Roel Tempelaar

Curriculum Vitae, dated Dec 18, 2023

Department of Chemistry
Northwestern University
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Evanston, IL 60208

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PROFESSIONAL INTERESTS

Spin chemistry, spintronics, chirality, photosynthetic energy transfer, time-resolved spectroscopy, mixed quantum–classical dynamics, tensor network states

PROFESSIONAL APPOINTMENTS

Northwestern University
Assistant Professor, Department of Chemistry — 2020 – present

Columbia University
Rubicon Postdoctoral Fellow, Department of Chemistry — 2015 – 2019
Advisor: David Reichman

EDUCATION

University of Groningen (The Netherlands)
PhD in Chemistry — 2011 – 2015
Advisors: Jasper Knoester & Thomas La Cour Jansen
Cum Laude

MSc in Physics — 2009 – 2011
Advisors: Jasper Knoester & Frank Spano (Temple University)

BSc in Physics — 2004 – 2009

HONORS & AWARDS

CAREER Award, National Science Foundation	2022
Postdoctoral Fellow Award, Penn Conference in Theoretical Chemistry	2016
Rubicon Postdoctoral Grant, Netherlands Organisation for Scientific Research	2016
Doctoral Thesis Award, Koninklijk Natuurkundig Genootschap, The Netherlands	2016
PhD with Distinction *Cum Laude* (Highest Honor at University of Groningen)	2015
Huygens Fellow, Dutch Ministry of Education, Culture, & Science	2010

INVITED TALKS

Purdue University	December 2023
Max Planck Institute for Polymer Research, Department "Molecular Spectroscopy"	November 2023
Midwest/Great Lakes Regional Meeting, American Chemical Society	October 2023
Meeting of the American Chemical Society	August 2023
Princeton University	April 2023
Meeting of the American Chemical Society	March 2023
TU Munich International Seminar: *Electron and Phonon Dynamics in Soft Optoelectronic Materials*	September 2022
Telluride Meeting: *Condensed Phase Dynamics*	July 2022
Meeting of the American Chemical Society	March 2022
CECAM Workshop: *Exciton Dynamics in Functional Materials*	December 2021
Telluride Meeting: *Quantum Effects in Condensed-phase Systems*	June 2021
Telluride Meeting: *Spatiotemporal Dynamics of Excitons*	June 2021
UC San Diego, Polariton Webinar Series	March 2021
UC Berkeley, Pitzer Center Seminar	September 2020
Northwestern University	February 2019
Rutgers University	January 2019
Harvard University	January 2019
Flatiron Institute, Center for Computational Quantum Physics	January 2018
Meeting of the American Chemical Society	August 2016
Penn Conference in Theoretical Chemistry	August 2016

PUBLICATIONS

Preprints

- B. Kramar, A. Bondarenko, B. Diroll, X. Wang, K. Schanze, L. Chen, R. Tempelaar, J. Hupp Unexpected Photo-driven Linker-to-Node Hole Transfer in a Zirconium-Based Metal–Organic Framework
  ChemRxiv, doi: 10.26434/chemrxiv-2023-9mxxc (2023)

- T.-L. Chen, A. Salij, K. Parrish, J. Rasch, P. Brown, A. Dhavamani, F. Urraci, G. Pescitelli, L. A. Aronica, F. Zinna, M. S. Arnold, M. R. Wasielewski, L. Di Bari, R. Tempelaar, R. Goldsmith *A Chiral Microcavity based on Apparent Circular Dichroism*
  ChemRxiv, doi: 10.26434/chemrxiv-2023-bqnl7 (2023)

- A. Krotz and R. Tempelaar
  Treating geometric phase effects in nonadiabatic dynamics
  arXiv:2206.13539 (2022)

Published (Northwestern)

1. A. H. Salij, R. H. Goldsmith, and R. Tempelaar
   Theory predicts 2D chiral polaritons based on achiral Fabry–Pérot cavities using apparent circular dichroism
   Nat. Commun. (Accepted)

2. M.-H. Hsieh, A. Krotz, and R. Tempelaar
   Ehrenfest Modeling of Cavity Vacuum Fluctuations and How to Achieve Emission from a Three-Level Atom
   J. Chem. Phys. 159, 221104 (2023)
   Selected as a Communication

3. C. K. Terry Weatherly, J. Provazza, E. A. Weiss, and R. Tempelaar
   Theory predicts UV/vis-to-IR photonic down conversion mediated by excited state vibrational polaritons
   Nat. Commun. 14, 4804 (2023)

4. S. Kumar, I. S. Dunn, S. Deng, T. Zhu, Q. Zhao, O. F. Williams, R. Tempelaar, and L. Huang
   Exciton annihilation in molecular aggregates suppressed through quantum interference
   Nat. Chem. 15, 1118 (2023)

5. M.-H. Hsieh, A. Krotz, and R. Tempelaar
   A mean-field treatment of vacuum fluctuations in strong light-matter coupling
   J. Phys. Chem. Lett. 14, 1253 (2023)

6. A. Bondarenko and R. Tempelaar
   Overcoming positivity violations for density matrices in surface hopping
   J. Chem. Phys. 158, 054117 (2023)

7. J. Provazza and R. Tempelaar
   Perturbation theory under the truncated Wigner approximation reveals how system-environment entanglement formation drives quantum decoherence
   Phys. Rev. A 106, 042406 (2022)

8. F. Unger, L. Moretti, J. Hausch, J. Bredehoeft, C. Zeiser, S. Haug, R. Tempelaar, N. J. Hestand, G. Cerullo, and K. Broch
   Modulating singlet fission by scanning through vibronic resonances in pentacene-based blends
   J. Am. Chem. Soc. 144, 20610 (2022)

9. A. Krotz and R. Tempelaar
   A reciprocal-space formulation of surface hopping
   J. Chem. Phys. 156, 024105 (2022)
   Selected for Emerging Investigators Special Collection

10. A. Salij, R. H. Goldsmith, and R. Tempelaar
    Theory of apparent circular dichroism reveals the origin of inverted and noninverted chiroptical response under sample flipping
    J. Am. Chem. Soc. 143, 21519 (2021)

11. A. Salij and R. Tempelaar
    Microscopic theory of cavity-confined monolayer semiconductors: Polariton-induced valley relaxation and the prospect of enhancing and controlling valley pseudospin by chiral strong coupling
    Phys. Rev. B 103, 035431 (2021)

12. A. Krotz, J. Provazza, and R. Tempelaar
A reciprocal-space formulation of mixed quantum–classical dynamics
J. Chem. Phys. 154, 224101 (2021)

13. J. Provazza, R. Tempelaar, and D. F. Coker
Analytic and numerical vibronic spectra from quasi-classical trajectory ensembles
J. Chem. Phys. 155, 014108 (2021)

14. C. Zeiser, C. Cruz, D. R. Reichman, M. Seitz, J. Hagenlocher, E. L. Chronister, C. J. Bardeen, R. Tempelaar, and K. Broch
Vacancy control in acene blends links exothermic singlet fission to coherence
Nat. Commun. 12, 5149 (2021)

15. J. Cao, R. J. Cogdell, D. F. Coker, H.-G. Duan, J. Hauer, U. Kleinekathöfer, T. L. C. Jansen, T. Mančal, R. J. D. Miller, J. P. Ogilvie, V. I. Prokhorenko, T. Renger, H.-S. Tan, R. Tempelaar, M. Thorwart, E. Thyrhaug, S. Westenhoff, and D. Zigmantas
Quantum biology revisited
Sci. Adv. 6, eaaz4888 (2020)

16. I. Schlesinger, N. E. Powers-Riggs, J. L. Logsdon, Y. Qi, S. A. Miller, R. Tempelaar, R. M. Young, and M. R. Wasielewski
Charge-transfer biexciton annihilation in a donor–acceptor co-crystal yields high-energy long-lived charge carriers
Chem. Sci. 11, 9532 (2020)

Published (before Northwestern)

17. B. Kloss, D. R. Reichman, and R. Tempelaar
Multiset matrix product state calculations reveal mobile Franck-Condon excitations under strong Holstein-type coupling
Phys. Rev. Lett. 123, 126601 (2019)

18. R. Tempelaar and T. C. Berkelbach
Many-body simulation of two-dimensional electronic spectroscopy of excitons and trions in monolayer transition metal dichalcogenides
Nat. Commun. 10, 3419 (2019)

19. I. S. Dunn, R. Tempelaar, and D. R. Reichman
Removing instabilities in the hierarchical equations of motion: Exact and approximate projection approaches
J. Chem. Phys. 150, 184109 (2019)

20. A. Oleson, T. Zhu, I. S. Dunn, D. Bialas, Y. Bai, W. Zhang, M. Dai, D. R. Reichman, R. Tempelaar, L. Huang, and F. C. Spano
Perylene diimide-based Hj-and hJ-aggregates: the prospect of exciton band shape engineering in organic materials
J. Phys. Chem. C 123, 20567 (2019)

21. R. Tempelaar and D. R. Reichman
Generalization of fewest-switches surface hopping for coherences
J. Chem. Phys. 148, 102309 (2018)

Selected as Editor's Pick

22. R. Tempelaar and D. R. Reichman
Vibronic exciton theory of singlet fission. III. How vibronic coupling and thermodynamics promote rapid triplet generation in pentacene crystals
J. Chem. Phys. 148, 244701 (2018)

Selected as Editor's Pick

23. E. Thyrhaug, R. Tempelaar, M. J. P. Alcocer, K. Žídek, D. Bína, J. Knoester, T. L. C. Jansen, and D. Zigmantas
Identification and characterization of diverse coherences in the Fenna–Matthews–Olson complex
Nat. Chem. 10, 780 (2018)

24. R. Tempelaar and D. R. Reichman
Vibronic exciton theory of singlet fission. II. Two-dimensional spectroscopic detection of the correlated triplet pair state
J. Chem. Phys. 146, 174704 (2017)

25. R. Tempelaar and D. R. Reichman
Vibronic exciton theory of singlet fission. I. Linear absorption and the anatomy of the correlated triplet pair state
J. Chem. Phys. 146, 174703 (2017)

26. R. Tempelaar, T. L. C. Jansen, and J. Knoester
Exciton–exciton annihilation is coherently suppressed in H-Aggregates, but not in J-aggregates
J. Phys. Chem. Lett. 8, 6113 (2017)

27. I. Breen, R. Tempelaar, L. A. Bizimana, B. Kloss, D. R. Reichman, and D. B. Turner
Triplet separation drives singlet fission after femtosecond correlated triplet pair production in rubrene
J. Am. Chem. Soc. 139, 11745 (2017)

28. R. Tempelaar, A. Halpin, P. J. M. Johnson, J. Cai, R. S. Murphy, J. Knoester, R. J. D. Miller, and T. L. C. Jansen
Laser-limited signatures of quantum coherence
J. Phys. Chem. A 120, 3042 (2016)

29. R. Tempelaar, L. J. A. Koster, R. W. A. Havenith, J. Knoester, and T. L. C. Jansen
Charge recombination suppressed by destructive quantum interference in heterojunction materials
J. Phys. Chem. Lett. 7, 198 (2016)

30. N. J. Hestand, R. Tempelaar, J. Knoester, T. L. C. Jansen, and F. C. Spano
Exciton mobility control through sub-Å packing modifications in molecular crystals
Phys. Rev. B 91, 195315 (2015)

31. A. Halpin, P. J. M. Johnson, R. Tempelaar, R. S. Murphy, J. Knoester, T. L. C. Jansen, and R. J. D. Miller
Two-dimensional spectroscopy of a molecular dimer unveils the effects of vibronic coupling on exciton coherences
Nat. Chem. 6, 196 (2014)

Featured as News & Views

32. R. Tempelaar, F. C. Spano, J. Knoester, and T. L. C. Jansen
Mapping the evolution of spatial exciton coherence through time-resolved fluorescence
J. Phys. Chem. Lett. 5, 1505 (2014)

33. R. Tempelaar, T. L. C. Jansen, and J. Knoester
Vibrational beatings conceal evidence of electronic coherence in the FMO light-harvesting complex
J. Phys. Chem. B 118, 12865 (2014)

34. R. Tempelaar, A. Stradomska, J. Knoester, and F. C. Spano
Anatomy of an exciton: Vibrational distortion and exciton coherence in H-and J-aggregates
J. Phys. Chem. B 117, 457 (2013)

35. R. Tempelaar, C. P. Van Der Vegte, J. Knoester, and T. L. C. Jansen
Surface hopping modeling of two-dimensional spectra
J. Chem. Phys. 138, 164106 (2013)

Selected as Editor's Pick

36. R. Tempelaar, A. Stradomska, J. Knoester, and F. C. Spano
Circularly polarized luminescence as a probe for long-range interactions in molecular aggregates
J. Phys. Chem. B 115, 10592 (2011)

RESEARCH SUPPORT

Current

Title: CAREER – Investigating Strong Electron-Phonon Interactions in Semiconducting Crystals Using Reciprocal-Space Quantum-Classical Modeling
Source: National Science Foundation
Role: PI
Amount: $601,980
Dates: April 1, 2022 – March 31, 2027

Title: Organic–Inorganic Nanostructure Design through Strong Light–Matter Coupling
Source: The International Institute for Nanotechnology
Role: Seed investigator
Amount: $97,374
Dates: September 1, 2023 – August 31, 2024

Title: EFRC – Center for Molecular Quantum Transduction
Source: Department of Energy
Role: Co-I (PI: Michael Wasielewski)
Amount: $12,400,000 / 15 investigators
Dates: September 1, 2020 – August 31, 2024

Title: NU-MRSEC
Source: National Science Foundation
Role: Seed investigator
Amount: 36 student months
Dates: December 1, 2021 – February 29, 2024

Completed

Title: High-mobility metal-organic frameworks through quantum design

Source: The International Institute for Nanotechnology
Role: Seed investigator
Amount: $110,000
Dates: February 1, 2021 – January 31, 2022

AFFILIATIONS

Investigator, Center for Molecular Quantum Transduction	2020 – present
Member, International Institute for Nanotechnology	2021 – present
Seed investigator, NU Materials Research Science and Engineering Center	2021 – present

TEACHING

CHEM 172: Accelerated General Physical Chemistry (undergraduate)

146 students, 4.16/6.00 course rating, 4.36/6.00 instructor rating	2023
123 students, 3.42/6.00 course rating, 3.48/6.00 instructor rating	2022

CHEM 442-1: Quantum Chemistry (graduate, curriculum revision)

24 students, 5.06/6.00 course rating, 5.50/6.00 instructor rating	2022
15 students, 5.18/6.00 course rating, 5.36/6.00 instructor rating	2021
10 students, 5.00/6.00 course rating, 5.50/6.00 instructor rating	2020

CHEM 448: Computational Chemistry (graduate, new curriculum development)

13 students, 5.00/6.00 course rating, 5.56/6.00 instructor rating	2021

ADVISING

PhD Students
Andrew Salij (2019 – present), Alex Krotz (2020 – present), Connor Terry Weatherly (2020 – present), Ming-Hsiu Hsieh (2021 – present), Chientzu Lin (2022 – present), Luis Sierra Ossa (2023 – present), Kyle Kairys (2023 – present)

Postdoctoral Scholars
Anna Bondarenko (2020 – present), Justin Provazza (2021 – 2022, currently at QSimulate), Antonio Garzon Ramirez (2023 – present), Ken Miyazaki (2023 – present)

UNIVERSITY SERVICE

Graduate admissions committee	2020 – present
General chemistry committee	2021 – present
Qualifying exam committee (12 graduate students)	2020 – present
Dissertation committee (4 students)	2021 – present
Teaching faculty search committee	2022
Teaching faculty search committee	2021

EXTERNAL SERVICE

Member, Early Career Advisory Board, Chemical Reviews — 2023 – present

Journal Reviewer
Peer reviewer for Nature Chemistry, Nature Communications, Proceedings of the National Academy of Sciences of the USA, Chemical Reviews, The Journal of the American Chemical Society, The Journal of Chemical Theory and Computation, ACS Omega, The Journal of Physical Chemistry, and The Journal of Chemical Physics — 2016 – present

Proposal Reviewer
Ad hoc reviewer for the National Science Foundation the Department of Energy, the American Chemical Society, the Swiss National Science Foundation — 2020 – present

Organizer
Chair, Organizing Committee Symposium on Information Science, Groningen, The Netherlands — 2009

OUTREACH

NSF-CAREER educational component (design phase) — 2022 - present

Addressing code illiteracy among economically-disadvantaged highschoolers in the Chicago area through developing/executing a smartphone-based programming course