美国北卡罗莱纳大学刘述斌教授学术报告

报告题目： **Density Functional Reactivity Theory: Its Recent Developments and Applications**

地点：中心会议室

主讲人：刘述斌 教授

时间：5月28日（周一）下午15:30-17:00

工作单位：湖 南 师 范 大 学

University of North Carolina at Chapel Hill

主讲人介绍

刘述斌教授1985年毕业于湖南师范大学化学系，获学士学位；1985-1988年在兰州大学化学系学习，获硕士学位；1988-1993年期间在湖南师范大学化学系工作，担任助教和讲师；1994-1996年赴美国北卡罗莱纳大学深造，从师于国际量子化学泰斗Robert G. Parr教授，获博士学位；1996-2000年分别在北卡罗莱纳大学和杜克大学从事博士后研究工作；2000年起任职于北卡罗来纳大学超算中心和太阳能研究中心，并于2004年起担任湖南师大讲座教授。研究方向为理论与计算化学，研究兴趣为密度泛函理论（DFT）与密度泛函活性理论（DFRT）的方法发展以及在材料和生物体系中的应用。发表论文150余篇，h因子30，荣获《国际量子化学杂志》Young Investigator等奖励。现担任《物理化学学报》等杂志编委和70多家国内外专业杂志评审。

报告摘要

Density functional reactivity theory as the chemical application of density functional theory is to appreciate and quantify molecular properties including stability, bonding and reactivity with simple density functionals. Examples of such simple functionals recently investigated in the literature are Shannon entropy, Fisher information, information gain and other quantities from information theory. This talk presents an overview about the theoretical framework of conceptual density functional theory and density functional reactivity theory. More attentions are paid to their applications in quantifying steric effect, electrophilicity, nucleophilicity, regioselectivity, and stereoselectivity. A new understanding about the nature and origin of *ortho/para* and *meta* group directing phenomena in electrophilic aromatic substitution reactions is outlined. Also presented are our recent results in the identification and determination of strong covalent interactions with bind orders equal to or larger than two, and cooperativity properties for weak interactions. A brief outlook of possible future developments is discussed at the end.

欢迎各位参加！

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