

# D. Vale Cofer-Shabica, Ph.D.

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## APPOINTMENTS

**Postdoctoral Researcher** Princeton University, Princeton, NJ, 2024–*Present*  
**Postdoctoral Researcher** University of Pennsylvania, Philadelphia, PA, 2019–2024  
**Director of Education** Banneker Institute, Harvard University, Cambridge, MA, 2019

## EDUCATION & TRAINING

**Ph.D. Theoretical Physical Chemistry** Brown University, Providence, RI, 2018  
**Certificate in Reflective Teaching** Brown University, Providence, RI, 2014  
**Sc.B. Chemical Physics** Brown University, Providence, RI, 2009

## SELECTED HONORS & AWARDS

**William R. Potter Prize for Doctoral Thesis of Outstanding Merit** 2018  
Brown University Department of Chemistry award for best dissertation

**2017 Editors' Choice article: Cofer-Shabica and Stratt [2017]** 2018  
*Journal of Chemical Physics* selection of the most innovative and influential articles of the year

**Elaine Chase Award for Leadership and Service** 2017  
Brown University Department of Chemistry award for outstanding student leadership

**William T. King Prize for Teaching Excellence** 2014  
Brown University Department of Chemistry award for best graduate teaching assistant

**Research Matters Speaker, Brown University's 250th anniversary** 2014  
Selected in University-wide competition for best graduate student talk for general audiences

**Teaching Fellowship** 2013, 2014, 2015  
Brown University Department of Chemistry competitive award for excellence in teaching

**Karen T. Romer Undergraduate Teaching and Research Award** 2008  
Brown University competitive award to fund undergraduate research

**Eagle Scout** 2004  
Boy Scouts of America rank for distinguished leadership and service

## PUBLICATIONS

Alec J. Coffman, Zuxin Jin, Junhan Chen, Joseph E Subotnik, and **D. Vale Cofer-Shabica**. On the use of QM/MM surface hopping simulations to understand thermally-activated rare event nonadiabatic transitions in the condensed phase. *Journal of Chemical Theory and Computation*, 2023. doi:10.1021/acs.jctc.3c00276.

Maximilian Menger, Yihan Shao, Ou Qi, Shirin Faraji, Joseph Subotnik, and **D. Vale Cofer-Shabica**. On the nature of hops, coordinates, and detailed balance for nonadiabatic simulations in the condensed phase. *Journal of Physical Chemistry A*, 2023. doi:10.1021/acs.jpca.3c03546.

**D. Vale Cofer-Shabica**, Vishikh Athavale, and Joseph E. Subotnik. To guess or not to guess excited state amplitudes during optimization and dynamics. *The Journal of Chemical Physics*, 159(12): 121101, 09 2023. doi:10.1063/5.0163571.

Jagna Witek, Joseph P. Heindel, Xingyi Guan, Itai Leven, Hongxia Hao, Pavithra Naullage, Allen LaCour, Selim Sami, M.F.S.J. Menger, **D. Vale Cofer-Shabica**, Shirin Faraji, Evgeny Epifanovsky, and Teresa Head-Gordon. M-chem: a modular software package for molecular simulation that spans scientific domains. *Molecular Physics*, 121(9-10):e2129500, 2023. doi:10.1080/00268976.2022.2129500.

**D. Vale Cofer-Shabica**, Maximilian F. S. J. Menger, Qi Ou, Yihan Shao, Joseph E. Subotnik, and Shirin Faraji. INAQS, a generic interface for nonadiabatic QM/MM dynamics: Design, implementation, and validation for GROMACS/Q-CHEM simulations. *Journal of Chemical Theory and Computation*, 18(8):4601–4614, 2022. doi:10.1021/acs.jctc.2c00204.

Hsing-Ta Chen, Junhan Chen, **D. Vale Cofer-Shabica**, Zeyu Zhou, Vishikh Athavale, Gregory Medders, Maximilian F. S. J. Menger, Joseph E. Subotnik, and Zuxin Jin. Methods to calculate electronic excited-state dynamics for molecules on large metal clusters with many states: Ensuring fast overlap calculations and a robust choice of phase. *Journal of Chemical Theory and Computation*, 18(6):3296–3307, 2022. doi:10.1021/acs.jctc.1c01304.

Evgeny Epifanovsky, . . . , **Vale Cofer-Shabica**, . . . , and Anna I. Krylov. Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *The Journal of Chemical Physics*, 155(8):084801, 2021. doi:10.1063/5.0055522.

**D. Vale Cofer-Shabica** and Richard M. Stratt. What is special about how roaming chemical reactions traverse their potential surfaces? Differences in geodesic paths between roaming and non-roaming events. *The Journal of Chemical Physics*, 146(21):214303, 2017. doi:10.1063/1.4984617.

J. M. Budarz, M. P. Minitti, **D. V. Cofer-Shabica**, B. Stankus, A. Kirrander, J. B. Hastings, and P. M. Weber. Observation of femtosecond molecular dynamics via pump-probe gas phase x-ray scattering. *Journal of Physics B: Atomic Molecular and Optical Physics*, 49(3), 2016. doi:10.1088/0953-4075/49/3/034001.

Michael P. Minitti, James M. Budarz, Adam Kirrander, Joseph Robinson, Thomas J. Lane, Daniel Ratner, Kenichiro Saita, Thomas Northey, Brian Stankus, **Vale Cofer-Shabica**, Jerome Hastings, and Peter M. Weber. Toward structural femtosecond chemical dynamics: Imaging chemistry in space and time. *Faraday Discussions*, 171:81–91, 2014. doi:10.1039/c4fd00030g.

## TALKS & POSTERS

|   |                |
|---|----------------|
| University of Pittsburgh, Pittsburgh, Pennsylvania. <b>Invited.</b> | January 2024.  |
| Texas A&M University, College Station, Texas. <b>Invited.</b>       | January 2024.  |
| Colorado School of Mines, Golden Colorado. <b>Invited.</b>          | December 2023. |
| ACS National Meeting, San Francisco, CA.                            | August 2023.   |

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| Photochemistry Gordon Conference, Lewiston, ME. poster.                            | July, 2023.     |
| ACS Northeastern Regional Meeting, Boston, MA.                                     | June 2023.      |
| University of Jyväskylä, Jyväskylä, Finland. <b>Invited.</b>                       | April 2023.     |
| Donor Acceptor Interactions Gordon Conference, Newport, RI. poster.                | July, 2022.     |
| Q-Chem Inc., Developer Workshop.   | May 2021.       |
| Q-Chem Inc., Webinar. <b>Invited.</b>  | November 2020.  |
| University of Oklahoma, Norman, OK. <b>Invited.</b>                                | February 2020.  |
| University of Jyväskylä, Jyväskylä, Finland. <b>Invited.</b>                       | December 2019.  |
| University of Groningen, Groningen, The Netherlands. <b>Invited.</b>               | December 2019.  |
| Warren Wilson College, Asheville, NC. <b>Invited.</b>                              | February 2019.  |
| Brown University, Providence, RI. Physical Chemistry Tea Session.                  | March 2017.     |
| Brown University, Providence, RI. Physical Chemistry Tea Session.                  | February 2016.  |
| American Chemical Society, Boston, MA. PHYS 554 poster.                            | August, 2015.   |
| Brown University, Providence, RI. Physical Chemistry Tea Session.                  | January 2015.   |
| Brown University, Providence, RI. Research Matters, <b>Invited.</b>                | September 2014. |
| Brown University, Providence, RI. Physical Chemistry Tea Session.                  | December 2013.  |
| Academic Magnet High School, Charleston, SC. Commencement Address, <b>Invited.</b> | May 2010.       |

## TEACHING

|  |                     |
|--|---------------------|
| <b>Banneker Institute, Harvard/Smithsonian Center for Astrophysics</b> | Cambridge, MA       |
| Instructor: <i>Social Justice in Science and the World</i>             | 2019                |
| Instructor: <i>How to think about programming for astrophysicists</i>  | 2018, 2019          |
| <b>Brown University Department of Chemistry</b>                        | Providence, RI      |
| Problem Session Facilitator: <i>Equilibrium, Rate, and Structure</i>   | 2014, 2015          |
| Problem Session Facilitator: <i>Introductory Chemistry</i>             | 2013, 2014          |
| Tutorial Assistant: <i>Equilibrium, Rate, and Structure</i>            | 2013                |
| Laboratory Teaching Assistant: <i>Equilibrium, Rate, and Structure</i> | 2012                |
| <b>Blackstone Academy Charter School</b>                               | Pawtucket, RI       |
| High School Math Teacher: <i>Calculus, Pre-calculus, Statistics</i>    | 2010–2011           |
| <b>The Metropolitan Regional Career and Technical Center</b>           | Providence, RI      |
| High School Math Teacher: <i>Algebra, Arithmetic</i>                   | 2009–2010           |
| <b>Kaplan Tutoring Services Inc.</b>                                   | Barrington, RI      |
| Science, Math, & Language Tutor  | 2008–2019           |
| <b>Camp Ho Non Wah, BSA</b>  | Wadmalaw Island, SC |
| Various positions including Program Director                           | 2001–2006           |

## TRAINEES MENTORED

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|--|----------------------|
| <b>Titouan Duston</b> (UPenn), First-year graduate student | 2023                 |
| <b>Vishikh Athavale</b> (UPenn), Graduate student          | 2022– <i>present</i> |

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| <b>Alec Coffman</b> (UPenn), Graduate student (now postdoc), 2 joint publications | 2020– <i>present</i> |
| <b>Jenn Derosa</b> (UPenn), Graduate student                                      | 2020– <i>present</i> |
| <b>Natasa Rohacs</b> (UPenn), Undergraduate summer researcher                     | 2020                 |
| <b>Layne Frechette</b> (Brown), Undergraduate, 2 years with group                 | 2013–2015            |

## SERVICE

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| <b>CSSM Trainee Advisory Board</b>                                       | 2021–2023 |
| Center for Sustainable Separation of Metals , University of Pennsylvania |           |
| <b>Inclusive Teaching Workshops</b>                                      | 2018      |
| Department of Physics, Brown University                                  |           |
| <b>Diversity and Inclusion Action Committee</b>                          | 2016–2018 |
| Department of Chemistry, Brown University                                |           |
| <b>WE Teach STEM Discussion Group</b>                                    | 2015–2018 |
| Teaching for and/or as women in STEM fields, Brown University            |           |
| <b>Stand Up for Graduate Student Employees</b>                           | 2013–2017 |
| Graduate student union organizer, Brown University                       |           |
| <b>Exhibition Night Judge</b>  | 2013–2019 |
| Blackstone Academy High School, Pawtucket, RI                            |           |
| <b>Graduate Student Recruitment</b>                                      | 2012–2017 |
| Department of Chemistry, Brown University                                |           |

## AFFILIATIONS

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|--------------------------------------|----------------------|
| <i>American Physical Society</i>     | 2018– <i>Present</i> |
| <i>Union of Concerned Scientists</i> | 2018– <i>Present</i> |
| <i>American Chemical Society</i>     | 2015– <i>Present</i> |