

# Professor Shervin Fatehi

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Department of Chemistry  
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## EDUCATION

PhD, University of California, Berkeley, 2010  
Major: Chemistry  
Dissertation Title: Excursions in Chemical Dynamics

Other, SB, Massachusetts Institute of Technology, 2004  
Major: Chemistry

## EMPLOYMENT

Assistant Professor, University of Texas Rio Grande Valley (August 2015)

Postdoctoral Fellow, University of Utah (September 1, 2013 - July 31, 2015)

Postdoctoral Researcher, University of Pennsylvania (January 5, 2011 - July 31, 2013)

## PUBLICATIONS

### Journal Articles

Yihan Shao, Zhengting Gan, Evgeny Epifanovsky, Andrew Gilbert, Michael Wormit, Joerg Kussmann, Shervin Fatehi, Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*. 113, no. 2 (2015): 184–215.

Shervin Fatehi and Ryan Steele. Multiple-Time Step Ab Initio Molecular Dynamics Based on Two-Electron Integral Screening. *Journal of Chemical Theory and Computation*. 11, no. 3 (2015): 884–898.

Joseph Subotnik, Ethan Alguire, Qi Ou, Brian Landry, and Shervin Fatehi. The Requisite Electronic Structure Theory To Describe Photoexcited Nonadiabatic Dynamics: Nonadiabatic Derivative Couplings and Diabatic Electronic Couplings. *Accounts of chemical research*. (2015)

Ethan Alguire, Shervin Fatehi, Yihan Shao, and Joseph Subotnik. Analysis of localized diabatic states beyond the Condon approximation for excitation energy transfer processes. *The Journal of Physical Chemistry A*. 118, no. 51 (2014): 11891–11900.

Qi Ou, Shervin Fatehi, Ethan Alguire, Yihan Shao, and Joseph Subotnik. Derivative couplings between TDDFT excited states obtained by direct differentiation in the Tamm-Dancoff approximation. *The Journal of chemical physics*. 141, no. 2 (2014): 024114.

Qi Ou, Shervin Fatehi, Ethan Alguire, Yihan Shao, and Joseph Subotnik. Publisher's Note: "Derivative couplings between TDDFT excited states obtained by direct differentiation in the Tamm-Dancoff approximation" [J. Chem. Phys. 141, 024114 (2014)]. *The Journal of chemical physics*. 141, no. 6 (2014): 069903.

Shervin Fatehi, Ethan Alguire, and Joseph Subotnik. Derivative couplings and analytic gradients for diabatic states, with an implementation for Boys-localized configuration-interaction singles. *The Journal of chemical physics*. 139, no. 12 (2013): 124112.

Xinle Liu, Shervin Fatehi, Yihan Shao, Brad Veldkamp, and Joseph Subotnik. Communication: Adjusting charge transfer state energies for configuration interaction singles: Without any parameterization and with minimal cost. *The Journal of chemical physics*. 136, no. 16 (2012): 161101.

Shervin Fatehi and Joseph Subotnik. Derivative couplings with built-in electron-translation factors: Application to benzene. *The Journal of Physical Chemistry Letters*. 3, no. 15 (2012): 2039–2043.

Shervin Fatehi, Ethan Alguire, Yihan Shao, and Joseph Subotnik. Analytic derivative couplings between configuration-interaction-singles states with built-in electron-translation factors for translational invariance. *The Journal of chemical physics*. 135, no. 23 (2011): 234105.

Craig Schwartz, Shervin Fatehi, Richard Saykally, and David Prendergast. Importance of electronic relaxation for inter-Coulombic decay in aqueous systems. *Physical review letters*. 105, no. 19 (2010): 198102.

Shervin Fatehi, Craig Schwartz, Richard Saykally, and David Prendergast. Nuclear quantum effects in the structure and lineshapes of the N<sub>2</sub> near-edge x-ray absorption fine structure spectrum. *The Journal of chemical physics*. 132, no. 9 (2010): 094302.

## Other

Shervin Fatehi. Excursions in Chemical Dynamics. (2010)

## Media Contributions

### Newspaper

Valley Morning Star. (May 03, 2017)

The Chronicle of Higher Education. (April 09, 2017)

Valley Morning Star. (April 06, 2016)

## PRESENTATIONS

Michael Carrillo, Shervin Fatehi, and Wei Lin. "Theoretical and Experimental Study of Cyclobutanecarboxylic Acid." UTRGV College of Sciences Student Conference, Edinburg, TX. (March 31, 2019)

Shervin Fatehi. "Toward a complete framework for non adiabatic dynamics with full configuration interaction," 73rd American Chemical Society Southwest Regional Meeting, American Chemical Society, Lubbock, TX. (October 30, 2017)

Shervin Fatehi. "Qualitative criteria and screening strategies for intermolecular Coulombic decay in solution," 72nd American Chemical Society Southwest Regional Meeting, American Chemical Society, Galveston, TX. (November 10, 2016)

Shervin Fatehi. "Qualitative criteria for energy transfer in solution," 24th Gordon Research Conference on Electron Donor–Acceptor Interactions, Gordon Research Conferences, Newport, RI. (August 8, 2016)

Shervin Fatehi. "Qualitative criteria for energy transfer in solution," 9th Congress of the International Society for Theoretical Chemical Physics, International Society for Theoretical Chemical Physics, Grand Forks, ND. (July 19, 2016)

Shervin Fatehi. "Qualitative criteria for energy transfer in solution," 1st Gordon Research Conference on Molecular Interactions & Dynamics, Gordon Research Conferences, Easton, MA. (July 12, 2016)

Shervin Fatehi. "Chemistry beyond Born–Oppenheimer and targeted energy transfer," Chemistry Department Seminar, The University of Texas Rio Grande Valley, Edinburg, TX. (May 11, 2015)

Shervin Fatehi. "Unusual physical principles for designing new materials and therapies," Chemistry Department Seminar, Jackson State University, Jackson, MS. (April 23, 2015)

Shervin Fatehi. "Chemistry beyond Born–Oppenheimer: Energy transfer in large molecules," Chemistry Department Seminar, Hofstra University, Hempstead, NY. (February 25, 2015)

Shervin Fatehi. "Multiple-timestep ab initio molecular dynamics: Correlation, screening, and beyond," Institute of High Performance Computing Seminar, Agency for Science, Technology, and Research, Singapore. (February 6, 2015)

Shervin Fatehi. "Beyond Born–Oppenheimer: The chemistry of electrons and nuclei moving together," Chemistry Department Seminar, William Paterson University, Wayne, NJ. (January 30, 2015)

Shervin Fatehi. "Inhibitory mechanisms in enzyme kinetics; a new approach to cancer treatment," Biology, Chemistry & Physics, and Mathematica Department Seminar, Northern State University, Aberdeen, SD. (January 22, 2015)

Shervin Fatehi. "Window screening and multiple-timestep ab initio molecular dynamics in Q-Chem," Q-Chem Developers' Meeting, Q-Chem, Inc., Berkeley, CA. (August 15, 2014)

Shervin Fatehi. "Multiple-timestep integration methods for ab initio molecular dynamics," 248th American Chemical Society National Meeting, American Chemical Society, San Francisco, CA. (August 10, 2014)

Shervin Fatehi. "Beyond critical points: Ab initio dynamics and sampling in Q-Chem," Q-Chem Webinar Series, Q-Chem, Inc., (February 19, 2014)

Shervin Fatehi. "Comprehensive analytic-gradient theory for localized-diabetic CIS states," 246th American Chemical Society National Meeting, American Chemical Society, Indianapolis, IN. (September 11, 2013)

Shervin Fatehi. "Qualitative criteria correctly predict targeted energy transfer in solution," 246th American Chemical Society National Meeting, American Chemical Society, Indianapolis, IN. (September 11, 2013)

Shervin Fatehi. "Targeted energy transfer: A new approach to cancer treatment," Chemistry Department Seminar, University of Tulsa, Tulsa, OK. (March 14, 2013)

Shervin Fatehi. "Derivative couplings made more physical—and cheaper," 4th New York Theoretical and Computational Chemistry Conference, City University of New York, New York, NY. (January 14, 2013)

Shervin Fatehi. "Derivative couplings made more physical—and cheaper," Andrew Rappe Group Meeting, University of Pennsylvania, Philadelphia, PA. (October 15, 2012)

Shervin Fatehi. "Derivative couplings made more physical—and cheaper," 244th American Chemical Society National Meeting, American Chemical Society, Philadelphia, PA. (August 20, 2012)

Shervin Fatehi. "Derivative couplings: How to get them, how to fix them, and why," Alán Aspuru-Guzik Group Meeting, Harvard University, Cambridge, MA. (May 7, 2012)

Shervin Fatehi. "Derivative couplings: How to get them, how to fix them, and why," Troy Van Voorhis Group Meeting, Massachusetts Institute of Technology, Cambridge, MA. (May 4, 2012)

Shervin Fatehi. "A perturbative universal correction operator for derivative couplings," 13th Berkeley Mini. Stat. Mech. Meeting, University of California, Berkeley, Berkeley, CA. (January 14, 2012)

Shervin Fatehi. "A perturbative universal correction operator for derivative couplings," Quantum Molecular Dynamics: A Conference in Honor of William H. Miller, Office of Naval Research, Berkeley, CA. (January 10, 2012)

Shervin Fatehi. "Analytical derivative couplings between configuration-interaction-singles states," Andrew Rappe Group Meeting, University of Pennsylvania, Philadelphia, PA. (September 27, 2011)

Shervin Fatehi. "Analytical derivative couplings between configuration-interaction-singles states," 3rd Gordon Research Conference on Time-Dependent Density Functional Theory, Gordon Research Conferences, Biddeford, ME. (August 15, 2011)

Shervin Fatehi. "Quantizing nuclear motion to improve predicted X-ray spectra: The N<sub>2</sub> test case," Facility for Theory of Nanostructured Materials Seminar, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA. (April 7, 2010)

Shervin Fatehi. "Expanding our ability to accurately simulate X-ray absorption spectra of aqueous systems," Department of Energy Review, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA. (March 10, 2010)

Shervin Fatehi. "Nuclear quantum effects in the structure and lineshapes of the N<sub>2</sub> NEXAFS spectrum," 11th Berkeley Mini. Stat. Mech. Meeting, University of California, Berkeley, Berkeley, CA. (January 8, 2010)

## **TEACHING**

### **Courses Taught**

Chemistry Capstone

Chemistry Seminar

Directed Research

General Chemistry II

General Chemistry II Lab

Physical Chemistry I

Physical Chemistry II

## Directed Student Learning

- Engaged Scholar Award "Characterizing the Mechanical Response of Molecules with Quantum Chemistry" , Department of Chemistry. (November 2018)
  - Engaged Scholar Award "Computational methods for understanding steric hindrance and near-field effects" , Department of Biology. (January 16, 2018 - July 31, 2018)
- Master's Thesis Committee Chair. Agapito Serrato, "Experimental and Computational Studies in Rotation and Proton Tunneling in Organic Molecules and Dimers" , Department of Chemistry. (September 1, 2016 - May 8, 2018)
- Engaged Scholar Award "Characterizing the Mechanical Response of Molecules with Quantum Chemistry" , Department of Chemistry. (September 8, 2017)
- Undergraduate Capstone/Senior Project. Jorge Garcia, "Signatures of Criticality in Spontaneous Neural Activity in Mice Retrosplenial Cortex" , Department of Chemistry. (October 14, 2016 - August 17, 2017)
- Engaged Scholar Award "Computational methods for understanding geometric effects in solutions after X-ray exposure" , Department of Biology. (January 16, 2017 - July 31, 2017)

## SERVICE

### Department Service

- Attendee, Meeting, Recording Secretary for Department Meetings. (January 2018)
- Committee Chair, Department Seminar. (September 2017)
- Committee Member, General Chemistry. (September 2017)
- Committee Member, Lecturer/Visiting or Clinical Faculty Search. (September 2017)
- Committee Chair, Library Liaison. (September 2017)
- Committee Member, Publicity. (September 2017)
- Committee Member, Strategic Plan/Program Review. (September 2017)
- Other, Department Webmaster. (February 2016)
- Other, Department Listserv Manager. (December 2015)
- Committee Member, Graduate Program. (September 2015)
- Committee Member, Three-Year Lecturer Search. (August 19, 2017 - July 31, 2018)
- Committee Member, Senior Lecturer Search. (August 19, 2017 - May 11, 2018)
- Committee Member, Chemistry Department Chair Search. (September 1, 2016 - August 31, 2017)
- Committee Co-Chair, Library Liaison. (September 1, 2015 - August 31, 2017)

### College Service

- Attendee, Meeting, 2018 College of Sciences Convocation. (August 22, 2018)

Attendee, Meeting, 2017 College of Sciences Convocation. (August 22, 2017)

Attendee, Meeting, 2016 College of Sciences Convocation. (August 24, 2016)

Attendee, Meeting, 2015 College of Sciences Convocation. (August 24, 2015)

### **University Service**

Attendee, Graduation, Spring 2019 Edinburg Commencement. (May 11, 2019)

Attendee, Graduation, Spring 2019 Lavender Graduation. (April 30, 2019)

Attendee, Graduation, Fall 2018 Edinburg Commencement. (December 15, 2018)

Grant Proposal Reviewer, Internal (November 14, 2018 - November 25, 2018)

Attendee, Convocation, 2018 Academic Affairs Convocation. (August 22, 2018)

Attendee, Graduation, Spring 2018 Edinburg Commencement. (May 12, 2018)

Attendee, Graduation, Fall 2017 Edinburg Commencement. (December 16, 2017)

Attendee, Graduation, Spring 2017 Brownsville Commencement. (May 12, 2017)

Attendee, Graduation, Fall 2016 Edinburg Commencement. (December 17, 2016)

Attendee, Convocation, 2016 Academic Affairs Convocation. (August 24, 2016)

Attendee, Graduation, Spring 2016 Edinburg Commencement. (May 14, 2016)

Attendee, Graduation, Fall 2015 Edinburg Commencement. (December 19, 2015)

Attendee, Convocation, 2015 President's Events. (August 11, 2015)

### **Development Activities Attended**

Workshop, "Small Teaching: Motivating and Growing," UTRGV Center for Teaching Excellence. (June 26, 2018)

Workshop, "Small Teaching: Practicing and Self-Explaining," UTRGV Center for Teaching Excellence. (June 19, 2018)

Workshop, "Small Teaching: Interleaving and Connecting," UTRGV Center for Teaching Excellence. (June 12, 2018)

Workshop, "Small Teaching: Retrieving and Predicting," UTRGV Center for Teaching Excellence. (June 5, 2018)

Workshop, "Civilian Response to Active Shooter Event (CRASE)," UTRGV Police Department. (May 10, 2018)

Workshop, "Designing Effective Group Projects," UTRGV Center for Teaching Excellence. (March 29, 2018)

Workshop, "Indiana University–Minority Serving Institutions STEM Initiative Faculty Research Development Institute," Indiana University. (July 24, 2017 - July 28, 2017)

• Write-In, "Faculty Summer Write-Ins," Faculty Writing Support Program. (June 28, 2017)

Workshop, "Session 6: Tenure and Promotion," Second Year Faculty Support Program. (April 4,

2017)

Workshop, "Session 5: Grant Writing Workshop," Second Year Faculty Support Program. (March 31, 2017)

Workshop, "2017 NSF Division of Chemistry Early Career Investigator Workshop," National Science Foundation Division of Chemistry. (March 20, 2017 - March 21, 2017)

Workshop, "Session 4: Distance Teaching and Learning," Second Year Faculty Support Program. (February 7, 2017)

Workshop, "Knowing Your Students and Helping Them Succeed," UTRGV Center for Teaching Excellence. (February 6, 2017)

Workshop, "Session 3: Developing a Service Profile," Second Year Faculty Support Program. (November 1, 2016)

Workshop, "ADVANCE Search Committee Training," UTRGV Division of Academic Affairs. (October 7, 2016)

Workshop, "Session 2: Research Collaborations," Second Year Faculty Support Program. (October 4, 2016)

Workshop, "Session 1: Introduction to Second Year Faculty Support," Second Year Faculty Support Program. (September 13, 2016)

Workshop, "Session 10: Career Mapping—Planning for Summer and Beyond," New Faculty Support Program. (April 19, 2016)

Workshop, "Grant Writing Workshop," New Faculty Support Program. (April 8, 2016)

Workshop, "Jumpstart your Research Career with an NSF CAREER Grant! Workshop II: Details on Writing an NSF CAREER Proposal," UTRGV Strategic Research Development. (April 8, 2016)

Workshop, "Session 8: Getting Published—Tools and Strategies," New Faculty Support Program. (March 29, 2016)

Workshop, "Jumpstart your Research Career with a NSF CAREER Grant!," UTRGV Strategic Research Development. (March 22, 2016)

Workshop, "Session 7: Navigating External Funding Sources," New Faculty Support Program. (February 23, 2016)

Workshop, "Session 6: Supporting Faculty & Student Success: Resources & Strategies," New Faculty Support Program. (February 2, 2016)

Seminar, "Session 2: Mentors & Mentees Networking Luncheon," New Faculty Support Program. (October 29, 2015)

Workshop, "Teaching Workshop: Enhancing Your Teaching Effectiveness," New Faculty Support Program. (October 16, 2015)

Workshop, "Session 2: Building Your Research Profile Through Internal Funding Sources," New Faculty Support Program. (September 22, 2015)

Workshop, "Session 1: Getting the Mentoring You Need," New Faculty Support Program. (September 8, 2015)

Tutorial, "2015 Faculty Portfolio Tool Training," Office of the Vice Provost for Faculty Affairs &

Diversity. (August 28, 2015)

Workshop, "New Faculty Orientation," New Faculty Support Program. (August 17, 2015 - August 18, 2015)

### **Professional Service**

Workshop Organizer , Southwest Theoretical and Computational Chemistry 2018 (October 30, 2017 - November 30, 2018)

Reviewer, Journal Article , The Journal of Physical Chemistry Letters , Washington , (August 7, 2015 - December 12, 2017)

Program Organizer , South Texas Section of American Chemical Society , Edinburg , (April 27, 2017)

Reviewer, Journal Article , Chemical Physics Letters (April 2012)

Reviewer, Journal Article , Molecular Physics (November 2007 - December 2007)

### **Professional Memberships**

Q-Chem, Inc. (Q-Chem) (June 2013)

American Chemical Society (ACS) (July 2006)

International Union of Pure and Applied Chemistry (IUPAC) (July 2006)

### **Public Service**

- Judge , Rio Grande Valley Regional Science & Engineering Fair , Brownsville , (February 13, 2016)
- Judge , Reynaldo G. Garza Elementary , McAllen , (December 4, 2015)
- Guest Speaker , Rosa Parks Elementary , Berkeley , (June 2, 2008)
- Guest Speaker , Rosa Parks Elementary , Berkeley , (March 14, 2008)