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Computational studies of catalytic reactions in various platforms: From organic reactions to metal-organic frameworks

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Even though chemistry is divided into many sub-disciplines for practical reasons, the physical principles used in computational chemistry underlie all branches of chemistry. In addition, to make finally developed reactions as well as even research phases greener, today, it is inevitable that computational chemistry is used in various scenes. Hence, computational chemistry has unlimited potential to contribute to the advancement of chemistry in a broad context. With this in mind, we are applying quantum chemistry, multi-scale QM/MM models, and many other advanced computational chemistry techniques to a variety of complex molecular systems such as metalloenzymes, porous materials, transition-metal catalysts, drugs/drug targets, porous coordination polymers/metal-organic frameworks and nanomaterials. In particular, using computational approaches and often with experimental coworkers, we seek to derive key insights into chemical reaction mechanisms and bonding patterns of complex molecules.

Biography

Hajime Hirao has received his BS and MS degrees from Kyoto University and his PhD from the University of Tokyo. He did his Post-doctoral studies at The Hebrew University of Jerusalem, Emory University and Kyoto University. He is currently an Assistant Professor at the Nanyang Technological University, Singapore. He is particularly interested in theoretical aspects of Chemical Reactions. Before starting his Post-doc training, he also worked for three years on Computer Assisted Drug Design at Novartis in Japan. These have made his research interest lie primarily in the application of computational chemistry to chemical reactions in bioinorganic chemistry, homogeneous/heterogeneous catalysis and medicinal chemistry.

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