CBC SEMINAR ANNOUNCEMENT

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Chemical Reactivity: From Computational Understanding to New Design

Understanding chemical reactivity is central to chemistry research and the development of novel chemical systems. The continued development of powerful computational methods has advanced the chemical reactivity understanding at the electronic level. By connecting reaction energetics, molecular orbital interactions, and spectroscopy together, computational chemistry can provide invaluable insights into the chemical reactivity. As such, a synergy between computation and experiment has tremendous potential for enabling new developments, which the current chemistry research has witnessed over the recent years. This talk will encompass the use of computational methods for a wide range of catalytic reactions to showcase different aspects of chemical reactivity. In particular, examples from organic electron donor promoted organocatalysis, non-noble metal based CO₂ hydrogenation, and oxo-iron mediated C–H and C=C oxidation reactions will be discussed. The elegant correlation between governing reaction steps, electronic structure, and reactivity will be highlighted. The case of oxo-iron complexes will demonstrate how spectroscopic results from magnetic circular dichroism (MCD), electron paramagnetic resonance (EPR), and Mössbauer spectroscopy correlate with the electronic structure and thereby help to decipher the complex structure-activity relations. Overall, this talk will exhibit high-end applications of advanced computational techniques, mainly based on correlated ab initio methods, to decipher the correlation between electronic structure, reactivity, and spectroscopic properties in chemical systems, which in turn trigger in silico design.

References

Date: 6th August 2018 (Monday)
Time: 2:00pm – 3:00pm
Venue: SPMS Research & Graduate Studies Office Conference Room
Host: Professor Shunsuke Chiba