

Seogjoo J. Jang, Ph.D.

Current Position: Professor, Department of Chemistry and Biochemistry
Queens College, City University of New York (CUNY)
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Education

Ph.D., Theoretical Chemistry (July 1995 - Dec. 1999)	University of Pennsylvania
Graduate Study in Chemistry and Physics (Sep. 1994 - June 1995)	Georgia Tech.
MS, Theoretical Chemistry (Mar. 1989 - Aug. 1993)	Seoul National University
(Leave of Absence due to military service during Mar. 1990 -Mar. 1992)	
BS, Chemistry (Mar. 1985 - Feb. 1989)	Seoul National University

Employment and Experience

Professor of Chemistry (Sep. 2012 - Present)	Queens College, CUNY
Chair, Department of Chemistry and Biochemistry (July 2018 - June 2021)	Queens College, CUNY
Associate Professor of Chemistry (Jan. 2010 - Aug. 2012)	Queens College, CUNY
Assistant Professor of Chemistry (Sep. 2005 - Dec. 2009)	Queens College, CUNY
Goldhaber Distinguished Fellow (Jan. 2003 - Aug. 2005)	Brookhaven National Laboratory
Postdoctoral Associate (Nov. 1999 - Dec. 2002)	Massachusetts Institute of Technology

Other current appointments

Korea Institute for Advanced Study (KIAS) Scholar (Jan. 2022 - Present)	Seoul, Korea
Faculty, Initiative for the Theoretical Sciences (Sep. 2011 - Present)	Graduate Center, CUNY
Doctoral Faculty of Physics (Jan. 2009 - Present)	Graduate Center, CUNY
Doctoral Faculty of Chemistry (Oct. 2005 - Present)	Graduate Center, CUNY

Other past appointments and experience

Visiting Professor, KAIST (Aug. 2022 - Feb. 2023)	Daejeon, Korea
Visiting Senior Research Scientist (Sep. 2012 - May 2014)	Columbia University
Visiting Research Scientist (June 2012 - Aug. 2012)	University of California, Berkeley
Guest Scientist (Sep. 2005 - Aug. 2014)	Brookhaven National Laboratory
Korean Military Service (Oct. 1990 - Mar. 1992)	Seoul, South Korea

Awards

Outstanding Community Service Award (2017)	KSEA
Camille Dreyfus Teacher-Scholar Award (2010 - 2015)	Dreyfus Foundation
Salute to Scholars (2010, 2011, 2014, 2016)	City University of New York
Faculty Early Career Development Award (2009 - 2014)	National Science Foundation
Goldhaber Distinguished Fellowship (2003 - 2005)	Brookhaven National Lab.
Chairman's Award for Academic Excellence (1996)	University of Pennsylvania

Research Expertise available for consulting: Solar Energy Conversion, Computational Chemistry, Energy/Charge Transfer Processes, Spectroscopy

Current Research Support

Seogjoo J. Jang, “Integrative computational investigation of the spectroscopy, dynamics, and controlling of molecular excitons in complex environments,” Department of Energy; Sep. 2020 - May 2025

Past Research Support

18. **Seogjoo J. Jang**, “Quantum dynamics methods for fluctuating systems in quantum environments: Development and Application,” National Science Foundation; July 2019 - June 2023
17. **Seogjoo J. Jang**, “Theoretical investigation of the distance dependence of resonance energy transfer in the presence of quantum coherence and nonequilibrium effects,” PSC-CUNY Grant; July 2019 - Dec. 2023
16. **Seogjoo Jang**, “Molecular level characterization of quantum design principles for efficient and robust exciton and charge migration,” Department of Energy, Office of Basic Energy Sciences, Program of Computational and Theoretical Chemistry (PCTC); Jan. 2016 - Dec. 2019
15. **Seogjoo Jang**, “Development of next generation quantum master equation and generalized master equation approaches,” National Science Foundation; May 2014 - Oct. 2017
14. **Seogjoo Jang**, “Large scale molecular level and quantum simulation of light harvesting complexes in photosynthetic purple bacteria,” PSC-CUNY Grant; July 2016 - June 2017
13. **Seogjoo Jang**, “Elucidating positive quantum effects for efficient energy and charge transfer dynamics in soft solar energy conversion systems,” Department of Energy, Office of Basic Energy Sciences, Program of Computational and Theoretical Chemistry Research (PCTC); Jan. 2013 - Dec. 2015
12. **Seogjoo Jang**, “Theory development and computational modeling of exciton and electron/hole migration in soft disordered environments,” Camille Dreyfus Teacher-Scholar Award; June 2010 - May 2015
11. **Seogjoo Jang**, “Kinetic Monte Carlo simulation of electron-hole pair dynamics in polymeric bulk heterojunction device,” PSC-CUNY grant; July 2010 - Dec. 2011
10. **Seogjoo Jang**, “Coarse-grained computational modeling of conjugated polymers at nanometer length scale,” User Proposal for linux cluster in the Center for Functional Nanomaterials, Brookhaven National Laboratory; Sep. 2009 -Dec. 2010
9. **Seogjoo Jang**, “Computational modeling and theory development of charge flow dynamics in photosynthetic units and conjugated polymer systems,” Department of Energy, Office of Basic Energy Sciences, Program of Computational and Theoretical Chemistry (PCTC); Sep. 2009 - Dec. 2012
8. **Seogjoo Jang**, “Theoretical modeling of the pump-probe anisotropy of coherent resonance energy transfer dynamics,” PSC-CUNY grant; July 2009 - Dec. 2010

7. **Seogjoo Jang**, “Synergistic theory development and computational modeling of the energy flow dynamics in soft optoelectronic molecules,” National Science Foundation, CAREER award; May 2009 - Apr. 2014
6. **Seogjoo Jang**, “Coarse-grained computational modeling of conjugated polymers,” Research Enhancement Grant, Queens College; July 2009 - Aug. 2010
5. **Seogjoo Jang**, “Theoretical investigation on the microscopic basis of the two-state model of the excess electron in saturated hydrocarbon liquids based on path integral simulation,” American Chemical Society Petroleum Research Foundation, Type G grant; July 2007 - Aug. 2010
4. **Seogjoo Jang**, “Theoretical development and application of path integral centroid methods for quantum dynamics simulation of condensed phase systems,” PSC-CUNY grant; July 2008 - June 2009
3. **Seogjoo Jang**, “Feynman path integral simulation of an excess electron in hydrocarbon liquids,” Research Enhancement Funding, Queens College; Nov. 2007 - May 2008
2. Zhonghua Yu and **Seogjoo Jang**, “Single Molecule Spectroscopy of Conjugated Organic Oligomers: A Joint Experimental and Theoretical Study,” CUNY Collaborative Research Grant; Sep. 2006 - Aug. 2008
1. **Seogjoo Jang**, “Quantum dynamical modeling and computation of the charge transport through single DNA duplexes,” PSC-CUNY grant; July 2006 - Dec. 2007

Recent Invited Talks and Seminars (2009 - Present)

88. Boston University (April, 2024)
87. University of Toronto (April, 2024)
86. City College, CUNY, New York (Apr. 2024)
85. American Chemical Society National Meeting, New Orleans (March, 2024)
84. Workshop on “Non-Markovian Quantum Dynamics,” Flatiron Institute, New York (Sep. 2023)
83. Workshop on “Quantum Dynamics and Spectroscopy of Functional Molecular Materials and Biological Photosystems,” Les Houches, France (Sep. 2023)
82. International Conference on Biological Physics, Seoul (August, 2023)
81. International Workshop on New Advances in Theoretical and Computational Molecular Sciences for Complex and Quantum Processes, Seoul (June, 2023)
80. Northwestern University, Evanston (May, 2023)
79. Duke University, Durham (April, 2023)
78. East Regional Photosynthesis Conference, Woods Hole (April, 2023)
77. American Chemical Society National Meeting, Indianapolis (March, 2023)

76. University of Seoul, Seoul, Korea (March, 2023)
75. Yonsei University, Seoul, Korea (March, 2023)
74. Korea University, Seoul, Korea (March, 2023)
73. Academy of Sinica and Taiwan National University, Taiwan (March, 2023)
72. KIAS Workshop on Quantum Information and Thermodynamics, Busan, Korea (December, 2022)
71. Chungbuk National University, Cheongju, Korea (November 2022)
70. Seoul National University, Seoul, Korea (November 2022)
69. Korean Advanced Institute of Science and Technology (KAIST), Daejeon, Korea (November 2022)
68. Telluride Workshop on “Spatio-temporal dynamics of excitons: Bridging the gap between quantum mechanics and applications,” Telluride, CO (September 2022)
67. Kyungpook National University, Daegu, Korea (July 2022)
66. Chung-Ang University, Seoul, Korea (July 2022)
65. American Chemical Society mid-Atlantic Regional Meeting, Ewing, NJ (June 2022)
64. American Chemical Society National Meeting, San Diego (March 2022)
63. Pacificchem 2021 Congress, Virtual (Dec. 2021)
62. Virtual Telluride Workshop on “Quantum Frontiers in Molecular Science” (July 2020)
61. Chinese Academy of Sciences and Peking University, Beijing, China (November 2019)
60. Nanjing University of Post and Telecommunication, Nanjing, China (November 2019)
59. University of Rochester, Rochester, NY (November 2019)
58. American Chemical Society National Meeting, San Diego, CA (August 2019)
57. 10th Triennial Congress of the International Society of Theoretical Chemical Physics, Tromsø, Norway (July 2019)
56. Telluride Workshop on “Quantum Dynamics and Spectroscopy in Condensed-Phase Materials and Bio-Systems,” Telluride, CO (June 2019)
55. DOE Research Meeting of the Computational and Theoretical Chemistry Program, Gaithersburg, MD (May 2019)
54. American Chemical Society National Meeting, Boston (Aug. 2018)
53. US-Korea Conference 2018, Queens, NY (Aug. 2018)
52. Chung-Ang University, Seoul, Korea (July 2018)
51. Korean Advanced Institute of Science and Technology (KAIST), Daejeon, Korea (July 2018)

50. Korea University, Seoul, Korea (July 2018)
49. Korean Institute for Advanced Study (KIAS), Seoul, Korea (July 2018)
48. Advanced Science Research Center, CUNY, New York (April 2018)
47. Mini-Workshop on Nonadiabatic Dynamics and Conical Intersections, New York University, New York (Nov. 2017)
46. US-Korea Conference 2017, Washington DC (Aug. 2017)
45. Workshop on “Quantum Dynamics and Spectroscopy of Functional Molecular Materials and Biological Photosystems,” Les Houches, France (May 2017)
44. DOE Research Meeting of the Computational and Theoretical Chemistry Program, Gaithersburg, MD (May 2017)
43. Korean Institute for Advanced Study (KIAS) Workshop on “Quantum Information and Thermodynamics,” Jeju, Korea (Nov. 2016)
42. Seoul National University, Seoul (Nov. 2016)
41. American Chemical Society National Meeting, Philadelphia (Aug. 2016)
40. Telluride Workshop on “Molecular Recognition and the Chemical Senses,” Telluride, CO (July 2016)
39. University of California at San Diego (May, 2016)
38. University of Toronto (April, 2016)
37. American Chemical Society National Meeting, San Diego (March, 2016)
36. Stony Brook University, Laufer Center (January, 2016)
35. Seoul National University, Seoul, Korea (August 2015)
34. Korea Institute for Advanced Study (KIAS), Seoul, Korea (August 2015)
33. Postech Symposium on “Chemistry and Light,” Pohang, Korea (August 2015)
32. Penn Computational and Theoretical Chemistry Conference, Philadelphia, PA (July 2015)
31. Telluride Workshop on “Quantum Effects in Condensed Phase Systems,” Telluride, CO (July 2015)
30. Telluride Workshop on “Quantum Dynamics and Spectroscopy in Condensed-Phase Materials and Bio-Systems,” Telluride, CO (June 2015)
29. “Recent Advances in Quantum Dynamics and Thermodynamics of Complex Systems,” the 15th ICQC Satellite Meeting, Beijing, China (June, 2015)
28. DOE Research Meeting of the Computational and Theoretical Chemistry Program, Annapolis, MD (Apr. 2015)
27. Rutgers University, Newark, NJ (Apr. 2015)

26. University of Chicago, Chicago, IL (Nov. 2014)
25. Carnegie Mellon University, Pittsburgh, PA (Apr. 2014)
24. Princeton University, Princeton, NJ (Oct. 2013)
23. University of Pennsylvania, Philadelphia, PA (Sep. 2013)
22. US-Korea Conference 2013, East Rutherford, NJ (Aug. 2013)
21. Telluride Workshop on “Nonequilibrium Phenomena, Nonadiabatic Dynamics, and Spectroscopy,” Telluride, CO (July 2013)
20. Telluride Workshop on “Quantum Dynamics and Spectroscopy in Condensed-Phase Materials and Bio-Systems,” Telluride, CO (July 2013)
19. Brookhaven National Lab., Center for Functional Nanomaterials User’s Meeting, Upton (May, 2013)
18. New York Theoretical and Computational Chemistry Conference, New York (Jan. 2013)
17. Arizona State University, Energy Research Frontier Center, Tempe (Oct., 2012)
16. American Chemical Society National Meeting, Philadelphia (Aug., 2012)
15. New York University, New York (May, 2012)
14. Hunter College, CUNY, New York (Feb. 2012)
13. City College, CUNY, New York (Nov. 2011)
12. College of Staten Island, CUNY, New York (Nov. 2011)
11. Symposium on “Quantum Biology - Applications of Physical and Chemical Methods in Biological Systems,” Boston, MA (Oct. 2011)
10. DOE Research Meeting of the Condensed Phase and Interfacial Molecular Science Program, Baltimore, MD (June 2011)
9. Brookhaven National Laboratory (May 2011)
8. University of Michigan (April 2011)
7. City College (Chemical Engineering) , CUNY (April 2011)
6. York College, CUNY (Mar. 2011)
5. Workshop on “Quantum Effects in Biological Systems,” Cambridge, MA (June 2010)
4. Canadian Chemical Society Conference on “Coherence and Decoherence in Molecular Systems,” Toronto, Canada (May 2010)
3. CECAM Workshop on “Theoretical, Computational, and Experimental Challenges to Exploring Coherent Quantum Dynamics in Complex Many-Body Systems,” Dublin, Ireland (May 2010)
2. Soft Materials Symposium: “The Future of Solar Technologies” (Moderator), New York Academy of Sciences (Jan. 2010)

1. Conference on Quantum Information and Quantum Control, Fields Institute, Toronto (Aug. 2009)

Mentoring

Postdoctoral Researchers

Dr. Pablo Ramos, Queens College (Sep. 2020 - Aug. 2023)
Dr. Ning Chen, Queens College (Feb. 2020 - June 2021)
Dr. Eva Rivera, Queens College (June, 2013 - May, 2017)
Dr. Daniel Montemayor, Queens College (June, 2013 - May, 2017)
Dr. Hiroko Ajiki, Queens College (part time) (July, 2013 - December, 2015)
Dr. Praveen Kumar, Queens College (Feb. 2010 - Sep. 2012)
Dr. Lei Yang, Queens College (Nov. 2008 - June 2012)

Ph.D. Students

Taner Ture, Chemistry Graduate Student, Queens College (June 2016 - Present)
Ning Chen, Chemistry Graduate Student, Queens College (June 2014 - Feb. 2020)
Murali Devi, Physics Graduate Student, Queens College (Apr. 2008 - May, 2016)
Marta Kowalczyk, Chemistry Graduate Student, Queens College (Jan. 2007 - March, 2013)

Undergraduate and Master's Students

Ryan Pangilinan, Master's degree, Physics, Queens College (July 2019 - December 2021)
Ester Aziz, BA and Master's program, Chemistry, Queens College (June 2014 - Dec., 2015)
Eric Steimez, BA, Computer Science, Queens College (Jan. 2014 - May, 2016)
Xun Huang, Master's degree, Chemistry, Graduate Center, CUNY (July 2009 - June, 2012)
Daniel Sangobawno, Chemistry Undergraduate Student, Queensborough Community College, CUNY (June 2009 - August 2009)
Alexis Estrada, Chemistry Undergraduate Student, Queens College, CUNY (June 2009 - May 2010)
Jin Bakalis, Chemistry Undergraduate Student, Queens College, CUNY (June 2009 - May 2010)
Andres Montoya Castillo, Undergraduate Student, Honors College, CUNY (June 2007 -May 2009) & Master's program, Physics Department, Queens College, CUNY (June 2009 - May 2011)
Michael Kirschenbaum, Undergraduate Student, Queens College (Jan. 2006 - Dec. 2007)

High School Students

Michael Kaplan, Bronx High School (Jan. 2007 -Jan. 2009) - Siemens Competition Semifinalist, Intel Talent Search Competition Semifinalist, New York City Science and Engineering Fair Finalist, and Intel International Science and Engineering Fair 4th place winner

Teaching

Quantum Chemistry and Spectroscopy (Spring, 2024)	Queens College, CUNY
Chemical Thermodynamics and Kinetics (Fall, 2023)	Queens College, CUNY
Quantum Chemistry (Fall, 2022)	KAIST
Quantum Chemistry and Spectroscopy (Spring, 2022)	Queens College, CUNY
Introductory Quantum Chemistry (Fall, 2021)	Graduate Center, CUNY

Quantum Chemistry and Spectroscopy (Spring, 2021)	Queens College, CUNY
Quantum Chemistry and Spectroscopy (Spring, 2020)	Queens College, CUNY
Quantum Chemistry and Spectroscopy (Spring, 2018)	Queens College, CUNY
Chemical Thermodynamics and Kinetics (Fall, 2017)	Queens College, CUNY
Quantum Chemistry and Spectroscopy (Spring, 2017)	Queens College, CUNY
Introductory Quantum Chemistry (Fall, 2016)	Graduate Center, CUNY
Molecular Quantum Mechanics (Spring, 2016)	Queens College, CUNY
Introductory Quantum Chemistry (Fall, 2015)	Graduate Center, CUNY
Quantum Chemistry and Spectroscopy (Spring, 2015)	Queens College, CUNY
Chemical Thermodynamics and Kinetics (Fall, 2014)	Queens College, CUNY
Quantum Chemistry and Spectroscopy (Spring, 2014)	Queens College, CUNY
Chemical Thermodynamics and Kinetics (Fall, 2013)	Queens College, CUNY
Quantum Chemistry and Spectroscopy (Spring, 2012)	Queens College, CUNY
Advanced Seminar (Fall, 2011)	Graduate Center, CUNY
Quantum Mechanics for Solar Energy Conversion (Fall, 2011)	Graduate Center, CUNY
Quantum Chemistry and Spectroscopy (Spring, 2011)	Queens College, CUNY
Introduction to Spectroscopy (Fall, 2010)	Graduate Center, CUNY
Chemical Thermodynamics and Kinetics (Fall, 2009)	Queens College, CUNY
Physical Chemistry II (Spring, 2009)	Queens College, CUNY
Seminar (Fall, 2008)	Queens College, CUNY
Physical Chemistry I (Fall, 2008)	Queens College, CUNY
Lectures on Spectroscopy (Spring, 2008)	Graduate Center, CUNY
Introductory Quantum Chemistry (Fall, 2007)	Graduate Center, CUNY
Seminar (Spring, 2007)	Queens College, CUNY
Physical Chemistry II (Spring, 2007)	Queens College, CUNY
Advanced Seminar (Spring, 2006)	Graduate Center, CUNY
Introduction to Spectroscopy (Spring, 2006)	Graduate Center, CUNY
Physical Chemistry II(Spring, 2006)	Queens College, CUNY

Synergistic Activity (Sep. 2005 - Present)

College Activity

- Dean Search Committee, Queens College, CUNY (Dec. 2018 - May, 2019)
- College Website Advisory Committee, Queens College, CUNY (Nov. 2018 - Present)
- Faculty Search Committee, Queens College, CUNY (Nov. 2017 - Apr. 2018)
- Faculty Search Committee, City College, CUNY (Nov. 2013 - Feb. 2014)
- Doctoral Program Restructuring Super Committee, CUNY (Sep. 2013 - Feb. 2014)
- Doctoral Program Restructuring Committee, Queens College, CUNY (Nov. 2012 - Jan. 2013)
- Tech Fee Committee, Queens College, CUNY (Nov. 2009 - Nov. 2011)
- Deputy Chair, Department of Chemistry and Biochemistry, Queens College, CUNY (July 2009 - June 2015)

- Personnel and Budget Committee, Department of Chemistry and Biochemistry, Queens College, CUNY (May 2009 - Present)
- Executive Committee, Chemistry Graduate Program, City University of New York (May 2009 - Present)
- Graduate Admission Committee (Mar. 2006 - Oct. 2008), Queens College, CUNY
- Faculty Hiring Committee (2005, 2006), Queens College, CUNY
- Academic Senate, Queens College, CUNY (2007 - 2008, 2017 - 2018)

Academic Activity

- Co-editor, Journal of Chemical Physics Special Issue on “Excitons: Energetics and Spatio-temporal dynamics” (April, 2020)
- Co-organization of Telluride Workshop on “Spatio-temporal dynamics of excitons: Bridging the gap between quantum mechanics and applications,” Telluride, CO (August, 2020, rescheduled for July 2021)
- Co-organization of Symposium on “Characterization, Detection & Application of Excitons in Chemistry” at the American Chemical Society National Meeting, Boston (August, 2018)
- Organization of Workshop on Theoretical and Computational Chemistry, Initiative for the Theoretical Sciences, Graduate Center, CUNY (May 2014-Present)
- Organization of Annual “New York Theoretical and Computational Chemistry Conference,” Graduate Center, CUNY (Jan. 2010 - 2013, May 2015)
- Organization of a CUNY theory meeting “Association of Theoretical and Computational Chemists at CUNY (ATaCCC)” (2006-2008, 2010 -Present)
- Organization of “Workshop on Computation, Simulation, and Modeling of molecular processes,” Graduate Center, CUNY (2007- 2008)
- Soft Materials Steering Committee, the New York Academy of Sciences (2006 - 2010)
- Chair, “Computers in Chemistry” Topical Group, New York Section of the American Chemical Society (Dec. 2008 - Present)
- Co-Chair, Computational Chemistry Program, 2008 mid-Atlantic regional meeting of the American Chemical Society & Organization of “Computational chemistry for the health of humanity and the planet,” 2008 mid-Atlantic regional meeting of the American Chemical Society, Queensborough Community College, CUNY (May 2008)

Activity for Korean-Scientists and Engineers Association

- Project Director, KSEA 46th Administration (July 2017-June 2018)
- Program Chair of KSEA Scientists’ and Engineers’ Early Career Development Workshop, Vienna, VA (Dec. 2017)

- Project Director, KSEA 45th Administration (July 2016-June 2017)
- Project Director, KSEA 42nd Administration (July 2013 - June 2014)
- Program Chair of KSEA Professional Development Workshop (ProDeW), Chicago, IL (March 2014)
- Technical Group B (Chemistry) Councilor, KSEA (July 2011 - June 2014)
- Hosting KSEA NY Metro Chapter's Math and Science Olympiad (KMSO) at Queens College (2007 - 2016, Fall)
- President, New York Metro Chapter of KSEA (July 2010 - June 2011)
- Senior Vice President, New York Metro Chapter of KSEA (July 2009 - June 2010)
- Vice President, New York Metro Chapter of KSEA (July 2007 - June 2009)

Review Activity for Professional Journals

- The Journal of Chemical Physics
- Physical Review Letters, A, B, and E
- The Journal of American Chemical Society
- The Journal of Physical Chemistry
- Chemical Physics
- Soft Matter, Royal Society
- Philosophical Transactions, Royal Society
- Department of Energy Proposals
- National Science Foundation proposals
- CUNY Collaborative grant proposals
- PSC-CUNY Proposals
- Physical Chemistry textbook by Atkins and de Paula, 9th Edition, Freeman and Company
- Physical Chemistry Chemical Physics, a Journal of Royal Society of Chemistry
- New Journal of Physics
- Nature Communications
- Nature Chemistry
- ACS Central Science
- Chem

- RSC Chemical Science
- PRX Quantum
- Advanced Quantum Technologies

Published Books

2. **Seogjoo J. Jang**; “Quantum Mechanics for Chemistry,” (DOI: <https://doi.org/10.1007/978-3-031-30218-3>; ISBN: 978-3-031-30217-6, 978-3-031-30220-6, 978-3-031-30218-3) (Springer Nature, 2023)
1. **Seogjoo J. Jang**; “Dynamics of Molecular Excitons,” Book in *Nanophotonics Series* (ISBN: 9780081023358) (Elsevier, 2020)

Published Journal Articles and Book Chapters

78. **Seogjoo J. Jang** and Young Min Rhee; “Fermi’s golden rule rate expression for transitions due to nonadiabatic derivative couplings in the adiabatic basis,” *Journal of Chemical Theory and Computation*, Submitted (2024)
77. Won Kyu Kim, Yoonji Lee, **Seogjoo J. Jang**, and Changbong Hyeon, ; “Kinetic model for the desensitization of G protein-coupled receptor,” *Journal of Physical Chemistry Letters*, Submitted (2024)
76. J. D. Schultz, J. L. Yuly, E. A. Arsenault, K. Parker, S. N. Chowdhury, R. Dani, S. Kundu, H. Nuomin, Z. Zhang, J. Valdiviezo, P. Zhang, K. Orcutt, **S. J. Jang**, G. R. Fleming, N. Makri, J. P. Ogilvie, M. J. Therien, M. R. Wasielewski, and D. N. Beratan, “Coherence in chemistry: foundations and frontiers,” *Chemical Reviews*, Accepted (2024)
75. Kwang Hyun Cho, **Seogjoo J. Jang**, and Young Min Rhee; “Dynamics embedding of effective harmonic normal mode vibrations in all-atomistic energy gap fluctuations: Case study of light harvesting 2 complex,” *Journal of Chemical Physics* **160**, 184104 (2024)
74. Taner M. Ture and **Seogjoo J. Jang**; “Simple and general unitarity conserving numerical real-time propagators of the time-dependent Schrödinger equation based on Magnus expansion,” *Journal of Physical Chemistry A* **128**, 2871 - 2882 (2024)
73. Pablo Ramos, Hannah Friedman, Barry Y. Li, Cesar Garcia, Ellen Sletten, and **Seogjoo J. Jang**; “Nonadiabatic derivative couplings through multiple Franck-Condon modes dictate the energy gap law for near and short-wave infrared dye molecules,” *Journal of Physical Chemistry Letters* **15**, 1802 - 1810 (2024)
72. Won Kyu Kim, Kiri Choi, Changbong Hyeon, and **Seogjoo J. Jang**; “General Chemical Reaction Network Theory for GPCR-based Olfactory Sensing: Elucidation of Odorant Mixture Effects and Agonist–Synergist Threshold,” *Journal of Physical Chemistry Letters* **14**, 8412 - 8420 (2023)
71. **Seogjoo J. Jang** and Young Min Rhee; “Modified Fermi’s golden rule rate expressions,” *Journal of Chemical Physics* **159**, 014101(2023)

70. Davinder Singh, **Seogjoo J. Jang**, and Changbong Hyeon; “Fundamental trade-off between the speed of light and the Fano factor of photon current in three-level lambda systems ,” *Journal of Physics A: Mathematical and Theoretical* **56**, 015001 (2023)
69. **Seogjoo J. Jang**; “Partially polaron-transformed quantum master equation for exciton and charge transport dynamics,” *Journal of Chemical Physics* **157**, 104107 (2022)
68. **Seogjoo J. Jang**, Irene Burghardt, Chao-Ping Hsu, and Christopher J. Bardeen, “Excitons: Energetics and spatiotemporal dynamics,” *Journal of Chemical Physics* **155**, 200401 (2021)
67. **Seogjoo J. Jang**; “A simple generalization of the energy gap law for nonradiative processes,” *Journal of Chemical Physics* **155**, 164106 (2021)
66. Andrew M Levine, Guiying He, Guan hong Bu, Pablo Ramos, Fanglue Wu, Aisha Soliman, Jacqueline Serrano, Dorian Pietraru, Christopher Chan, James D Batteas, Marta Kowalczyk, **Seogjoo J. Jang**, Brent L Nannenga, Matthew Y Sfeir, Esther H R. Tsai, and Adam B Braunschweig; “Efficient Free Triplet Generation Follows Singlet Fission in Diketopyrrolopyrrole Polymorphs with Goldilocks Coupling,” *Journal of Physical Chemistry C* **125**, 12207 - 12213 (2021)
65. Kara Ng, Megan Webster, William P Carbery, Nikunj Kumar Visaveliya, Pooja Gaikwad, **Seogjoo J. Jang**, Ilona Kretschmar, and Dorte M Eisele; “Frenkel excitons in heat-stressed supramolecular nanocomposites enabled by tunable cage-like scaffolding,” *Nature Chemistry* **12**, 1157 - 1164 (2020)
64. Lei Yang and **Seogjoo J. Jang**; “Theoretical investigation of non-Förster exciton transfer mechanisms in perylene diimide donor, phenylene bridge, and terrylene diimide acceptor systems,” *Journal of Chemical Physics* **153**, 144305 (2020)
63. Ning Chen, Murali Devi, and **Seogjoo J. Jang**; “Computational modeling of charge hopping dynamics along a disordered one-dimensional wire with energy gradients in quantum environments,” *Journal of Chemical Physics* **153**, 054109 (2020)
62. **Seogjoo J. Jang**; “Fourth order expressions for the electronic absorption lineshape of molecular excitons,” *Journal of Chemical Physics (Special Issue on Open System Quantum Dynamics)*, **151**, 044110 (2019)
61. Marta Kowalczyk, Ning Chen, and **Seogjoo J. Jang**; “Comparative computational study of electronic excitations of neutral and charged small oligothiophenes and their extrapolations based on simple models,” *ACS Omega* **4**, 5758-5767 (2019)
60. **Seogjoo J. Jang**; “Effects of donor-acceptor quantum coherence and non-Markovian bath on the distance dependence of resonance energy transfer,” *Journal of Physical Chemistry C* **123**, 5767-5775 (2019)
59. **Seogjoo J. Jang**; “Robust and fragile quantum effects in the transfer kinetics of delocalized excitons between B850 units of LH2 complexes,” *Journal of Physical Chemistry Letters* **9**, 6576-65 83 (2018)
58. **Seogjoo J. Jang** and Benedetta Mennucci; “Delocalized excitons in natural light harvesting complexes,” *Reviews of Modern Physics* **90**, 035003 (2018)

57. Ji Hyun Bak, **Seogjoo J. Jang**, and Changbong Hyeon, "Implications for human odor sensing revealed from the statistics of odorant-receptor interactions," *PLOS Computational Biology* **14**, e1006175 (2018)
56. Daniel Montemayor, Eva Rivera, and **Seogjoo J. Jang**; "Computational modeling of exciton-bath Hamiltonians for light harvesting 2 and light harvesting 3 complexes of purple photosynthetic bacteria at room temperature," *Journal of Physical Chemistry B* **122**, 3815-3825 (2018)
55. **Seogjoo Jang** and Gregory A. Voth; "Non-uniqueness of quantum transition state theory and general dividing surfaces in the path integral space," *Journal of Chemical Physics* **146**, 174106 (2017)
54. **Seogjoo Jang** and Changbong Hyeon; "Kinetic model for the activation of mammalian olfactory receptor," *Journal of Physical Chemistry B*, **121** 1304 (2017)
53. **Seogjoo Jang** "Bridging the gap between coherent and incoherent resonance energy transfer dynamics by quantum master equations in the polaron picture," in *Ultrafast Dynamics at the Nanoscale: Biomolecules and Supramolecular Assemblies* (Edited by Stefan Haacke and Irene Burghardt, Pan Stanford, Singapore) (2016)
52. **Seogjoo Jang**; "Generalized quantum Fokker-Planck equation for photo induced nonequilibrium processes with positive definiteness condition," *Journal of Chemical Physics* **144**, 214102 (2016)
51. **Seogjoo Jang** and Gregory A. Voth; "Can quantum transition state theory be defined as an exact $t=0+$ limit?," *Journal of Chemical Physics* **144**, 084110 (2016)
50. Eric Block, **Seogjoo Jang**, Victor Batista, and Hanyi Zhuang; "Reply to Turin *et al.*: Vibrational theory of olfaction is implausible," *Proceedings of the National Academy of Sciences, USA* **112**, E3155 (2015)
49. Eric Block, **Seogjoo Jang**, Hiroaki Matsunami, Sivakumar Sekharan, B er enice Dethier, Mehmed Z. Ertem, Sivaji Gundala, Yi Pan, Shengju Li, Zhen Li, Stephene N. Lodge, Mehmet Ozbil, Huihong Jiang, Sonia F. Penalba, Victor Batista, and Hanyi Zhuang; "Implausibility of the vibrational theory of olfaction," *Proceedings of the National Academy of Sciences, USA*, **112**, E2766 (2015)
48. **Seogjoo Jang** and Andr es Montoya-Castillo; "Charge hopping dynamics along a disordered chain in quantum environments: Comparative study of different rate kernels," *Journal of Physical Chemistry B* **119**, 7659 (2015)
47. **Seogjoo Jang**, Eva Rivera, and Daniel Montemayor; "Molecular level design principle behind optimal sizes of photosynthetic LH2 complex: Taming disorder through cooperation of hydrogen bonding and quantum delocalization," *Journal of Physical Chemistry Letters* **6**, 928 (2015)
46. **Seogjoo Jang**, Stephan Hoyer, Birgitta Whaley, and Graham R. Fleming; "Generalized master equation with non-Markovian multichromophoric F orster resonance energy transfer for modular exciton densities," *Physical Review Letters* **113**, 188102 (2014)
45. **Seogjoo Jang**, Hoda Hossein-Nejad, and Gregory D. Scholes; "Generalized F orster resonance energy transfer," in *Quantum Effects in Biology* (Edited by Masoud Mohseni, Yasser Omar, Gregory Engel and Martin Plenio, Cambridge University Press, Cambridge, UK) (2014)

44. Alireza Shabani, Masoud Mohseni, **Seogjoo Jang**, Akihito Ishizaki, Martin Plenio, Patrick Rebentrost, Alan Aspuru-Guzik, Jianshu Cao, Seth Lloyd, and Robert Silbey; "Open quantum system approaches to biological systems," in *Quantum Effects in Biology* (Edited by Masoud Mohseni, Yasser Omar, Gregory Engel, and Martin Plenio, Cambridge University Press, Cambridge, UK) (2014)
43. **Seogjoo Jang**, Anton Sinitskiy, and Gregory A. Voth; "Can the ring polymer molecular dynamics method be interpreted as real time quantum dynamics?," *Journal of Chemical Physics* **140**, 154103 (2014)
42. **Seogjoo Jang**; "Real time quantum dynamics pre-averaged over imaginary time path integral: A formal basis for both Centroid Molecular Dynamics and Ring Polymer Molecular Dynamics," arXiv: 1308.3805 (2013)
41. **Seogjoo Jang**, Timothy Berkelbach, and David R. Reichman; "Coherent quantum dynamics in donor-bridge-acceptor nonadiabatic processes: Beyond the hopping and super-exchange mechanisms," *New Journal of Physics*, **15**, 105020 (2013)
40. Praveen Kumar and **Seogjoo Jang**; "Emission lineshapes of the B850 band of light-harvesting 2 (LH2) complex in purple bacteria: A second order time-nonlocal quantum master equation approach," *Journal of Chemical Physics* **138**, 135101 (2013)
39. **Seogjoo Jang** and Yuan-Chung Cheng; "Resonance energy flow dynamics of coherently delocalized excitons in biological and macromolecular systems: Recent theoretical advances and open issues," Wiley Interdisciplinary Reviews (WIREs) on Computational Molecular Science (*Invitational expert review article*) **3**: 84-104 (2013)
38. **Seogjoo Jang**; "Nonadiabatic quantum Liouville and master equations in the adiabatic basis," *Journal of Chemical Physics (Special Issue on Nonadiabatic Dynamics)* **137**, 22A536 (2012)
37. Lei Yang, Murali Devi, and **Seogjoo Jang**; "Polaronic quantum master equation theory of inelastic and coherent resonance energy transfer for soft systems" *Journal of Chemical Physics* **137**, 024101 (2012)
36. **Seogjoo Jang**; "Multistep quantum master equation theory for response functions in four wave mixing electronic spectroscopy of multichromophoric macromolecules," *Bulletin of the Korean Chemical Society* (Invitational contribution for a special edition) **33**, 997 (2012)
35. **Seogjoo Jang**, Robert J. Silbey, Ralf Kunz, Clemens Hofmann, and Jürgen Köhler; "Is there elliptic distortion in the light harvesting complex 2 of purple bacteria?" *Journal of Physical Chemistry B*, **115**, 12947 (2011)
34. Paiboon Sreearunothai, Alexis Estrada, Sadayuki Asaoka, Marta Kowalczyk, **Seogjoo Jang**, Andrew Cook, Jack Preses, and John Miller; "Triplet transport to and trapping by acceptor end groups on conjugated polyfluorene chains," *Journal of Physical Chemistry C*, **115**, 19569 (2011)
33. **Seogjoo Jang**; "Theory of multichromophoric coherent resonance energy transfer: A polaronic quantum master equation approach," *Journal of Chemical Physics*, **135**, 034105 (2011)
32. Lei Yang, Stefano Caprasecca, Benedetta Mennucci, and **Seogjoo Jang**; "Theoretical investigation of the mechanism and dynamics of intramolecular coherent resonance energy transfer in soft molecules: A case study of dithia-anthracenophane," *Journal of the American Chemical Society*, **132**, 16911 (2010)

31. **Seogjoo Jang**; “Theory of coherent resonance energy transfer for coherent initial condition,” *Journal of Chemical Physics*, **131**, 164101 (2009)
30. **Seogjoo Jang**, Yuan-Chung Cheng, David R. Reichman, and Joel D. Eaves; “Theory of coherent resonance energy transfer,” *Journal of Chemical Physics* **129**, 101104 (2008)
29. Vijayakumar Ramalingam, Maciej E. Domaradzki, **Seogjoo Jang**, and Rajeev S. Muthyala; “Carbonyl groups as molecular valves to regulate chloride binding to squaramides,” *Organic Letters* **10**, 3315 (2008)
28. **Seogjoo Jang**; “Generalization of the Förster resonance energy transfer theory for quantum mechanical modulation of the donor-acceptor coupling,” *Journal of Chemical Physics* **127**, 174710 (2007)
27. **Seogjoo Jang**, Marshall D. Newton, and Robert J. Silbey; “Multichromophoric Förster resonance energy transfer from B800 to B850 in the light harvesting complex 2: Evidence for subtle energetic optimization by purple bacteria,” *Journal of Physical Chemistry B* **111**, 6807 (2007)
26. **Seogjoo Jang** and Marshall D. Newton; “Closed form expressions of quantum electron transfer rate based on the stationary phase approximation,” *Journal of Physical Chemistry B* **110**, 18996 (2006)
25. **Seogjoo Jang**; “Path-integral centroid dynamics for general initial conditions: A nonequilibrium projection operator formulation,” *Journal of Chemical Physics* **124**, 064107 (2006)
24. **Seogjoo Jang** and Marshall D. Newton; “Theory of torsional non-Condon electron transfer: A generalized spin-boson Hamiltonian and its nonadiabatic limit solution,” *Journal of Chemical Physics* **122**, 024501 (2005)
23. Eitan Geva, **Seogjoo Jang**, and Gregory A. Voth; “Quantum Rate Theory: A Path Integral Centroid Perspective,” in *Encyclopedia of Materials Modeling: Vol. I, Fundamental Models and Methods*, S. Yip, Editor (Springer-Verlag, 2005)
22. **Seogjoo Jang**, Marshall D. Newton, and Robert J. Silbey; “Multichromophoric Förster resonance energy transfer,” *Physical Review Letters* **92**, 218301 (2004)
21. **Seogjoo Jang** and Robert J. Silbey; “Single complex line shapes of the B850 band of LH2,” *Journal of Chemical Physics* **118**, 9324 (2003)
20. **Seogjoo Jang** and Robert J. Silbey; “Theory of single molecule line shapes of multichromophoric macromolecules,” *Journal of Chemical Physics* **118**, 9312 (2003)
19. **Seogjoo Jang** and Jianshu Cao; “Optimal quantum control in dissipative environments : General formalism and perturbative limits,” in *Laser Control and Manipulation of Molecules (ACS Symposium Series)* **821**, 132 (2002)
18. **Seogjoo Jang**, Jianshu Cao, and Robert J. Silbey; “On the temperature dependence of molecular line shapes due to linearly coupled phonon bands,” *Journal of Physical Chemistry B* **106**, 8313 (2002)
17. **Seogjoo Jang**, Jianshu Cao, and Robert J. Silbey; “Fourth order quantum master equation and its Markovian bath limit,” *Journal of Chemical Physics* **116**, 2705 (2002); **117**, 10428 (2002)

16. **Seogjoo Jang**, Younjoon Jung, and Robert J. Silbey; “Nonequilibrium generalization of Förster-Dexter theory for excitation energy transfer,” *Chemical Physics* **275**, 319 (2002)
15. **Seogjoo Jang**, Soonmin Jang, and Gregory A. Voth; “Applications of higher order composite factorization schemes in imaginary time path integral simulations,” *Journal of Chemical Physics* **115**, 7832 (2001)
14. **Seogjoo Jang**, Sara E. Dempster, and Robert J. Silbey; “Characterization of the static disorder in the B850 band of LH2,” *Journal of Physical Chemistry B* **105**, 6655 (2001)
13. Sara E. Dempster, **Seogjoo Jang**, and Robert J. Silbey; “Single molecule spectroscopy of disordered circular aggregates: A perturbation analysis,” *Journal of Chemical Physics* **114**, 10015 (2001)
12. **Seogjoo Jang** and Jianshu Cao; “Nonadiabatic instanton calculation of multistate electron transfer reaction rate: Interference effects in three and four states systems,” *Journal of Chemical Physics* **114**, 9959 (2001)
11. David R. Reichman, Pierre-Nicholas Roy, **Seogjoo Jang**, and Gregory A. Voth; “A Feynman path centroid dynamics approach for the computation of time correlation functions involving nonlinear operators,” *Journal of Chemical Physics* **113**, 919 (2000)
10. **Seogjoo Jang** and Gregory A. Voth; “A relationship between centroid dynamics and path integral quantum transition state theory,” *Journal of Chemical Physics* **112**, 8747 (2000)
9. **Seogjoo Jang**, Charles D. Schwieters, and Gregory A. Voth; “A modification of path integral quantum transition state theory for asymmetric and metastable potentials,” *Journal of Physical Chemistry A* **103**, 9527 (1999)
8. Soonmin Jang, **Seogjoo Jang**, and Gregory A. Voth; “Quantum molecular dynamics simulations of low-temperature high energy density matter : Solid p – H₂/Li and p – H₂/B,” *Journal of Physical Chemistry A* **103**, 9512 (1999)
7. Pierre-Nicholas Roy, **Seogjoo Jang**, and Gregory A. Voth; “Feynman path centroid dynamics for Fermi-Dirac statistics,” *Journal of Chemical Physics* **111**, 5303 (1999)
6. **Seogjoo Jang** and Gregory A. Voth; “A derivation of centroid molecular dynamics and other approximate time evolution methods for path integral centroid variables,” *Journal of Chemical Physics* **111**, 2371 (1999)
5. **Seogjoo Jang** and Gregory A. Voth; “Path integral centroid variables and the formulation of their exact real time dynamics,” *Journal of Chemical Physics* **111**, 2357 (1999)
4. **Seogjoo Jang** and Gregory A. Voth; “Response to Comment on Simple reversible Molecular Dynamics algorithms for Nosé-Hoover chain dynamics,” *Journal of Chemical Physics* **110**, 3626 (1999)
3. **Seogjoo Jang** and Gregory A. Voth; “Lithium impurity recombination in solid *para*-hydrogen: A path integral quantum transition state theory study,” *Journal of Chemical Physics* **108**, 4098 (1998)
2. **Seogjoo Jang** and Gregory A. Voth; “Simple reversible Molecular Dynamics algorithms for Nosé-Hoover chain dynamics,” *Journal of Chemical Physics* **107**, 9514 (1997)

1. **Seogjoo Jang**, Kook Joe Shin, and Sangyoub Lee; “Effects of excitation migration and translational diffusion in the luminescence quenching dynamics,” *Journal of Chemical Physics* **102**, 815 (1995)