Curriculum Vitae (official UNC format)

a) Personal

Name: Yosuke Kanai

b) Education

2006-2009	Postdoctoral Research	University of California at Berkeley
2006	Ph.D. in Theoretical Chemistry	Princeton University
2003	M.A. in Theoretical Chemistry	Princeton University
2001	B.S. (Honors) in Chemistry	University of Tennessee at Knoxville

c) Professional experience

2011- Professor (2022-), Assoc. Professor (2017-2022), Asst. Professor (2011-2017)
Department of Chemistry

Adjunct Professor (2022-)
Department of Physics and Astronomy
University of North Carolina at Chapel Hill

2019- Editorial Advisory Board
Journal of Physical Chemistry Letters (American Chemical Society)

2016- Graduate Faculty (Term member)
Department of Chemistry
Duke University

2011-2014 Visiting Scientist
2009-2011 Lawrence Fellow, Quantum Simulations Group
Condensed Matter and Materials Division
Lawrence Livermore National Laboratory

2006-2009 BNNI Postdoctoral Scholar
(Advisor: Prof. Jeffrey C. Grossman – currently at MIT)
Berkeley Nanosciences and Nanoengineering Institute (BNNI)
University of California at Berkeley

2001-2006 Graduate Student Researcher
(Advisors: Prof. Annabella Selloni / Prof. Roberto Car)
Department of Chemistry
Princeton University

1999-2001 Undergraduate Student Researcher
(Advisor: Prof. Robert J. Hinde)
Department of Chemistry
University of Tennessee at Knoxville

d) Honors

2022 Pariser Global Lectureship for Innovation in Physical Sciences, Sigma Xi Society

2016-2021 INCITE Award, Department of Energy
2016 Outstanding Junior Faculty Award in Computational Chemistry, American Chemical Society
2013 R. J. Reynolds Junior Faculty Development Award, UNC
2012 ACS-PRF Doctoral New Investigator Award
2009-2011 Lawrence Fellow, Lawrence Livermore National Laboratory
2006-2009 BNNI Postdoctoral Scholar, University of California at Berkeley
2001 Science and Engineering First Year Fellowship, Princeton University
2001 Dreyfus Undergraduate Research Award (Senior Award), University of Tennessee at Knoxville
2000 Dreyfus Undergraduate Research Award (Junior Award), University of Tennessee at Knoxville

e) Biography and Products of Scholarship

1. Refereed papers/articles

76. *Molecular Control of Floquet Topological Phase in Non-adiabatic Thouless Pumping*
R. Zhou and Y. Kanai
J. Phys. Chem. Lett., 14, 8205 (2023).

75. *Structure and Electronic Tunability of Acene Alkylamine Based Layered Hybrid Organic-inorganic Perovskites from First Principles*
R. Song, C. Liu, Y. Kanai, D. Mitzi, V. Blum
Phys. Rev. Materials, 7, 084601 (2023).

74. *Spin-Orbit-Coupling-Induced Band Splitting in 2D Hybrid Organic-Inorganic Perovskites: Importance of Organic Cations*
S. Bhattacharya and Y. Kanai
Phys. Rev. Materials*,* 7, 055001 (2023).

73. *Electronic Excitation Response of DNA to High-Energy Proton Radiation in Water*
C. Shepard, D. C. Yost, and Y. Kanai
Phys. Rev. Lett.*,* 130, 118401 (2023).
- Featured with Viewpoint in Physics Magazine and selected as Editor's Suggestion.

72. *Quantum Confinement and Decoherence Effect on Excited Electron Transfer at Semiconductor-Molecule Interface: A First-Principles Dynamics Study*
J. C. Wong, and Y. Kanai
J. Phys. Chem. C*,* 127, 1, 532 (2023).

71. *Electron Dynamics in Extended Systems within Real-time Time-Dependent Density Functional Theory*
A. Kononov, C. Lee, T. Pereira do Santos, B. Robinson, Y. Yao, Y. Yao, X. Andrade, A. D. Baczewski, E. Constantinescu, A. A. Correa, Y. Kanai, N. Modine, A. Schleife
MRS Comm.*,* 12, 1002 (2022).

70. *Nuclear-Electronic Orbital Approach to Quantization of Protons in Periodic Electronic Structure Calculations*
J. Xu, R. Zhou, Z. Tao, C. Malbon, V. Blum, S. Hammes-Schiffer, Y. Kanai
J. Chem. Phys.*,* 156, 224111 (2022).

69. *Nonlinear Electronic Excitation in Water under Proton Irradiation: A First Principles Study*
C. Shepard and Y. Kanai
Phys. Chem. Chem. Phys., 24, 5598 (2022).

68. *All-electron BSE@GW Method for K-edge Core Electron Excitation Energies*
Y. Yao, D. Golze, P. Rinke, V. Blum, Y. Kanai
J. Chem. Theor. Comp., 18, 1569 (2022).

67. *First-Principles Dynamics Study of Excited Hole Relaxation in DNA*
J. C. Wong and Y. Kanai
ChemPhysChem, 23, 92 (2022).

66. *All-electron Real-time and Imaginary-time Time-dependent Density Functional Theory within Numeric Atom-centered Basis Function Framework*
J. Hekele, Y. Yao, Y. Kanai, V. Blum, P. Kratzer,
J. Chem. Phys., 155, 154801 (2021).

65. *Simulating Electronic Excitation and Dynamics with Real-time Propagation Approach to TDDFT within Plane-wave Pseudopotential Formulation*
C. Shepard, R. Zhou, D. C. Yost, Y. Yao, Y. Kanai
J. Chem. Phys., 155, 100901(2021).
- Perspective article (invited). 2021 Editor's Choice.

64. *Nuclear Quantum Effect and Its Temperature Dependence in Liquid Water from Random Phase Approximation via Artificial Neural Network*
Y. Yao and Y. Kanai
J. Phys. Chem. Lett., 12, 6354 (2021).

63. *First-Principles Demonstration of Non-adiabatic Thouless Pumping of Electrons in a Molecular System*
R. Zhou, D. C. Yost, Y. Kanai
J. Phys. Chem. Lett., 12, 4496 (2021).

62. *Dynamical Transition Orbitals: A Particle-Hole Description in Real-time TDDFT Dynamics*
R. Zhou and Y. Kanai
J. Chem. Phys., 154, 054107 (2021).

61. *Enabling Aqueous NiO Photocathodes by Passivating Surface Sites that Facilitate Proton-Coupled Charge Transfer*
A. Taggart, J. Evans, L. Li, K. Lee, J. Dempsey, Y. Kanai, J. Cahoon
ACS Applied Energy Material, 3, 10702 (2020).

60. *Temperature Dependence of Nuclear Quantum Effects on Liquid Water via Artificial Neural Network Model Based on SCAN meta-GGA Functional*
Y. Yao and Y. Kanai
J. Chem. Phys., 153, 044114 (2020).

59. *First-Principles Modeling of Electronic Stopping in Complex Matter under Ion Irradiation*

D. C. Yost, Y. Yao, Y. Kanai
J. Phys. Chem. Lett., 11, 229 (2020).
- Perspective article (invited)

58. *All-electron Ab Initio Bethe-Salpeter Equation Approach to Neutral Excitations in Molecules with Numeric Atom-Centered Orbitals*
C. Liu, J. Kloppenburg, Y. Yao, X. Ren, H. Appel, Y. Kanai, V. Blum
J. Chem. Phys. 152, 044105 (2020).

57. *Excitation Energy-Dependent Photocurrent Switching in a Single-Molecule Photodiode*
B. Shan, A. Nayak, O. F. Williams, D. C. Yost, N. F. Polizzi, Y. Liu, N. Zhou, Y. Kanai, A. Moran, M. J. Therien, T. J. Meyer
Proc. Natl. Acad. Sci., 116, 16198 (2019).

56. *K-shell Core Electronic Excitation in Electronic Stopping of Protons in Water from First Principles*
Y. Yao, D. C. Yost, Y. Kanai
Phys. Rev. Lett., 123, 066401 (2019).

55. *Propagation of Maximally Localized Wannier Functions in Real-Time TDDFT*
D. C. Yost, Y. Yao, Y. Kanai
J. Chem. Phys., 150, 194113 (2019); Erratum, J. Chem. Phys., 151, 139901 (2019).

54. *Electronic Excitation Dynamics in DNA under Proton and α-particles Irradiation*
D. C. Yost and Y. Kanai
J. Am. Chem. Soc., 141, 5241 (2019).

53. *Modeling Electron Injection at Semiconductor-Molecule Interfaces using First-Principles Dynamics Simulation: Effects of Nonadiabatic Coupling, Self-Energy, and Surface Models*
L. Li and Y. Kanai
J. Phys. Chem. C, 123, 13295 (2019).

52. *Size Dependence and Role of Decoherence in Hot Electron Relaxation within Fluorinated Silicon Quantum Dots: A First-Principles Study*
J. C. Wong, L. Li, Y. Kanai
J. Phys. Chem. C, 122, 29526 (2018).

51. *Tunable Semiconductors: Control over Carrier States and Excitations in Layered Hybrid Organic-Inorganic Perovskites*
C. Li, W. Huhn, K. Du, A. Vazquez-Mayagoitia, D. Dirkes, W. You, Y. Kanai, D. B. Mitzi, V. Blum
Phys. Rev. Lett., 121, 146401 (2018).

50. *Modeling Plasmon-Induced Hot-Carrier Transfer*
L. Li and Y. Kanai
Chem, 4, 937 (2018).
- Invited commentary.

49. *Dependence of Hot Electron Transfer on Surface Coverage and Adsorbate Species at Semiconductor-Molecule Interfaces*

L. Li and Y. Kanai
Phys. Chem. Chem. Phys. 20, 12986 (2018).

48. *Free Energy Profile of NaCl in Water: First-Principles Molecular Dynamics with SCAN and ωB97X-V Exchange-Correlation Functionals*
Y. Yao and Y. Kanai
J. Chem. Theor. Comp., 14, 884 (2018).

47. *Examining Real-time TDDFT Non-equilibrium Simulation for the Calculation of Electronic Stopping Power*
D. Yost, Y. Yao, Y. Kanai
Phys. Rev. B, 96, 115134 (2017).

46. *Plane-wave Pseudopotential Implementation and Performance of SCAN meta-GGA Exchange-Correlation Functional for Extended Systems*
Y. Yao and Y. Kanai
J. Chem. Phys., 146, 224105 (2017).

45. *Examining the Effect of Exchange-Correlation Approximations in First-Principles Dynamics Simulation of Interfacial Charge Transfer*
L. Li, J. C. Wong, Y. Kanai
J. Chem. Theor. Comp., 13, 2634 (2017).

44. *Electronic Excitation Dynamics in Liquid Water under Proton Irradiation*
K. G. Reeves and Y. Kanai
Sci. Rep., 7, 40379 (2017).

43. *Diffusion Quantum Monte Carlo Study of Martensitic Phase Transition Energetics: The Case of Phosphorene*
K. G. Reeves*, Y. Yao*, Y. Kanai *Equal contributions
Chem. Phys., 145, 124705 (2016)

42. *Electronic Stopping for Protons and α-particles from First Principles Electron Dynamics: The case of silicon carbide*
D. C. Yost and Y. Kanai
Phys. Rev. B, 94, 115107 (2016).

41. *Passivation of Nickel Vacancy Defects in Nickel Oxide Solar Cells by Targeted Atomic Deposition of Boron*
C. Flynn, S. McCullough, L. Li, C. Donley, Y. Kanai, J. Cahoon
J. Phys. Chem. C, 120, 16568 (2016).

40. *Electronic Stopping Power in Liquid Water for Protons and α-particles from First Principles*
K. G. Reeves, Y. Yao, Y. Kanai
Phys. Rev. B (*Rapid Comm.*), 94, 041108(R) (2016).

39. *Excited Electron Dynamics at Semiconductor-Molecule Type-II Heterojunction Interface: First-Principles Dynamics Simulation*

L. Li and Y. Kanai
J. Phys. Chem. Lett., 7, 1495 (2016).

38. *Site-Selective Passivation of Defects in NiO Solar Photocathodes by Targeted Atomic Deposition*
F. J. Cory, S. M. McCullough, E. Oh, L. Li, C. C. Mercado, B. H. Farnum, W. Li, C. L. Donley, W. You, A. J. Nozik, J. R. McBride, T. J. Meyer, Y. Kanai, J. F. Cahoon
ACS Applied Materials and Interfaces, 8, 4754 (2016).

37. *Communication: Modeling of Concentration Dependent Water Diffusivity in Ionic Solutions: Role of Intermolecular Charge Transfer*
Y. Yao, M. L. Berkowitz, Y. Kanai
J. Chem. Phys., 143, 241101 (2015).

36. *Role of Surface Termination on Hot Electron Relaxation in Silicon Quantum Dots: A First Principles Dynamics Simulation Study*
K. Reeves, A. Schleife, A. A. Correa, Y. Kanai
Nano Lett., 15, 6429 (2015).

35. *Antiferromagnetic Structures and Electronic Energy Levels at Reconstructed NiO(111) Surfaces: A DFT+U Study*
L. Li and Y. Kanai
Phys. Rev. B, 91, 235304 (2015).

34. *Accurate Atomistic First-Principles Calculations of Electronic Stopping*
A. Schleife, Y. Kanai, A. A. Correa
Phys. Rev. B, 91, 014306 (2015).

33. *Reptation Quantum Monte Carlo Calculation of Charge Transfer: The Na-Cl Dimer*
Y. Yao and Y. Kanai
Chem. Phys. Lett., 618, 236 (2015).
- *Frontiers Article* (invited) and featured on the cover.

32. *Electronic and Optical Properties of Polypyridylruthenium Derivatized Polystyrenes:Multi-level Computational Analysis of Metallo-Polymeric Chromophore Assemblies*
Z. Watson, S. Keinan, Y. Kanai
Phys. Chem. Chem. Phys., 17, 1776 (2015).

31. *Quantum Dynamics Simulation of Electrons in Materials on High-Performance Computers*
A. Schleife, E. W. Draeger, V. Anisimov, A. A. Correa, Y. Kanai
Computing in Science and Engineering, 16, 54 (2014).
- Perspective article (invited) for Advances in Leadership Computing issue.

30. *Importance of Excitonic Effect in Charge Separation at Quantum-Dot/Organic Interface: First-Principles Many-Body Calculations*
D. Lee, J. L. Dubois, Y. Kanai
Nano Lett., 14, 6884 (2014).

29. *Scaling and Spatial Analysis of Dielectric Response in Cadmium Selenide Nanowires*

Y. Kanai and G. Cicero
Phys. Rev. B, 90, 165417 (2014).

28. *Exploring the Potential of Fulvalene Dimetals as Platforms for Molecular Solar Thermal Energy Storage: Computations, Syntheses, Structures, Kinetics, and Catalysis*
K. Borjesson, D. Coso, V. Gray, J. C. Grossman, J. Guan, C. B. Harris, N. Hertkorn, Z. Hou, Y. Kanai, D. Lee, J. P. Lomont, A. Majumdar, S. K. Meier, S. C. Nguyen, R. A. Segalman, V. Srinivasan, W. B. Tolman, N. Vinokurov, K. P. C. Vollhardt, T. W. Weidman
Chemistry: A European Journal, 20, 1 (2014).

27. *Role of Charge Transfer in Water Diffusivity in Aqueous Ionic Solutions*
Y. Yao, Y. Kanai, M. Berkowitz
J. Phys. Chem. Lett., 5, 2711 (2014).

26. *Theoretical Oxidation State Analysis of Ru-(Bpy)$_3$: Influence of Water Solvation and Hubbard Correction in First Principles Calculations*
K. G. Reeves and Y. Kanai
J. Chem. Phys., 141, 024305 (2014).

25. *Modeling Time-Coincident Ultrafast Electron Transfer and Solvation Processes at Molecule-Semiconductor Interfaces*
L. Li*, P. Giokas*, Y. Kanai, A. Moran *Equal contributions
J. Chem. Phys., 140, 234109 (2014).

24. *Dependence of Water Dynamics on Molecular Adsorbates near Hydrophobic Surface: A First Principles Molecular Dynamics Study*
D. Lee, E. Schwegler, Y. Kanai
J. Phys. Chem. C, 118, 8508 (2014).

23. *Atom Transfer Radical Polymerization Preparation and Photophysical Properties of Polypyridylruthenium Derivatized Polystyrenes*
Z. Fang, A. Ito, S. Keinan, Z. Chen, Z. Watson, J. Rochette, Y. Kanai, D. Taylor, K. S. Schanze, T. J. Meyer
Inorg. Chem., 52, 8511 (2013).

22. *Role of Four-Fold Coordinated Titanium and Quantum Confinement in CO_2 Reduction at Titania Surface*
D. Lee and Y. Kanai
J. Am. Chem. Soc. (*Comm.*), 134, 20266 (2012).

21. *Plane-wave Pseudopotential Implementation of Explicit Integrators for Time-Dependent Kohn-Sham Equations in Large Scale Simulations*
A. Schleife, E. W. Draeger, Y. Kanai, A. A. Correa
J. Chem. Phys., 137, 22A546 (2012).
- Invited submission for special topic issue on Non-adiabatic Dynamics.

20. *Biomimetic Carbon Nanotubes for Catalytic CO_2 Hydrolysis: First Principles Investigation on Role of Oxidation State and Metal Substitution in Porphyrin*

D. Lee and Y. Kanai
J. Phys. Chem. Lett., 3, 1369 (2012).

19. *X-ray Transient Absorption and Picosecond IR Spectroscopy of (Fulvalene)tetracarbonyl-diruthenim on Photoexcitaion*
M. R. Harpham, S. C. Nguyen, Z. Hou, J. C. Grossman, C. B. Harris, M. W. Mara, A. B. Stickrath, Y. Kanai, A. M. Kolpak, D. Lee, D. Liu, J. P. Lomont, K. Moth-Poulsen, N. Vinokuro, L. X. Chen, K. P. C. Vollhardt
Angew. Chem. Int. Ed., 51, 7692 (2012).

18. *Cooperative Chiral Adsorption of Styrene Molecules on the Si(001)-c(2x4) Surface: First Principles Investigation of Reaction Mechanisms*
N. Takeuchi and Y. Kanai
J. Phys. Chem. C, 115, 14213 (2011).

17. *Single-Molecule-Resolved Structural Changes Induced by Temperature and Light in Surface-Bound Organometallic Molecules Designed for Energy Storage*
J. Cho, L. Berbil-Bautista, I. Pechenezhskiy, N. Levy, S. K. Meier, V. Srinivasan, Y. Kanai, J. C. Grossman, K. P. C. Vollhardt, M. F. Crommie
ACS Nano, 5, 3701 (2011).

16. Mechanism of Thermal Reversal of the (Fulvalene)tetracarbonyldiruthenium Photoisomerization :Toward Molecular Solar-Thermal Energy Storage
Y. Kanai, V. Srinivasan S. K. Meier, K. P. C. Vollhardt, J. C. Grossman
Angew. Chem. Int. Ed., 49, 8926 (2010).

15. *Theory and Simulation of Nanostructured Materials for Photovoltaic Applications*
Y. Kanai, J. B. Neaton, J. C. Grossman
Computing in Science and Engineering (*Computational Nanoscience and Nanotechnology* Issue), 12, 18 (2010).

14. *Toward Accurate Reaction Energetics for Molecular Line Growth at Surface: Quantum Monte Carlo and Density Functional Theory Calculations*
Y. Kanai and N. Takeuchi
J. Chem. Phys., 131, 214708 (2009).

Prior to Independent Career: Graduate and Post-doctoral Work (Princeton and UC Berkeley)

13. *Surface Radical Chain Reaction Revisited: Comparative Investigation of Styrene and 2,4-dimethyl-styrene on hydrogenated Si(001) surface from Density Functional Theory Calculations*
N. T. Takeuchi, Y. Kanai, A. Selloni
J. Phys. Chem. C, 114, 3981 (2010).

12. *Charge Separation in Nano-scale Photovoltaic Materials: Recent Insights from First Principles Electronic Structure Theory*
Y. Kanai, Z. Wu, J. C. Grossman,

J. Mater. Chem., 20, 1053 (2010).

11. *Atomistic Oxidation Mechanism of a Carbon Nanotube in Nitric Acid*
Y. Kanai, V. R. Khalap, P. G. Collins, J. C. Grossman
Phys. Rev. Lett. 104, 066401 (2010).

10. *Role of Exchange in Density Functional Theory for Weakly–Interacting Systems: Quantum Monte Carlo analysis of Electron Density and Interaction Energy*
Y. Kanai and J. C. Grossman
Phys. Rev. A 80, 032504 (2009).

9. *Quantum Monte Carlo Calculations of Energy-Level Alignments at Hybrid Interface: Role of Many-Body Effects*
Z. Wu, Y. Kanai, J. C. Grossman
Phys. Rev. B (*Rapid Comm.*) 79, 201309R (2009).

8. *Role of Semiconducting and Metallic Tubes in P3HT/Carbon Nanotube Photovoltaic Heterojunctions: Density Functional Theory Calculations*
Y. Kanai and J. C. Grossman
Nano Lett. 8, 908 (2008).

7. *Insights on Interfacial Charge Transfer across P3HT/Fullerene Photovoltaic Heterojunction from Ab Initio Calculations*
Y. Kanai and J. C. Grossman
Nano Lett. 7, 1967 (2007).

6. *Testing the TPSS meta-GGA Exchange Correlation Functional in Calculations of Transition States and Reaction Barriers*
Y. Kanai, X. Wang, A. Selloni, R. Car
J. Chem. Phys. 125, 234104 (2006).

5. *Competing Mechanisms in the Optically Activated Functionalization of the Hydrogen Terminated Si(111) Surface*
Y. Kanai and A. Selloni
J. Am. Chem. Soc. (*Comm.*) 128, 3892 (2006).

4. *A Theoretical Study of Biotin Chemisorption on Si-SiC(001) Surfaces*
Y. Kanai, G. Cicero, A. Selloni, R. Car, G. Galli
J. Phys. Chem. B, 109, 13656 (2005).

3. *Role of Molecular Conjugation in Surface Radical Reaction of Aldehydes with H-Si(111): First Principles Study*
Y. Kanai, N. Takeuchi, R. Car, A. Selloni
J. Phys. Chem. B, 109, 18889 (2005).

2. *Surface Reaction of Alkynes and Alkenes with H-Si(111): A Density Functional Theory Study*
N. Takeuchi, Y. Kanai, A. Selloni
J. Am. Chem. Soc. 126, 15890 (2004).

1. *First Principles String Molecular Dynamics: Efficient Approach for Finding Chemical Reaction Pathways*
Y. Kanai, A. Tilocca, A. Selloni, R. Car
J. Chem. Phys. 121, 3359 (2004)

2. Invited Seminars and Presentations

72. FHI-aims Developers' and Users' Meeting, Hamburg, Germany, 8/2/2023
71. Theoretical Chemistry Seminar, UC Irvine, CA, USA, 7/13/2023
70. TDDFT Workshop, Rutgers Newark, NJ, USA, 7/6/2023
69. American Physical Society National Meeting, Las Vegas, NV, USA, 3/7/2023
68. Department of Physics and Astronomy Colloquium, UNC, NC, USA, 1/30/2023
67. Physical Chemistry Seminar, Univ. Wisconsin at Madison, WI, USA, 10/4/2022
66. International Conference on Recent Progress in Many-Body Theories XXI, NC, USA, 9/15/2022
65. American Chemical Society National Meeting, Chicago, IL, USA, 8/22/2022
64. Zasshikai Seminar, Department of Chemistry, The University of Tokyo, Japan, 7/21/2022
63. Southeast Theoretical Chemistry Association Annual Meeting, Atlanta, GA, USA 5/20/2022
62. Pariser Global Lectureship for Innovation in Physical Sciences, Sigma Xi Society, 4/19/2022
61. CECAM Workshop: Real-time quantum dynamics in photo-stimulated processes: experiment and theory, Beijing, China, postponed.
60. Triangle Molecular Simulation Society Workshop, Durham, NC, USA, 4/16/2022
59. NC Photochemistry 2021, NC, USA 10/23/2021
58. CECAM Workshop: Non-homogeneous matter under ionizing radiations, Paris, postponed
57. Triangle Hard Matter Workshop, Online, 12/7/2020
56. Materials and Chemical Science and Technology Seminar, National Renewable Research Laboratory, Golden, CO, USA, 3/6/2020
55. American Chemical Society National Meeting, San Diego, CA, USA, 8/26/2019
54. Theoretical Chemistry Seminar, Kyoto University, Japan, 5/23/2019
53. Applied Physics seminar, Osaka University, Japan, 5/22/2019
52. American Chemical Society National Meeting, Orlando, FL, USA, 3/31/2019
51. Theory/Computation Seminar (Chem/Phys/Chem-Eng.), Univ. Tennessee, USA, 2/22/2019
50. Materials Theory Seminar, Oak Ridge National Laboratory, TN, USA, 2/21/2019
49. Int'l Symposium on Ab Initio Electron Dynamics Simulation, Tsukuba, Japan, 11/16/2018
48. International Materials Research Congress, Cancun, Mexico, 8/19/2018
47. Dept. of Applied Physics Seminar, Politechnico Di Torino, Turin, Italy, 07/03/2018
46. Atomistic Simulation Theory Seminar, International Center for Theoretical Physics, Trieste, Italy, 6/27/2018
45. Condensed Matter Seminar, Int'l. School for Advanced Studies (SISSA), Trieste, Italy, 6/20/2018
44. Joint 2018 Annual Workshop on Recent Developments in Electronic Structure Methods (ES2018) and 2018 Penn Conference in Theoretical Chemistry (PCTC2018), U. Penn., PA, USA, 6/12/2018
43. Excited State Processes in Electronic and Bio Nanomaterials Conference (ESP 2018), Santa Fe, NM, USA, 6/5/2018
42. NSF Software Infrastructure for Sustained Innovation Program PI Meeting, Washington DC, USA, 4/30/2018
41. Chemistry-Physics Joint Department Colloquium, Wake Forest University, NC, USA, 1/24/2018

40. CPMD 2017 Workshop, Tsukuba, Japan, 10/19/2017
39. CECAM Workshop: Charge carrier dynamics in nanostructures: optoelectronic and photo-stimulated processes, Bremen, Germany, 10/10/2017
38. Physics Department Colloquium, University of North Carolina at Chapel Hill, NC, USA, 8/28/2017
37. Telluride Workshop: Excited States, CO, USA, 7/17/2017
36. American Chemical Society National Meeting, San Francisco, CA, USA, 4/02/2017
35. Southeastern Regional Meeting of American Chemical Society, Columbia, SC, USA, 10/23/2016
34. NC Photochem 2016 Symposium, North Carolina State Univ., NC, USA, 10/1/2016
33. Theoretical/Physical Chemistry Seminar, Northwestern University, IL, USA, 10/10/2016
32. NSF KI-Net Conference: Mathematical and Computational Methods in Quantum Chemistry, Yale Univ., USA, 5/13/2016
31. Physics Department Seminar, Temple University, PA, USA, 4/27/2016
30. Physical Chemistry Seminar, Massachusetts Institute of Technology, MA, USA, 4/12/2016
29. American Physical Society National Meeting, Baltimore, MD, USA, 3/15/2016
28. Chemical Physics Seminar, California Institute of Technology, CA, USA, 10/20/2015
27. Physical/Theoretical Chemistry Seminar, University of Southern California, CA, USA, 10/19/2015
26. Physical Chemistry Seminar, University of Washington, Seattle, WA, USA, 9/30/2015
25. SPIE Meeting: Photonics and Optics, CA, USA, 8/12/2015
24. Computational Chemistry and Material Science Summer Institute – Lawrence Livermore National Lab., CA, USA, 7/20-21/2015
23. Excited States and Dynamics Workshop, Telluride, USA, 7/13/2015
22. Center of Research Excellence in Complex Materials Seminar, Michigan State Univ., USA, 4/2/2015
21. Condensed Matter Theory Seminar (Physics/Chemistry/MSE), Univ. of Michigan, USA, 3/30/2015
20. Theory Facility Seminar – Molecular Foundry, Lawrence Berkeley Lab, CA, USA, 12/12/2014
19. Department of Chemistry Seminar, Duke University, NC, USA, 11/20/2014
18. Department of Applied Physics Seminar, University of Tokyo, Japan, 7/29/2014
17. International Materials Research Congress, Cancun, Mexico, 8/12/2013
16. Southeast Theoretical Chemistry Association Annual Meeting, Auburn, AL, USA, 5/10/2013
15. Chemistry Department Seminar, North Carolina State University, NC, USA, 9/28/2012
14. Solar Fuels, Science, Engineering, and Policy, Duke University, NC, USA, 1/11/2012
13. Chemistry and Physics of Nano-crystalline Surface Workshop, Berkeley, CA, USA, 10/6/2011
12. American Chemical Society National Meeting, CO, USA, 8/29/2011
11. Condensed Matter Physics Seminar, SISSA (International School of Advanced Studies), Trieste, Italy, 7/27/2010
10. DARPA Microsystems Technology Office PI review meeting, San Francisco, CA, USA, 7/22/2010
9. Materials Science and Engineering Department Colloquium, U.C. Berkeley, CA, USA, 10/22/2009
8. Frontiers of Advanced Materials Seminar, Central Michigan University, 4/10/2009
7. American Chemical Society National Meeting, UT, USA, 3/26/2009
6. American Physical Society National Meeting, PA, USA, 3/17/2009
5. International Conference on Surfaces, Materials, and Vacuum, Veracruz, Mexico, 9/29/2008
4. Materials Research Society National Meeting, CA, USA, 3/27/2008
3. CCMC Colloquium, Universidad Nacional Autonoma de Mexico, Ensenada, Mexico, 11/23/2007
2. Physics Department Seminar, Politecnico Di Torino, Turin, Italy, 6/27/2007
1. Roberto Car 60th Birthday Symposium, Trieste, Italy, 6/22/2007

f) Teaching activities

1. Course Assignments

(21) Spring 2023, Chem 482L "Physical Chemistry Lab: Computational" (24 students)
(20) Fall 2022, Chem 486 "Introduction to Quantum Chemistry" (18 students)

(19) Spring 2022, Chem 482L "Physical Chemistry Lab: Computational" (35 students)
(18) Fall 2021, Chem 486 "Introduction to Quantum Chemistry" (9 students)
(17) Spring 2021, Chem 481 "Physical Chemistry I: Thermodynamics" (27 students)
(16) Spring 2020, Chem 482L "Physical Chemistry Lab: Computational" (30 students)
(15) Fall 2019, Chem 488 "Quantum Chemistry (Advanced)" (7 students)
(14) Spring 2019, Chem 481L, "Physical Chemistry Lab: Computational" (43 students)
(13) Fall 2018, Chem 481 "Physical Chemistry I: Thermodynamics" (50 students)
(12) Spring 2018, Chem 481 "Physical Chemistry I: Thermodynamics" (35 students)
(11) Fall 2017, Chem 486 "Introduction to Quantum Chemistry" (6 students)
(10) Spring 2017, Chem 481L "Physical Chemistry Lab: Computational" (41 students)
(9) Fall 2016, Chem 783 "Special Topics in Physical Chemistry" (7 students)
(8) Fall 2015, Chem 481L "Physical Chemistry Lab: Computational" (40 students)
(7) Spring 2015, Chem 481L "Physical Chemistry Lab: Computational" (26 students)
(6) Fall 2014, Chem 486 "Introduction to Quantum Chemistry" (6 students)
(5) Spring 2014, Chem 481 "Physical Chemistry I: Thermodynamics" (26 students)
(4) Fall 2013, Chem 486 "Introduction to Quantum Chemistry" (7 students)
(3) Spring 2013, Chem 481 "Physical Chemistry I: Thermodynamics" (24 students)
(2) Fall 2012, Chem 486 "Introduction to Quantum Chemistry" (11 students)
(1) Fall 2011, Chem 486 "Introduction to Quantum Chemistry" (9 students)

3. Research Group

I. Current Members

Dr. Jianhang Xu	Post-doctoral Researcher	PhD: Temple Univ. / BS: USTC (China)
Chris Shepard	PhD Student	BS: University of Richmond
Sampreeti Bhattachrya	PhD Student	BS: Indian Institute of Technology at Kanpur
Ruiyi Zhou	PhD Student	BS: Univ. of Hong Kong
John Bost	PhD Student	BS: Davidson College
Thomas Carney	PhD Student	BS: NCSU
Nicholas Boyer	Undergraduate Student	UNC Class of 2025

II. Former Members

Ruyi Song	Visiting PhD Student (2019-2023)	BS: Peking University, PhD : Duke University Subsequently: Post-doc at Stanford
Aidan Thomas	REU Undergrad (2023)	BS: MidAmerican Nararene University
Kiran Lucas	REU Undergrad (2022)	BS: Brown University
Lily Al-Omari	Undergrad (2019-2020)	UNC Class of 2022
Dr. Jian-Cheng Wong	PhD Student (2015-2021)	AB: Cornell University Subsequently: Post-doc at the Institute of Physics (FZU) of the Czech Academy of Sciences
Harvey Liu	Undergrad (2020-2021)	BS: UNC Subsequently: Graduate student in Comp. Sci. at UNC
Dr. Yi Yao	Post-doc (2019-2021)	Subsequently: Research Scientist at Duke
	PhD Student (2012-2018)	PhD: UNC / BS: USTC (China) Subsequently: Post-doc at UNC and Duke
Dr. Dillon Yost	PhD Student (2014-2019)	BS: Berry College Subsequently: Post-doc at MIT

Dr. Garnet Liu	Vis. PhD Student (2017-2019)	BS: Nanjing University (China) Subsequently: Senior Researcher at TSMC
Samuel Slattery	Researcher (2017-2018)	BS: UNC Subsequently: PhD student (chem.) at Virginia Tech
Dr. Lesheng Li	PhD Student (2012-2018)	PhD: UNC / MS/BS: Xi'an Jiaotong University (China) Subsequently: Post-doc at Princeton Univ.
Philip Straughn	Undergrad (2015-2017)	BS: UNC Subsequently: Technician at UNC Medical School
Jacob Engel	Vis. Undergrad (2017)	BS: Rice Univ.
Dr. Kyle Reeves	PhD Student (2011-2016)	PhD: UNC / BS: Univ. of Mass., Amherst Subsequently: Post-doc at UPMC-Paris 6 (France)
Dr. Donghwa Lee	Post-doc (2010-2014)	PhD: University of Florida Subsequently: Assistant Professor at Chonnam National University (Korea)
Zoe Watson	Undergrad (2012-2014)	BS: UNC Subsequently: PhD student (chem.) at UC Berkeley
David Guarino	Undergrad (2013-2014)	BS: UNC Subsequently: Graduate student (financial math.) at University of Chicago
Zhenya Hu	Undergrad (2013-2014)	BS: UNC Subsequently: Employment at Sanofi Genzyme (Boston)
Dr. Andre Schleife	Post-doc (2011-2013)	PhD: Friedrich Schiller University (Germany) Subsequently: Assistant Professor (MSE) at UIUC
Matt Dutra	Undergrad (2011-2012)	BS: UNC Subsequently: PhD student (chem.) at UT Knoxville

III. Awards, Honors, and Special Recognition Received by Group Members

(12) Nicolas Boyer (undergraduate)	Chapel Family Undergraduate Research Award (UNC), 2022
(11) Ruiyi Zhou (PhD student)	Bost Fellowship (UNC), 2021
(10) Dr. Yi Yao (Post-doc)	Best Poster Award, Triangle Hard Matter Workshop, 2020
(9) Dillon Yost (PhD student)	Venable Award (UNC), 2019
(8) Yi Yao (PhD student)	James T. Dobbins Fellowship (UNC), 2017
(7) Kyle Reeves (PhD student)	Induction to Frank Porter Graham Honor Society (UNC), 2015
(6) Dillon Yost (PhD student)	NSF Graduate Research Fellowship, 2015
(5) Kyle Reeves (PhD student)	Outstanding Poster Prize, ES2014 Workshop 2014
(4) Zoe Watson (undergraduate)	Carrie Largent Award for Research Excellence (UNC), 2013
(3) Kyle Reeves (PhD student)	NSF Graduate Research Fellowship, 2013
(2) Yi Yao (PhD student)	Francis P. Venable Fellowship (UNC), 2012
(1) Zoe Watson (undergraduate)	Jason D. Altom Memorial Award for Undergrad. Research (UNC), 2012

h) Professional Service

1. Service to Discipline

- FHI-aims Advisory Board member, MS1P, 2023-
- Editorial Advisory Board member, Journal of Physical Chemistry Letters (ACS), 2019-
- Graduate Faculty (term member), Dept. of Chemistry, Duke University, 2016-
- Organizer/Lecturer, "2021 HybriD3 Theory Training Workshop", Online, 1/19-21/2021

- Organizer/Lecturer, "2018 HybriD3 Theory Training Workshop", Durham, NC, 9/28-29/2018
- Co-lead for IRG3, Research Triangle MRSEC, 2016-2017
- Member, Theory Facility Proposal Study Panel, Molecular Foundry, LBNL, 2011-2014
- Organizer, "High-Performance Computing and Electronic Structure Calculations in Materials Research" Japan Society of Applied Physics-Materials Research Society Joint Symposia, Kyoto, Japan, 9/16-20/2013
- Organizing Committee member for Solar Energy + Technology, Conference Chair, "Solar Hydrogen and Nanotechnology VIII" SPIE Optics + Photonics Meeting, San Diego, CA, 8/25-29/2013
- Director, Computational Chemistry and Materials Science Summer Institute, LLNL, 2009-2011
- Instructor: CECAM Spectra2010 Tutorial, SISSA (International School of Advanced Studies), Italy, 7/23-31/2010
- Lecturer/Mentor, Workshop on Global Innovation and Training of Young Leaders, Osaka University San Francisco Center, 2010, CA, USA
- Panel Member, DOE workshop for "Computational Research Needs in Alternative & Renewable Energy", 9/19-21/2007, Rockville, MD
- Technical Coordinator, *Berkeley PV Idea Lab* (bi-weekly experiment-theory discussion meetings on photovoltaic research), U.C. Berkeley, 2006-2009
- Proceeding editor for *MRS proceedings* and *Proceedings of SPIE*
- Merit reviewer for *CINECA* (Italy)
- PhD thesis examiner for Indian Institutes of Science Education and Research (India)
- Proposal reviewer for *Department of Energy*, *National Science Foundation*, *ACS Petroleum Research Fund*, *Leverhulme Trust* (UK), and *Netherlands Organization for Scientific Research (NWO).*
- Manuscript reviewer for *J. Am. Chem. Soc., J. Chem. Phys., J. Phys. Chem. Lett./A/B/C, ACS Nano, Nano Lett., Phys. Rev. B, J. Phys. D, Chem. Phys. Lett., App. Phys. Lett., Semi. Sci. Tech., Appl. Surf., Sci., Surf. Sci., Int. J. Quant. Chem., PNAS, Chem, Comp. Phys. Comm., Eur. Phys. J. B, Can. J. Phys.* and *Nature Comm.*

2. Departmental/University Service at UNC

- Research Computing Advisory Committee (University-wide), Oct. 2015-present
- Physical Chemistry Division Lead, Aug. 2022-present
- Faculty Mentoring Committee for Prof. Zhiyue Lu, Jan. 2020-present
- Colloquium Committee, Aug. 2021-present
- Undergraduate Studies Committee, Aug. 2021-present
- Theoretical Chemistry Faculty Search Committee (Chair), Oct. 2022-Mar. 2023
- Condensed Matter Physics Faculty Search Committee (Dept. Physics/Astronomy) Sept. 2021-May. 2022
- Graduate Studies Committee, Aug. 2011-Jul. 2012, Aug. 2013-May. 2021
- Pariser-Parr Lecture organizer, 2015, 2018, and 2022
- Physical Chemistry Division Contact, Aug. 2018-Jul. 2020
- Tenure-Track Faculty Search Committee (Chair), Spt. 2018-Mar. 2019
- Theoretical Chemistry Faculty Search Committee (Chair), Oct. 2017-Apr. 2018
- Undergraduate Lab Committee, Aug. 2014-Aug. 2017
- Analytical Chemistry Faculty Search Committee, Sept. 2016-Dec. 2016
- Chemistry Library Liaison, Aug. 2012-Jul. 2013
- Recruiting Committee, Aug. 2012-Jul. 2013
- PhD Thesis Committee for

Zhenyu Ouyang (2023), Lauren McRae (2023), Jack Sundberg (2022), Ninghao Zhou (2021), Jacob Pawlik (2021), Jian Cheng Wong (2021), Thomas Kolb (2020), Olivia Williams (2020), Dillon Yost (2019), Seokhyoung Kim (2019), Emma Cating-Subramanian (2018), Jun Hu (2018), Zhenkun Guo (2018), Thomas Cheshire (2018), Lesheng Li (2018), Yi Yao (2018), Melissa Gish (2018), Taylor Moot (2018), Christopher Pinion (2017), Tom Celano (2017), Dangxing Chen (Math, 2017), Zachary Morseth (2016), Kyle Reeves (2016), Paul Giokas (2016), Joe Christesen (2016), Brian Molesky (2016), Jordan Womick (2012), Stephen Miller (2012)

- PhD Thesis Committee at Duke University for
  Ruyi Song (2023), Tong Zhu (2020), Garnett Liu (2019)
- External PhD Thesis Committee member for
  Ritesh Pant (2023, IISER Bhopal – India), Clara Salvini (2023, Politecnico Di Torino, - Italy), Manish Kumar (2021, IISER Bhopal – India).
- B.S. Honors Thesis Committee for
  Siona Benjamin (2023), Ran Gao (2022), Ashton Hines (2022), Jake Evans (2019), Edgar Faison (2018), Philip Straughn (2017), Alexander Krois (2012), Zoe Watson (2012)