

# Roel Tempelaar

Curriculum Vitae, dated October 16, 2024

Department of Chemistry  
Northwestern University  
2145 Sheridan Road  
Evanston, IL 60208

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## PROFESSIONAL INTERESTS

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Quantum materials, spintronics, spin chemistry, chirality, strong light-matter coupling, time-resolved spectroscopy, mixed quantum-classical dynamics, tensor network states

## PROFESSIONAL APPOINTMENTS

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### Northwestern University

Assistant Professor, Department of Chemistry 2020 – present

### Columbia University

Rubicon Postdoctoral Fellow, Department of Chemistry 2015 – 2019  
*Advisor: David Reichman*

## EDUCATION

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### 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

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Cadence/OpenEye Outstanding Junior Faculty Award, ACS COMP Division 2024  
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

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University of Chicago, Center for Theoretical Chemistry October 2024  
Stanford University, Department of Chemistry September 2024  
Columbia University, Department of Chemistry September 2024  
Meeting of the American Chemical Society August 2024  
Gordon Research Conference: *Electron Donor-Acceptor Interactions* July 2024  
Telluride Meeting: *Condensed Phase Dynamics* July 2024  
Telluride Meeting: *Spatiotemporal Dynamics of Excitons* June 2024  
Cornell University, Department of Materials Science & Engineering April 2024  
Purdue University, Department of Chemistry 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, Department of Chemistry 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, Department of Chemistry February 2019  
Rutgers University, Department of Chemistry January 2019  
Harvard University, Department of Chemistry 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

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### Preprints

- K. A. Parrish, A. Salij, K. R. Kamp, M. I. B. Utama, E. Smith, M. C. Hersam, K. R. Poepfelmeier, R. H. Goldsmith, and R. Tempelaar  
*Differential Absorption of Circularly Polarized Light by a Centrosymmetric Inorganic Crystal*  
*ChemRxiv*: doi: 10.26434/chemrxiv-2024-hj1fl (2024)

- B. Kramar, A. Bondarenko, B. Diroll, X. Wang, K. Schanze, L. Chen, R. Tempelaar, and 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)

### Published (Northwestern)

1. A. Krotz and R. Tempelaar  
*Mixed quantum-classical modeling of exciton-phonon scattering in solids: Application to optical linewidths of monolayer MoS<sub>2</sub>*  
*J. Chem. Phys.* 161, 044117 (2024)
2. W. J. Chang, H. Zheng, C. Terry Weatherly, J. Provazza, P. Liu, E. Weiss, N. Stern, and R. Tempelaar  
*Dark State Concentration Dependent Emission and Dynamics of CdSe Nanoplatelet Exciton-Polaritons*  
*ACS Nano* 18, 20226 (2024)
3. K. Miyazaki, A. Krotz, and R. Tempelaar  
*Mixed Quantum–Classical Dynamics Under Arbitrary Unitary Basis Transformations*  
*J. Chem. Theory Comput.* 20, 6500 (2024)  

Featured as an ACS Editors' Choice
4. R. Tempelaar  
*Topological Materials Go Meta*  
*Chem. Rev.* 124, 7536 (2024)
5. 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, and R. Goldsmith  
*A 2D chiral microcavity based on apparent circular dichroism*  
*Nat. Commun.* 15, 3072 (2024)
6. A. Krotz and R. Tempelaar  
*Treating geometric phase effects in nonadiabatic dynamics*  
*Phys. Rev. A* 109, 032210 (2024)
7. 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.* 15, 340 (2024)
8. 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
9. 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)

10. 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)
  11. 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)
  12. A. Bondarenko and R. Tempelaar  
*Overcoming positivity violations for density matrices in surface hopping*  
**J. Chem. Phys.** 158, 054117 (2023)
  13. 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)
  14. 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)
  15. A. Krotz and R. Tempelaar  
*A reciprocal-space formulation of surface hopping*  
**J. Chem. Phys.** 156, 024105 (2022)
- Selected for Emerging Investigators Special Collection**
16. 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)
  17. 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)
  18. A. Krotz, J. Provazza, and R. Tempelaar  
*A reciprocal-space formulation of mixed quantum-classical dynamics*  
**J. Chem. Phys.** 154, 224101 (2021)
  19. J. Provazza, R. Tempelaar, and D. F. Coker  
*Analytic and numerical vibronic spectra from quasi-classical trajectory ensembles*  
**J. Chem. Phys.** 155, 014108 (2021)
  20. 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)
  21. 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. Thyryhaug, S. Westenhoff, and D. Zigmantas  
*Quantum biology revisited*  
**Sci. Adv.** 6, eaaz4888 (2020)

22. 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)**

23. 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)
24. 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)
25. 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)
26. 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 H<sub>j</sub>- and h<sub>J</sub>-aggregates: the prospect of exciton band shape engineering in organic materials*  
*J. Phys. Chem. C* 123, 20567 (2019)
27. 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**
28. 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**
29. E. Thyryhaug, R. Tempelaar, M. J. P. Alcocer, K. Židek, 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)
30. 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)
31. 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)

32. 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)
33. 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)
34. 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)
35. 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)
36. 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)
37. 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

38. 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)
39. 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)
40. 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)
41. 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

42. 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

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### Current

*Title:* EFRC – Center for Molecular Quantum Transduction  
*Source:* Department of Energy  
*Role:* Co-I (PI: Michael Wasielewski)  
*Amount:* \$14,500,000 / 15 investigators  
*Dates:* August 1, 2024 – July 31, 2028

*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:* International Institute for Nanotechnology  
*Role:* Seed investigator  
*Amount:* \$195,000  
*Dates:* September 1, 2023 – August 31, 2024

### Completed

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

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

*Title:* High-mobility metal-organic frameworks through quantum design  
*Source:* International Institute for Nanotechnology  
*Role:* Seed investigator  
*Amount:* \$110,000  
*Dates:* February 1, 2021 – January 31, 2022

## AFFILIATIONS

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Faculty Affiliate, Paula M. Trienens Institute for Sustainability & Energy	2024 – present
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 – 2024

## TEACHING

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CHEM 172: Accelerated General Physical Chemistry (undergraduate)  
162 students, 4.26/6.00 course rating, 4.54/6.00 instructor rating 2024  
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

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### Postdoctoral Scholars

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

### Graduate Students

Andrew Salij (2019 – 2024), 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)

### Undergraduate Students

Ethan Byrd (2024 – present)

## UNIVERSITY SERVICE

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Graduate admissions committee 2020 – present  
General chemistry committee 2021 – present  
Teaching faculty search committee 2022  
Teaching faculty search committee 2021

### **Dissertation Committee**

Samantha Harvey (2021), Shawn Irgen-Giorgio (2021), Jonathan Schultz (2022), Alanna Felts (2023), Chelsea Mueller (2023), Jana Butman (2023), Ray Fu (2023), Paige Brown (2024), Eric Qian (2024)

### **Qualifying Exam Committee**

Ray Fu (2020), Jana Butman (2020), Alanna Felts (2020), Dillon Edwards (2020), Geyao Gu (2021), Jonah Greenberg (2021), Maya Pathuri (2022), Chelsie Greene (2022), Jonathan Palmer (2023), Zachery Mast (2023), Tse-Min Chiang (2023), Nathan Sinai (2024), Georgia Mantel (2024), Cathryn Murphy (2024), Kathryn Peinkofer (2024)

### **Prospectus Exam Committee (Physics Department)**

Ethan Garvey (2024)

## **EXTERNAL SERVICE**

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

### **Journal Reviewer**

Peer reviewer for Nature Chemistry, Nature Communications, Communications Physics, Proceedings of the National Academy of Sciences of the USA, Chemical Reviews, The Journal of the American Chemical Society, Chirality, Chemistry of Materials, Nano Letters, The Journal of Chemical Theory and Computation, ACS Omega, Physical Chemistry Chemical Physics, 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**

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NSF-CAREER educational component (design phase) 2022 - present  
*Addressing code illiteracy among economically-disadvantaged highschool students in the Chicago area by developing/executing a smartphone-based programming course*