凝聚态物理-北京大学论坛

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Classical and quantum computations for electronic structures of molecules

李振东 教授

时间：12月24日（星期四）15:00—16:30
地点：北京大学物理大楼中212大教室

报告人简介（Aboutspeaker）：李振东，2009年于北京大学取得化学学士学位，2014年于北京大学取得物理化学博士学位。2014-2016年于普林斯顿大学进行博士后研究，2016-2018年于加州理工学院进行博士后研究。2019年加入北京师范大学化学学院工作。目前主要研究兴趣为发展高精度电子结构理论、算法与程序。

摘要 (Abstract) : Recent experimental advances in quantum information science have raised a fundamental question for chemistry - whether quantum computation will change the simulation of molecules in a transformative way in the near future. In this talk, I will first review the major classical and quantum algorithms proposed in the past and access their advantages as well as difficulties in solving the electronic structure problem of molecules. Then, I will present our recent works towards delineating the boundary of classical simulations of strongly correlated molecules such as the P-cluster and FeMo-cofactor in nitrogenase using tensor network states (TNS)[1,2,3]. Finally, I will discuss our recent progress in designing efficient quantum algorithms for computing molecular response properties[4].

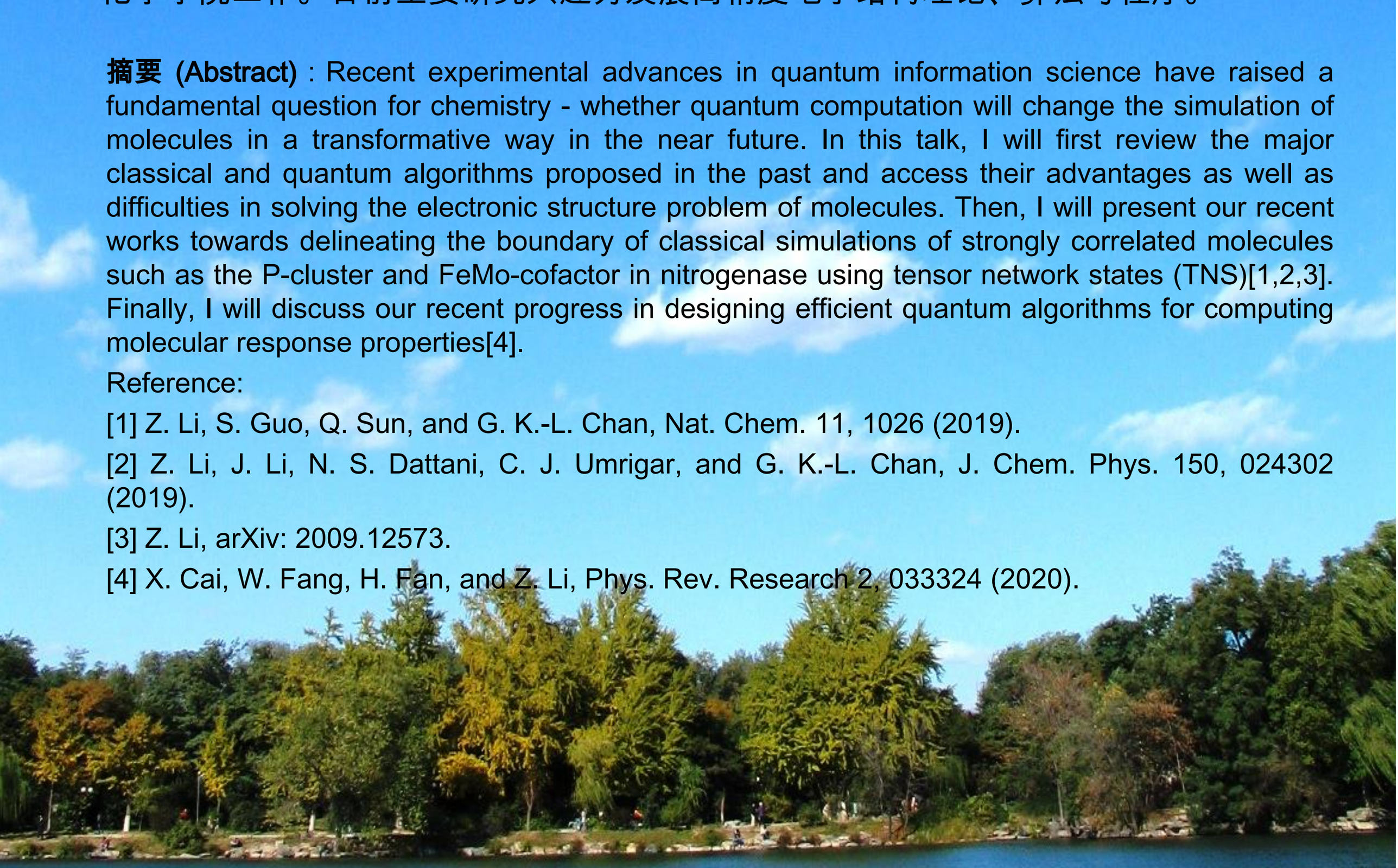
Reference:

[1] Z. Li, S. Guo, Q. Sun, and G. K.-L. Chan, Nat. Chem. 11, 1026 (2019).

[2] Z. Li, J. Li, N. S. Dattani, C. J. Umrigar, and G. K.-L. Chan, J. Chem. Phys. 150, 024302 (2019).

[3] Z. Li, arXiv: 2009.12573.

[4] X. Cai, W. Fang, H. Fan, and Z. Li, Phys. Rev. Research 2, 033324 (2020).



邀请人:陈基 ji.chen@pku.edu.cn

http://www.phy.pku.edu.cn/icmp/xsjl/njtwl__bjdxlt.htm