

## **PKU-UChicago Joint Series: Symposium on Theoretical Chemistry**

**Lecture 4:** When Quantum Computing Meets DFT

### **Speakers:**

David A. Mazziotti, University of Chicago  
Chen Li, Peking University

### **Time:**

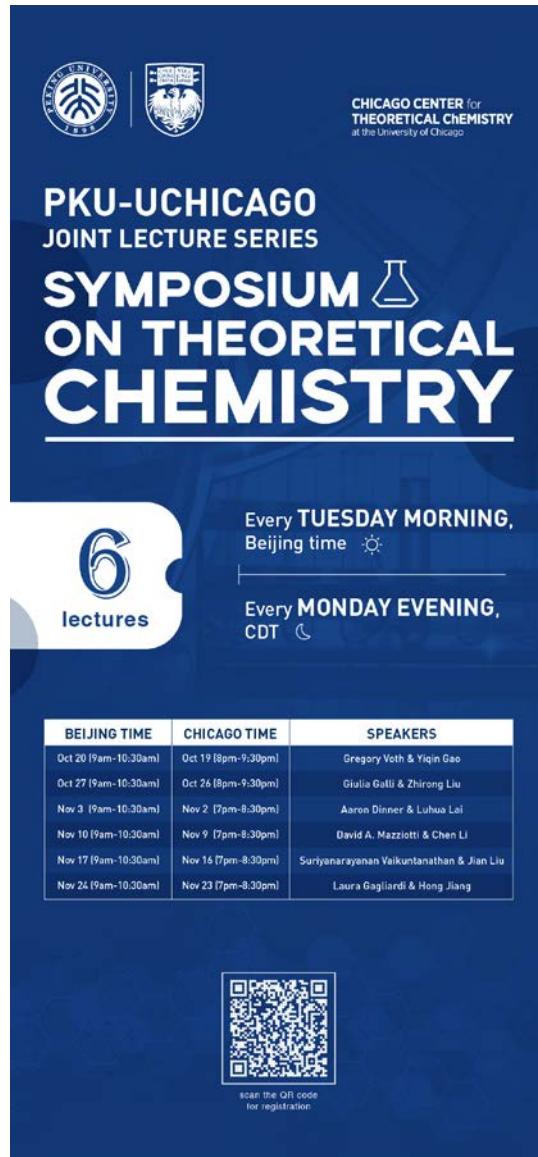
November 9, 7:00 pm (CDT)  
November 10, 9:00 am (Beijing time)

**Series Description:** The Symposium on Theoretical Chemistry will explore the concepts and underlining principles of chemistry through discourse between faculty from the Chicago Center for Theoretical Chemistry at the University of Chicago and Peking University. The series will create an open dialogue about computational theories and methods, and their applications. The symposium will advance conversations in the field of modern theoretical chemistry and include discussions on biophysics, quantum dynamics, electronic structure theory and non-equilibrium statistical mechanics, among others.

Speakers from this joint lecture series are co-chaired by faculty members from Peking University and the University of Chicago. The lectures will be held every Tuesday morning Beijing time and every Monday evening Chicago time. Please scan the QR code or click the link below for registration.

### **Registration Link:**

[https://uchicago.zoom.us/webinar/register/WN\\_eGh5QNeSQKGL-KKFwCF0sA](https://uchicago.zoom.us/webinar/register/WN_eGh5QNeSQKGL-KKFwCF0sA)





**David Mazziotti** is a Professor at the University of Chicago in the Department of Chemistry and the James Franck Institute. He received his Bachelor's degree in Chemistry from Princeton University in 1995 and his Ph.D. in Chemical Physics from Harvard University in 1999. He performed postdoctoral research at Duke University and Princeton University. He has been awarded the David and Lucile Packard Fellowship in Science and Engineering and the Microsoft Newton Award for his development of advanced methods for strongly correlated quantum systems. Professor Mazziotti's research interests include electronic structure and properties of strongly correlated molecules and materials, quantum information, and quantum computing.

**Title:** Exciton Condensate of Photons on a 53-Qubit Quantum Computer

**Abstract:** Quantum computation promises an exponential speedup of certain classes of classical calculations through the preparation and manipulation of entangled quantum states. So far most molecular simulations on quantum computers, however, have been limited to small numbers of particles. Here we prepare a highly entangled state on a 53-qubit IBM quantum computer, representing 53 particles, which reveals the formation of an exciton condensate of photon particles and holes. While elusive for more than 50 years, such condensates were recently achieved for electron-hole pairs in graphene bilayers and metal chalcogenides. Our result with a photon condensate has the potential to further the exploration of this new form of condensate that may play a significant role in realizing efficient room-temperature energy transport.



**Chen Li** is a junior faculty at the College of Chemistry and Molecular Engineering, Peking University. He received his bachelor's degree in chemistry and math from Peking University in 2011. After that, he pursued his PhD study in density functional theory at Duke University under the supervision of Prof. Weitao Yang, and obtained his Ph. D. degree in 2016. In 2017, he joined the Max Planck Institute of Microstructure Physics in Germany as a postdoc research scientist and worked with Prof. Hardy Gross on the topic of time dependent density functional theory beyond Born-Oppenheimer approximation. In 2019, he followed Prof. Gross and moved to the Fritz Haber Center for Molecular Dynamics at Hebrew University of Jerusalem in Israel. In September 2020, He finished his postdoc

and joined the chemistry department of Peking University as an assistant professor. Prof. Li is engaged in developing density functional theory methods, aiming at predicting properties of atoms, molecules and solid state materials, and capturing transition state intermediates in chemical reactions. Moreover, by developing time dependent density functional theory involving both electrons and nuclei and treating them quantum mechanically, he aims at describing nonadiabatic reaction mechanisms, particularly chemical reactions after photo-excitation and catalytic processes.

**Title:** From Self-Interaction Correction to Delocalization-Error Correction, a Paradigm Change in Constructing Density Functional Approximations

**Abstract:** The most commonly used density functional approximations (DFAs) have been known to suffer from diversified problems in various density functional theory calculations. For several decades, the deficiencies of DFAs have been attributed to the self-interaction error. Recently, we revisited these deficiencies and have been able to unify a large class of problems through the perspective of delocalization error. For achieving a universal elimination of delocalization error, we developed a localized orbital scaling correction (LOSC) framework, which accurately characterizes the distributions of global and local fractional electrons, and is thus capable of correcting system energy, energy derivative and electron density in a self-consistent and size-consistent manner. The LOSC-DFAs lead to systematically improved results, including the dissociation of cationic species, the band gaps of molecules and polymer chains, the energy and density changes upon electron addition and removal, and photoemission spectra. Our novel approach leads to a change of the paradigm in constructing density functional approximations.