

**Project Title:****Theoretical Modeling of Surface/Interface States in Topological Materials****Name:** OWei Fan**Laboratory at RIKEN:** Computational Condensed Matter Physics Lab

## 1. Introduction

Ruddlesdon-Popper series of iridates have attracted much intense research interests in the past several years due to a subtle interplay between spin, orbital and lattice degree of freedom. As a result, due to strong spin-orbital interaction (SOI), a half filled effective total angular momentum basis ( $J_{\text{eff}}=1/2$  basis) are the key players in low energy physics instead of pure spin basis ( $S=1/2$ ). Many novel physics have been reported including SOI driven metal-insulator transitions (MIT), special magnetic order and possible topological phases under strain engineering. To a natural generalization, iridates based interfaces or superlattices are also interesting due to controllable quantum phase transition may be realized by adjusting interface carrier density. Recently, RIKEN researcher Dr. Matsuno successfully fabricated a  $[(\text{SrIrO}_3)_m, \text{SrTiO}_3]$  superlattice and found MIT when  $m$  is down below 4. In order to understand the physics of this special superlattice, we carried out first principles calculations and tight binding Hamiltonian model analysis.

## 2. Calculation method

In the present study, a  $[(\text{SrIrO}_3)_m, \text{SrTiO}_3]$  superlattice was constructed and first principles calculations were performed to investigate the intriguing metal-insulator transition (MIT) with respect of decreasing  $m$ . Calculations were carried out by Vienna Ab initio Simulation Package (VASP) and Full Potential Linearized Augmented Wave code (ELK). To study the electronic properties of superlattice, local density approximation (LDA) +  $U$  + spin orbit coupling (SOC) calculations of  $\text{SrIrO}_3$  bulk was first carried out to test the validity of results. As  $\text{Ir}^{4+}$  has a  $5d^5$  configuration, the SOC is

large ( $\sim 0.5$  eV) and correlation should be small due to the fact of extended feature of  $5d$  orbitals. We choose  $U$  to be 1eV (We also tested other values later). All the calculations were performed on Massively Parallelized PC and Memory sharing UPC clusters of RICC.

## 3. Result

It was found a semi-metal ground state due to the co-operation of large SOC and correlation ( $U$ ), which is in consistent with literatures. Meanwhile, a Dirac point like line-node protected by crystal symmetry was found in the semi-metal phase. To search for possible topological phases based on this line-node might be one interesting direction for the future research of this project. On the other hand, if  $U$  is increased to a certain amount, a gap can be opened making the bulk a magnetic insulator. By far, all of the bulk calculations were in good agreement with literatures. Then, the superlattice was constructed according to the proposed structure in the recent experimental paper. According to the experiment, the mismatch between lattice constants of  $\text{SrTiO}_3$  and  $\text{SrIrO}_3$  leads to an in-plane rotation of  $\text{IrO}_6$  octahedral from cubic perovskite. This rotation gives rise to a Dzyaloshinski-Moriya (DM) interaction and induced an in-plane weak ferromagnetism when  $m$  is less than 4. The superlattice became a magnetic insulator when  $m < 4$ . It was suggested that correlation  $U$  has been enhanced due to the reduced dimensionality. Indeed, using a larger  $U$ , our first principles calculations realized the magnetic insulator phase, which is in consistent with the reported results. Based on these calculations, the future work may concentrate on evaluation of in-plane strain to DM interaction as well as correlation  $U$ , and model Hamiltonian study will be

carried out based on parameters extracted from first-principles calculations. The results will help to understand the interface physics composed of complex 5d transition metal oxides.

#### 4. Conclusion

From first principles calculations, there are two main conclusions: 1) the MIT is sensitive to SOI and U. The magnetic structure is very sensitive to the distortion of  $\text{IrO}_6$  octahedral; 2) possible topological phase transition may be realized by strain engineering.

#### 5. Future work

Density functional theory based calculations are very efficient on RICC. We will continue working on first principle calculations of topological phase realization of  $\text{SrIrO}_3$  based interface or superlattice. Meanwhile, to investigate the effect of electron correlation, we will also try to perform LDA+DMFT calculations.