# The 246th MANA Special Seminar

## Understanding of Electron Transfer through a Single Molecule

Chair: Dr. Kohei Uosaki (MANA PI)


## Prof. Jianwei Zhao

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In this talk, I will focus on the electron transfer through a Metal-Molecule-Metal junction. After a short literature survey of the modern experimental characterization of single molecule electron transfer, I will present the theoretical studies in this field by using density functional theory (DFT) combined with non-equilibrium Green function (NEGF) method. The electronic structure of the molecule is described by the DFT theory, and electron transport of the molecular system is calculated using the NEGF method. On the basis of the studies of a series of linear and cyclic conjugated molecules, an electron transfer pathway model will be proposed. Inspired by the classical semiconductor theory, we have designed a series of molecular rectifiers. It has been found that the efficient molecular rectification can be achieved by changing the electron transport pathway, such as proton transfer, the decoupling between molecule and electrode, and the asymmetric molecule-electrode connection. The difference between semiconductor diode and molecular diode will be compared as well.


***Venue:*** **Seminar Room #431, 4F, MANA Bldg.,**

***Date:*** **February 3rd, Friday** ***Time:*** **14:30-15:15**

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