

# 凝縮系物理学ゼミナール

## Condensed Matter Seminar

Date: 13:30-15:00, Wednesday, 26 July 2023

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Title: Electronic structure and superconductivity of electron-doped FeSe intercalates

Speaker: Dr. Makoto Shimizu (Condensed Matter Theory Group)

### Abstract:

The van-der-Waals gap of FeSe-based superconductors can be intercalated with a variety of inorganic and organic compounds that modify the electron doping level of the iron layers. Parts of these electron-doped FeSe-based materials show high- $T_c$  superconductivity. However, the microscopic mechanism has been controversial; whether it is spin fluctuations, nematic fluctuations or combinations of them. Especially in  $\text{Li}_x(\text{C}_3\text{N}_2\text{H}_{10})_{0.37}\text{FeSe}$  where a wide range of doping level,  $0.06 \leq x \leq 0.68$ , is realized.  $T_c$  shows maximum at  $x = 0.37$  ( $T_c = 46$  K), and it shows a dome. We study the electronic structure by performing DFT calculations. We analyze the superconductivity both from itinerant electron and localized moment perspectives. As results, sign-changing s-wave is enhanced by stripe type AFM spin fluctuations, and  $T_c$  grows by the electron doping. In high-doping region, the stripe type AFM fluctuations are destabilized toward bicollinear AFM, which explains why  $T_c$  decreases for  $x > 0.37$ .