High-Throughput Computational Screening for Excellent Organic Light-Emitting Materials, Multiscale Charge Transport Simulation, and DNP-NMR Analysis

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In this talk, three topics will be presented. First topic is high-throughput screening. Historically, enormous effort and time have been exhausted for the development of new materials with better performances than before. High-throughput computational screening is one of the excellent ways to improve the situation. We will show our recently-developed simple high-throughput computational screening method for the development of emitter materials in organic light-emitting diodes. Using the screening method, we have developed highly efficient light-emitting materials and devices.

Secondly, we will show our recent study on multiscale charge transport simulations based on the combination of quantum chemical calculations, molecular dynamics simulations, and kinetic Monte Carlo simulations. Our latest simulation provides excellent agreement with experimentally-obtained hole and electron mobilities without using any adjustable parameters.

Third topic is dynamic nuclear polarization (DNP) enhanced solid-state NMR (DNP-ssNMR). ssNMR is a powerful technique for analyzing the structure and dynamics of materials with atomic resolution. However, most ssNMR studies are based on bulk samples and reports on thin film samples are quite rare due to the lower sensitivity than other analytical methods such as mass spectrometry, infrared spectroscopy, and Raman spectroscopy. To resolve this, various techniques have been developed; applications of high field magnets, cryogenic detection systems, and so on. Among them, DNP-ssNMR has recently attracted considerable attention as an excellent technique. Fortunately, we successfully introduced a brand-new DNP-ssNMR spectrometer in our campus in FY2017. This spectrometer provides theoretically 660 times and experimentally more than 200 times higher NMR signals compared to conventional ones. In this talk, we will introduce this DNP-NMR spectrometer and show some experimental results. Also, we would like to propose joint researches using this DNP-ssNMR.

Our recent publications related to today's topics

[1] H. Kaji, *et al.*, *Nat. Commun.*, **2015**, *6*, 8476.
[2] K. Suzuki, *et al.*, *Angew. Chem. Int. Ed.*, **2015**, *54*, 15231.
[3] T. Miwa, *et al.*, *Sci. Rep.*, **2017**, *7*, 284.
[4] Y. Wada, *et al.*, *Appl. Phys. Lett.*, **2015**, *107*, 183303.
[5] Y. Wada, *et al.*, *Adv. Mater.*, **2018**, *30*, 1705641.
[6] F. Suzuki, *et al.*, *J. Mater. Chem. C*, **2015**, *3*, 5549.
[7] H. Uratani, *et al.*, *Sci. Rep.*, **2016**, *6*, 39128.
[8] F. Suzuki, *et al.*, *Sci. Rep.*, **2018**, *8*, 5203.
[9] S. Kubo and H. Kaji, *Sci. Rep.*, **2018**, *8*, 13462.
[10] K. Suzuki, *et al.*, *Angew. Chem. Int. Ed.*, **2017**, *56*, 14842.