Yosuke Kanai, Ph.D.

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. Honor in Chemistry	University of Tennessee at Knoxville

Professional experience

2017-present	Associate Professor (w/ tenure, granted in March 2017)
2011-2017	Assistant Professor Department of Chemistry University of North Carolina at Chapel Hill
2011-2014	Visiting Scientist Condensed Matter and Materials Division Lawrence Livermore National Laboratory
2009-2011	Lawrence Fellow 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

Honors and Awards

2016 Outstanding Junior Faculty Award in Computational Chemistry, American Chemical Society
2013 R. J. Reynolds Junior Faculty Development Award, UNC
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

Refereed Publications

47. "Examining Real-time TDDFT Non-equilibrium Simulation for the Calculation of Electronic Stopping Power" D. Yost, Y. Yao, and Y. Kanai, Phys. Rev. B in press (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 and 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, J. Chem. Phys., 145, 124705 (2016) *Equal contributions.

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).

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).

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, J. Chem. Phys., 140, 234109 (2014). *Equal contributions

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).

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 (Feature Article-Invited)" 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)

Invited Presentations

39. Chemistry-Physics Join Department Colloquium, Wake Forest University, NC, USA, 1/24/2018
38. CPMD 2017 Workshop, Tsukuba, Japan, 10/18-20/2017
37. CECAM/Psik Workshop: Charge carrier dynamics in nanostructures: optoelectronic and photo-stimulated processes, Germany, 10/9-13/2017
36. Physics Department Colloquium, University of North Carolina at Chapel Hill, NC, USA, 8/28/2017
35. Telluride Workshop: Excited States, USA, 7/17-21/2017
34. American Chemical Society National Meeting, San Francisco, USA, 4/02/2017
33. Southeastern Regional Meeting of American Chemical Society, Columbia, SC, USA, 10/23/2016
32. NC Photochem 2016 Symposium, North Carolina State Univ., NC, USA, 10/1/2016
31. Theoretical/Physical Chemistry Seminar, Northwestern University, IL, USA, 10/10/2016
30. NSF KI-Net Conference: Mathematical and Computational Methods in Quantum Chemistry, Yale Univ., USA, 5/13/2016
29. Physics Department Seminar, Temple University, PA, USA, 4/27/2016

28. Physical Chemistry Seminar, Massachusetts Institute of Technology, MA, USA, 4/12/2016
27. American Physical Society National Meeting, Baltimore, USA, 3/15/2016
26. Chemical Physics Seminar, California Institute of Technology, CA, USA, 10/20/2015
25. Physical/Theoretical Chemistry Seminar, University of Southern California, CA, USA, 10/19/2015
24. Physical Chemistry Seminar, University of Washington, WA, USA, 9/30/2015
23. SPIE Meeting: Photonics and Optics, CA, USA, 8/12/2015
22. Computational Chemistry and Material Science Summer Institute – Lawrence Livermore National Lab., CA, USA, 7/20-21/2015
21. Excited States and Dynamics Workshop, Telluride, USA, 7/13/2015
20. Center of Research Excellence in Complex Materials Seminar, Michigan State Univ., USA, 4/2/2015
19. Condensed Matter Theory Seminar (Physics/Chemistry/MSE), Univ. of Michigan, USA, 3/30/2015
18. Theory Facility Seminar – Molecular Foundry, Lawrence Berkeley Lab, CA, USA, 12/12/2014
17. Department of Chemistry Seminar, Duke University, NC, USA, 11/20/2014
16. Department of Applied Physics Seminar, University of Tokyo, Japan, 7/29/2014
15. International Materials Research Congress, Cancun, Mexico, 8/12/2013
14. Southeast Theoretical Chemistry Association Annual Meeting, Auburn, AL, USA, 5/10/2013
13. Chemistry Department Seminar, North Carolina State University, NC, USA, 9/28/2012
12. Solar Fuels, Science, Engineering, and Policy, Duke University, NC, USA, 1/11/2012
11. Chemistry and Physics of Nano-crystalline Surface Workshop, Berkeley, CA, USA, 10/6/2011
10. American Chemical Society National Meeting, CO, USA, 8/29/2011
9. Condensed Matter Physics Seminar, SISSA (International School of Advanced Studies), Trieste, Italy, 7/27/2010
8. Materials Science and Engineering Department Colloquium, U.C. Berkeley, CA, USA, 10/22/2009
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

Professional Service

1. Service to Discipline

- Co-lead for IRG3, Research Triangle MRSEC, 2016-2017
- Term Member, Graduate Faculty, Duke University, 2016-2021
- 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
- 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).
- Proposal reviewer for *Department of Energy*, *National Science Foundation*, *ACS Petroleum Research Fund*, and *Netherlands Organisation for Scientific Research (NWO).*
- Manuscript reviewer for *J. Am. Chem. Soc., J. Chem. Phys., J. Phys. Chem. B/C, ACS Nano, Nano Lett., Phys. Rev. B, J. Phys. D, Chem. Phys. Lett., App. Phys. Lett., J. Phys. Chem. Lett., Semi. Sci. Tech., Appl. Surf., Sci., Surf. Sci., Int. J. Quant. Chem., PNAS, and Nature Comm.*.

2. Departmental/University Service at UNC

- Graduate Studies Committee, Aug. 2011-Jul. 2012, Aug. 2013-present
- Undergraduate Lab Committee, Aug. 2014-present
- Analytical Chemistry Faculty Search Committee, Sept. 2016-Dec. 2016
- 2015 Pariser-Parr Lecture organizer
- Chemistry Library Liaison, Aug. 2012-Jul. 2013
- Recruiting Committee, Aug. 2012-Jul. 2013
- Research Computing Advisory Committee, Oct. 2015-present

Mentoring

Jian-Chen Wong	PhD Student (2015-)	BA: Cornell University
Dillon Yost	PhD Student (2014-)	BS: Berry College
Lesheng Li	PhD Student (2012-)	MS/BS: Xi'an Jiaotong University (China)
Yi Yao	PhD Student (2012-)	BS: USTC (China)
Philip Straughn	Undergrad (2015-2017)	BS: UNC Subsequently: Technician at UNC Medical School
Jacob Engel	Visiting Undergrad (2017)	BS: Emory Univ.
Dr. Kyle Reeves	PhD Student (2011-2016)	PhD: UNC / BS: Univ. of Mass., Amherst Subsequently: Post-doc at UPMC-Paris 6 (France)
Dr. Andre Schleife	Post-doc (2011-2013)	PhD: Friedrich Schiller University (Germany) Subsequently: Assistant Professor (MSE) at UIUC
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)
Matt Dutra	Undergrad (2011-2012)	BS: UNC Subsequently: PhD student (chem.) at UT Knoxville

Research Grants

NSF (CISE-OAC), "NSCI: SI2-SSE: Time Stepping and Exchange-Correlation Modules for Massively Parallel Real-time Time-dependent DFT", 2017-2020, $500K ($250K Kanai's share), lead-PI (2 PIs).

NSF (DMR-DMREF), "DMREF: HybriD3: Discovery, Design, Dissemination of Organic-Inorganic Hybrid Semiconductor Materials for Optoelectronic Applications", 2017-2021, $1.5M ($244K Kanai's share), co-PI (6 PIs).

NSF (CHE-CTMC), "First-Principles Simulation of Electronic Excitation Dynamics in Water and DNA under Proton Irradiation", 2016-2019, $373K, PI (single PI).

DOE, "UNC EFRC: Center for Solar Fuels", 2014-2018, $10.8M ($216K Kanai's share), co-PI (18 PIs).

ACS-PRF, "Dynamics and Kinetics of Carbon Dioxide in Nano-porous Materials Environment from Quantum Molecular Dynamics Simulations", 2012-2016, $100K, PI (single PI).

DOE, "UNC-CH EFRC: Solar Fuels and Next Generation Photovoltaics: ARPA Funding", 2012-2014, $73K (Kanai's share), Participant.

DARPA (MTO), "Quantum Mechanical Modeling in Support for Tip-based Nanofabrication", 2010-2013, $321K, PI (single PI).

UNC, "First Principles Quantum Dynamics of Electrons in Complex Materials for Solar Energy Conversion", 2013, $7K, PI (single PI).

DOE, "Multiscale Capability for Exploring Transport Phenomena in Battery", 2011-2013, $73K (Kanai's share), co-PI (5 PIs).

Significant Computational Resource Grants

2017 DOE INCITE Award, "Electronic Stopping in Condensed under Ion Irradiation", 140 million hours lead-PI (3 PIs)

2016 DOE INCITE Award, "Electronic Response to Particle Radiation in Condensed Matter", 75 million hours co-PI (4 PIs)

2011~, DOE, NERSC, 1~4 million hours/year, single-PI