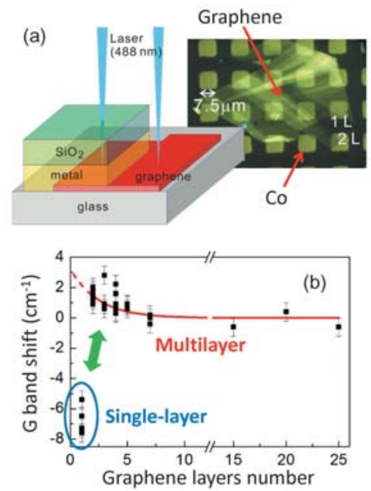


Fig. 1 (a) Schematic drawing and optical image of the micro-patterned graphene/Co sample with the $SiO_2$/Co/graphene/glass layer structure in the bright areas. The graphene sheet contains more than ten regions with various layers numbers (L) (e.g., 1 L, 2 L), as can be seen from the color. (b) Graphene layers number dependence of the G band shift induced by the heterostructure formation with Co.

### References

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