Assoc. Prof Hajime Hirao

Department of Biology and Chemistry, City University of Hong Kong, Hong Kong, China

Abstract:

The physical principles used in computational chemistry underlie all branches of chemistry; as such, computational chemistry has unlimited potential to contribute to the advancement of fundamental chemistry in every different subdiscipline as well as to finding solutions to critical challenges that humankind faces today, such as healthcare and energy/environmental issues. With this in mind, our computational exploration of chemistry applies quantum chemistry, multiscale QM/MM and QM/QM approaches, and many other advanced computational chemistry techniques to a broad range of complex molecular systems such as metalloenzymes, transition-metal catalysts, drugs/drug targets, metal-organic frameworks (MOFs), and nanomaterials. In particular, using computational approaches and often with experimental collaborators, we seek to derive information about chemical reaction mechanisms and bonding patterns of these complex molecules. We are also developing efficient computational methods and algorithms, in the hope that our new computational methods will expand the capability of computational chemistry and thereby enable one to simulate the behavior of complex molecular systems with higher reliability and predictability in the future.