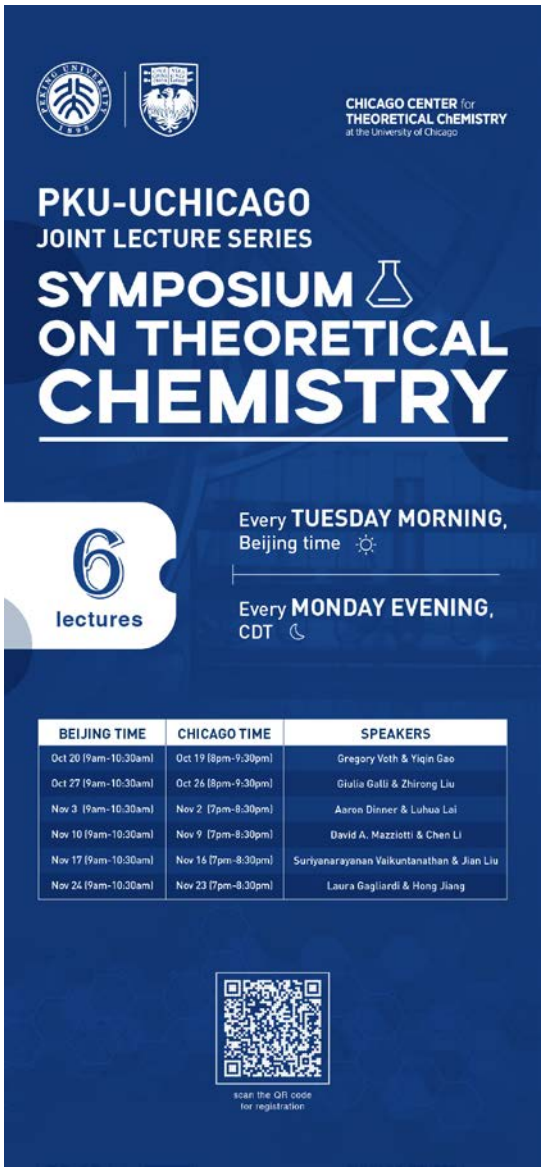
PKU-UChicago Joint Series: Symposium on Theoretical Chemistry

Lecture 6: Strong Correlation and Band Structure

Speakers:
Laura Gagliardi, University of Chicago
Hong Jiang, Peking University

Time:
November 23, 7:00 pm (CDT)
November 24, 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-KKFWcFOsA

Laura Gagliardi is the Richard and Kathy Leventhal Professor of Chemistry and Molecular Engineering at the University of Chicago. She was born and raised in Italy, and she pursued her undergraduate and graduate education there. She earned her Ph.D. in theoretical chemistry at the University of Bologna in 1997. She was then postdoctoral research associate at the University of Cambridge, UK. Gagliardi became an assistant professor at the University of Palermo in 2002. In 2005, she became associate professor at the University of Geneva in Switzerland, and in 2009 she joined the University of Minnesota as a professor of chemistry. She was director of the Nanoporous Materials Genome Center from 2012 to 2014 and has been director of the Inorganometallic Catalyst Design Center since 2014. She was the director of the Chemical Theory Center from 2011 to 2020. She was appointed as Distinguished McKnight University Professor in 2014 and awarded a McKnight Presidential Endowed Chair in 2018. In 2020, she joined the University of Chicago as the Richard and Kathy Leventhal Professor with a joint appointment at the Department of Chemistry, Department of Chemistry, Pritzker School of Molecular Engineering, and the James Franck Institute. She is the director of the Chicago Center for Theoretical Chemistry Gagliardi is a theoretical quantum chemist who is internationally known for her contributions to the development of electronic structure methods and their use for understanding complex chemical systems. Particularly impressive and impactful has been her work in the challenging area of strongly correlated systems that require a so-called multi-reference (MR) treatment, i.e., the total wavefunction must comprise many individual terms. Her long-term goal is to advance these methods so that they can be employed to study energy-relevant chemical systems and materials. Gagliardi has received many recognitions from the chemistry community, including the Peter Debye Award in Physical Chemistry from the American Chemical Society in 2020; the Award in Theoretical Chemistry from the Physical Chemistry Division of the American Chemical Society in 2019, the Humboldt research award in 2018, and the Bourke Award of the Royal Society of Chemistry in 2016. Moreover, she is an Elected Member of the American Academy of Arts and Sciences (2020), the International Academy of Quantum Molecular Science (2019) and Academia Europaea (2018). She also serves as an Associate Editor for the most prestigious journal in the field of theoretical chemistry, the Journal of Chemical Theory and Computation of the American Chemical Society.

Title: Electronic Structure Challenges for Strongly Correlated Systems

Abstract: I will give an overview of the challenges that modern electronic structure theory faces in describing strongly correlated chemical systems from molecules to materials. Our latest progress in combining density matrix renormalization group with pair-density functional theory as a new way to calculate correlation energy [1] will be discussed, together with the recent development of density matrix embedding methods based on multireference solvers for molecules[2], [3] and materials[4]. Applications to compounds containing transition metals and excited states will be presented.

[1] P. Sharma, V. Bernales, S. Knecht, D. G. Truhlar, and L. Gagliardi, Density matrix renormalization group pair-density functional theory (DMRG-PDFT): singlet–triplet gaps in polyacenes and polyacetylenes, Chem. Sci., 10, 2019, pp 1716-1723

[2] M. R. Hermes and L. Gagliardi, Multiconfigurational Self-Consistent Field Theory with Density Matrix Embedding: The Localized Active Space Self-Consistent Field Method, J. Chem. Theory Comput., 15, 2019, pp 972–986

[3] M. R. Hermes, R. Pandharkar, and L. Gagliardi, The Variational Localized Active Space Self-Consistent Field Method, J. Chem. Theory Comput., 16, 2020, 4923-4937

[4] Hung Q. Pham, Matthew R. Hermes, Laura Gagliardi Periodic Electronic Structure Calculations With Density Matrix Embedding Theory J. Chem. Theory Comput., 16, 2020, pp 130-140

Hong Jiang received his bachelor and doctor degrees of science from Peking University, and worked as a post-doctorial research fellow at Duke University (with Prof. Weitao Yang), University of Frankfurt (with Prof. Eberhard Engel), and Fritz-Harber Institute der MPG (with Prof. Matthias Scheffler). In 2009 he joined the faculty of College of Chemistry at Peking University, and has become a tenured associate professor since 2014. He has been working on the development and applications of first-principles electronic structure theory for materials including, in particular, the all-electron GW method based on augmented planewaves and first-principles approaches to strongly correlated systems.

Title: First-principles approaches to electronic band structure of materials

Abstract: Electronic band structure properties of materials play key roles in solar energy conversion related applications, but their first-principles prediction poses a long-standing challenge. The GW method in many-body perturbation theory and the hybrid functional method in density-functional theory (DFT) are among the most accurate first-principles approaches to electronic band structure of insulating materials, but there are still several important open issues in their practical application. In this talk I will first address the challenges of numerically accurate GW calculation based on our recent systematic investigation of the effects of including high-energy local orbitals (HLOs) in the linearized augmented plane waves (LAPW)-based GW calculations for both weakly and strongly correlated materials [1-4]. It is shown that both the accuracy of unoccupied states and the completeness in the summation of states are crucial for numerically accurate GW calculation [2]. Using LAPW+HLOs basis can significantly improve the performances of the semi-local density functional approximation based GW0 approach to weakly correlated semiconductors [2,3]. The consideration of HLOs in the GW based on DFT plus the Hubbard U correction (GW0@DFT+U) approach can significantly improve the description of electronic band structure of strongly correlated d- and f-electron oxides [4]. I will also present our recent work on the development of system-tuned hybrid functional that takes into account both dielectric and metallic screenings, which is found to be able to describe the band gaps of narrow-, medium-, and wide-gap insulating systems with comparably good performances [5].

[1] H. Jiang, R. I. Gomez-Abal, X. Li, et al. Computer Phys. Commun.,184, 348(2013).

[2] H. Jiang and P. Blaha, Phys. Rev. B, 93, 115203(2016).

[3] M.-Y. Zhang and H. Jiang, Phys. Rev. B. 100, 205123(2019)

[4] H. Jiang, Phys. Rev. B, 97, 245132(2018).