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Computational tools for studying complex molecular systems

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Quantum mechanics (QM) and molecular mechanics (MM) are two major approaches to study drug-related molecular systems and other complex systems. It is also possible to combine QM and MM or even QM and a different level of QM (QM'). Within these core methodological frameworks, many things can be done to derive insights into a variety of molecular systems. In this presentation, I intend to explain some of our recent attempts.

Biography

Hajime Hirao has received his BEng and MEng degrees from Kyoto University and his PhD from The University of Tokyo. He did his Post-doctorate at The Hebrew University of Jerusalem, Emory University and Kyoto University. Prior to that, he has worked for three years at the Novartis Institute in Japan. Currently, he is an Associate Professor at The City University of Hong Kong, China. Over the years, he has been interested in computational and theoretical aspects of chemistry, especially chemical reactions.

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