GOETHE UNIVERSITÄT
FRANKFURT AM MAIN
Fachbereich Physik
Institut für Theoretische Physik

CONDENSED MATTER THEORY SEMINAR

Subject: **First-principles description of correlated materials with strong spin-orbit coupling: the analytic continuation and branching ratio calculation**

Speaker: **Dr. Jae-Hoon Sim, Department of Physics, KAIST, Daejeon 34141, Republic of Korea**

Date & time: **Friday, February 1st, 2019 at 3.15 p.m.**

Venue: **Seminar room 1.114**

The DFT+DMFT combined with the continuous-time quantum Monte Carlo (CT-QMC) impurity solver is one of the successful approaches to describe correlated electron materials. However, analytic continuation of the QMC data written in the imaginary frequency to the real axis is a difficult numeric problem mainly due to the ill-conditioned kernel matrix. While the maximum entropy method is one of the most suitable choices to gain information from the noisy input data, its applications to the materials with strong spin-orbit coupling are limited by the non-negative condition of the output spectral function. In the first part of this talk, I will discuss the newly developed method for analytic continuation problem, the so-called maximum quantum entropy method (MQEM) [1]. It is the extension of the conventional method, introducing quantum relative entropy as a regularization function. The application of the MQEM for a prototype $j_{\mathrm{eff}} = 1/2$ Mott insulator, Sr_2IrO_4, shows that it provides a reasonable band structure without introducing a material specific basis set. I will also introduce the application of machine learning technique to the same problem [2]. In the second part, a simple technique to calculate the branching ratio from the first-principles calculation will be discussed [3]. The calculated ⟨L·S⟩ and branching ratio of the different 5*d* iridates, namely Sr_2IrO_4, Sr_2MgIrO_6, Sr_2ScIrO_6, and Sr_2TiIrO_6 are in good agreement with recent experimental data. Its reliability and applicability are also carefully examined in the wider material classes.

[1] J.-H. Sim and M. J. Han, Phys. Rev. B 98, 205102 (2018).
[2] H. Yoon, J.-H. Sim, and M. J. Han, Phys. Rev. B 98, 245101 (2018).
[3] J.-H. Sim, H. Yoon, S. H. Park, and M. J. Han, Phys. Rev. B 94, 115149 (2016).