武汉物数所理论交叉学术交流系列报告

（第一一八期）

QM and QM/MM Studies of Enzymatic Reactions: Mechanism and Selectivity

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频标楼 4 楼报告厅

报告人简介：廖荣臻 2010 年获瑞典斯德哥尔摩大学博士学位，2011.2-2012.12 在德国马普煤炭研究所从事博士后研究，2013.1-2014.12 在瑞典斯德哥尔摩大学有机化学系从事博士后研究，2014.12 起受聘为华中科技大学化学化工学院教授。主要从事计算催化方法学、酶催化反应机理的理论、人工合成光合系统理论等方向的研究，并取得了卓越的成就。在如 Chem. Rev., PNAS，Angew. Chem. Int. Ed., Chem. Sci., ACS Catal. 等杂志上发表文章 50 余篇。

Abstract: The understanding of the catalytic function of enzymes at an atomistic level is of both fundamental and practical interest. Quantum-chemical calculations have been shown to be a complement and alternative to experimental studies in elucidating the reaction mechanism of enzymes. In this talk, five examples will be presented, namely acetylene hydratase, formaldehyde ferredoxin oxidoreductase, benzoyl-CoA epoxidase, aldoxime dehydratase, and fosfomycin resistance protein A. For these enzymes, the calculations are able to rationalize the reactivity and explain the various selectivities, including chemoselectivity, regioselectivity, stereoselectivity, metal preference (W vs Mo), and oxidation state preference (Fe2+ vs Fe3+).

1. Rong-Zhen Liao, Per E. M. Siegbahn. Chem. Sci. 2015, 6, 2754-2764.
2. Rong-Zhen Liao, Per E. M. Siegbahn. ACS Catal. 2014, 4, 3937-3949.
3. Rong-Zhen Liao, Jian-Guo Yu, Fahmi Himo. Proc. Natl. Acda. Sci. U.S.A. 2010, 107, 22523-22527.