

Dr. Gregory Smith

Associate Professor of Chemistry and Biochemistry
Cullen Trust for Higher Education / Dolores Welder-Mitchell Chair
University of Saint Thomas, Houston, TX

Education

2013 PhD, Chemistry (Minor: Nanoscience and Microsystems)

University of New Mexico, Albuquerque, NM
Advisor: Distinguished Professor Hua Guo
Thesis: *Simulations of Chemical Catalysis*

1999 BS, Chemistry (Minor: Physics)

Northeastern University, Boston, MA

Professional Experience

2022-present Associate Professor of Chemistry and Biochemistry

2026-present Cullen Trust for Higher Education/Dolores Welder-Mitchell Chair
University of Saint Thomas, Houston, TX

2018-2022 Assistant Professor of Physical Chemistry

Southern Oregon University, Ashland, OR

2017-2018 Adjunct Assistant Professor of Physical Chemistry

Southern Oregon University, Ashland, OR

2015-2017 Postdoctoral Teaching Fellow

Ithaca College, Ithaca, NY

2014-2015 Visiting Lecturer II

University of New Mexico, Albuquerque, NM

2012-2014 Part-time Instructor

Central New Mexico C.C., Albuquerque, NM

2010-2012 Teaching Assistant

University of New Mexico, Albuquerque, NM

2008-2010 Research Assistant

University of New Mexico, Albuquerque, NM

2008 Graduate Internship

Biogen Idec, Cambridge, MA

2004-2006 Chemist

NM Department of Health, Scientific Lab Division, Albuquerque, NM

2002-2003 Analytical Chemist

Johnson & Johnson, Piscataway, NJ

1999-2001 Product Development Chemist

National Starch and Chemical, Bridgewater, NJ

Teaching

Current Courses

Physical Chemistry I and II - Full-year sequence covering the major areas of physical chemistry: thermodynamics, statistical mechanics, kinetics, kinetic molecular theory, and quantum mechanics with applications to spectroscopy.

Physical Chemistry Lab I - Covers experiments in thermodynamics, kinetics, spectroscopy, and computational chemistry. Emphasis on formal reports, error analysis, and Python based data analysis.

Computational Chemistry - Advanced elective covering molecular modeling across length scales. Serves as an introduction to scientific programming in Python and to molecular visualization. Classical methods include molecular mechanics and docking. Quantum methods include basis sets, Hartree-Fock, post-HF, and semi-empirical methods. Covers molecular representations (SMILES, InChI, 3D structures) and visualization (PyMOL and VMD).

General Chemistry I and II - Full year sequence for majors, STEM fields, and pre-professional track.

General Chemistry Lab I and II - Companion lab for General Chemistry - focus on lab technique, calculations and data analysis, and scientific writing.

Chemical Communications - Introduction to searching the scientific literature, reference management, scientific ethics, professional development, and scientific communication, including literature reviews, scientific posters and scientific presentations.

Previous courses taught:

- Scientific Methods for Scientists - Introductory Chemistry - General Physics Laboratory I and II

Curricular Leadership & Innovation

- **Led transition to OpenStax** as the primary textbook in General Chemistry I/II (2024-2025), improving accessibility and reducing student costs.
- **Spearheaded adoption of ALEKS**, an adaptive homework platform; developed standardized template assignments for faculty use and provided ongoing technical support.
- **Redesigned General Chemistry Lab I** to scaffold formal report writing: implemented weekly mini-assignments (introduction, methods, results, discussion) leading to a capstone lab report. Resulted in significant improvement in average report scores from 5.3 ± 3.0 (2022) to 8.2 ± 1.7 (2024).
- **Pioneered AI-integrated pedagogy** in laboratory courses: piloted use of Blackboard AI tools for revision feedback on formal lab reports (Spring 2025); co-developing rubrics and protocols with Dr. Stubbert.
- **Evaluated and recommended implementation of a diagnostic math placement exam**, correlated with student outcomes in General Chemistry I/II; results published internally (weak correlation in Gen Chem I, moderate-to-strong in Gen Chem II).
- **Developed and launched** the new elective course *Computational Chemistry* (Fall 2025), including full curriculum, Python tutorials, Jupyter Notebooks, assignments, and exams.

Research Interests

Computational Biochemistry - Classical and quantum simulations of biomolecules, enzyme reaction mechanisms, QM/MM, enhanced sampling methods, molecular docking, and scientific computing.

Antibiotic Discovery - Computational modeling of key enzyme targets in *mycobacterium tuberculosis*. Elucidating reaction mechanisms to find transition state structures and using docking and structure similarity to discover potential selective inhibitors.

Chemical Education Research - Design, implementation, and evaluation of RAG-powered AI tools in chemistry education; assessing their impact on student writing quality and conceptual retention through scaffolding lab report assignments.

Research Students

Current Students (projects in development)

Santiago Pirela - Feb 2026-present

Fatima Carbajal - Feb 2026-present

Hannah Le - May 2026-present

Madeline Contreras - May 2026-present

Previous Students

Christopher Lubrano | Feb 2025 - May 2026

Project: RAG-Based AI Tutoring System for OpenStax Chemistry Textbook

Developed document parsing workflows to convert PDF textbook chapters into structured Markdown, then processing chunks and metadata for use in Retrieval-Augmented Generation (RAG). Presented findings at departmental and university seminars, and presented a poster at the Spring 2026 ACS National Meeting.

Ryan Nguyen | August 2024 - May 2026

Project: Antibiotic Target Identification in Mycobacterium tuberculosis

Mapped metabolic pathways of *M. tuberculosis*, identifying essential enzymes in cell wall synthesis (e.g. FASII, arabino-galactan and peptidoglycan synthesis pathways). Currently Pursuing MD at Canadian School of Medicine in the Dominican Republic.

Nicolas Le | Aug 2024 - May 2026

Project: Revision and Standardization of General Chemistry Lab Manuals

Conducted comprehensive audit of CHEM 1141/1142 lab handouts; identified inconsistencies, outdated procedures, and unclear instructions. Produced first-pass revisions aligned with current lab practices, improving clarity and instructor usability. Authored updated procedural guides for 8+ experiments.

Katie Crouch | Sept 2023 - May 2024

Project: IR Spectra Prediction of Fatty Acid Derivatives

Applied DFT methods (PBEh-3c) to compute vibrational spectra; correlated theoretical peaks with experimental FTIR data. Contributed to dataset used for machine learning model training in collaboration with Dr. Chandra.

Margaret Edozie | July 2023 - May 2024

Project: IR Spectra Prediction of Fatty Acid Derivatives

Performed computational modeling and data analysis for a library of saturated and unsaturated fatty acids. Developed Python scripts to automate peak identification and error analysis from Gaussian output. Currently pursuing PharmD at University of Houston.

Roberto Gonzalez | Sept 2022 - May 2023

Project: MM-PBSA Binding Energy Calculations for Enzyme-Ligand Complexes

Calculated binding free energies using Molecular Mechanics Poisson-Boltzmann Surface Area method. Completed calculations for two of three target complexes; authored comprehensive technical report on methodology and results.

Edward Gutierrez | Aug 2022 - May 2023

Project: Physical Chemistry lab experiment revision

Helped critique and revise upper-division physical chemistry experiments. Successfully updated and validated laboratory protocols, improving clarity.

Jack Diab | Sept 2020 - Jun 2022

Project: Reaction Path Mapping of Epoxide Hydrolase B using QM/MM calculations.
Currently pursuing PhD at UCLA.

Christopher Evancich | Sept 2019 - Jun 2021

Project: Bioprospecting molecules for activity against FadD32: A computational approach.

Bobby Chisum | Sept 2019 - Jun 2021

Project: Investigating Hydration of Epoxide Hydrolase B using the 3D-RISM method.

Brian Lee | Sept 2018 - Jun 2019

Project: Computational Analysis of Human Soluble Epoxide Hydrolase

Danielle Adler | Sept 2017 - Jun 2018

Project: Evaluating histidine protonation states in Epoxide Hydrolase B.

Grants

Funded

Robert A. Welch Foundation Departmental Research Grant

M. Steiger (PI), R. Chandra, J.A. Palasota, O.A. Ulloa, G. Smith

Funding supports department-wide research infrastructure and undergraduate research initiatives in computational chemistry, spectroscopy, and educational innovation.

June 1, 2024-May 31, 2027 | \$165,000

Robert A. Welch Foundation Departmental Equipment Grant

M. Steiger (PI), R. Chandra, O.A. Ulloa, J.A. Palasota, G. Smith

Funds acquisition of lab instrumentation to support undergraduate research.

2024-2025 | \$75,000

Not funded

"Incorporating Generative AI Tools in the University Chemistry Curriculum"

G. Smith (Co-PI), R. Stubbart (Co-PI), R. Chandra (Supporting), J. Hochman (Supporting).

Proposed a randomized controlled study to evaluate the impact of cloud-based vs. local LLMs + RAG systems on student writing, concept retention, and AI literacy in General Chemistry labs.

Spencer Foundation | Submitted June 2025 | \$245,921 (Unfunded)

"Improving Undergraduate STEM Education Hispanic Serving Institutions HSI Pilot Project: UST STEM Familia"

Steiger, M. (Principal), Simmons Nout, A. D. (Co-Principal), Smith, G. (Co-Principal)

Proposed comprehensive support system targeting C-DFW rates in introductory STEM courses through academic advising, identity development, and curricular alignment - particularly for Hispanic and low-income students.

University of St. Thomas (Federal IUSE) | Submitted 2024 | \$99,325 (Unfunded)

Department of Education, Fund for the Improvement of Postsecondary Education (FIPSE): Advancing Artificial Intelligence to Improve Educational Outcomes of Postsecondary Students

Multi-department effort with contributions from Chemistry, Theology/Philosophy, Education, and Business. Chemistry participants: R. Chandra (Narrative), G. Smith (Project Plan), R. Stubbart (Planning/Revising)

University of St. Thomas (Federal IUSE) | Submitted Dec 2025 | \$245,180 (Unfunded)

Service

Academic Advising

2023-Present: Incoming Freshman Advising (Spring/Summer)

- Guided incoming first-year students in course registration, major exploration, and STEM pathway planning.

2024-Present: Undergraduate Academic Advisor, Department of Chemistry

- Advised 8 undergraduates in 2024, 23 students by 2025, and 25 students in 2026, including declared majors and undeclared STEM track students. Conducted individual advising meetings each term; performed graduation audits for seniors; coordinated with registrar on degree substitutions and curriculum exceptions.

Search Committees

In the role of Search Committee Member

2025-2026 : Chemical Engineering Faculty Position - Successful hire

2024-2025 : Biochemistry Faculty Position - Successful hire

2024-2025 : Generalist/Inorganic Chemistry Faculty Position - Successful hire

2024-2025 : Organic Chemistry Faculty Position - Successful hire

2023-2024 : Organic Chemistry Faculty Position - no candidate selected

Departmental Service

2023-Present : Safety Committee Member, Department of Chemistry - Regularly attended monthly meetings to review chemical storage, waste disposal protocols, equipment safety, and lab access policies.

2024-2025 : Committee on Reducing D/W/F Rates in Introductory STEM Courses - Collaborated with faculty from Biology and Chemistry to design a placement and remediation pilot program for students underprepared in math/chemistry fundamentals. Recommended implementation of a diagnostic exam and targeted academic support modules, piloted in Fall 2024. Produced an internal report correlating math placement exam results with success in General Chemistry I (weak correlation) and General Chemistry II (moderate to strong correlation).

2025-Present: Faculty Advisor, ACS Student Chapter - Advised student-led American Chemical Society chapter; organized and chaperoned trip to the 2025

ACS National Meeting in San Diego for three undergraduate presenters. Supported poster preparation, travel logistics, and networking opportunities.

University & Professional Service

2023: Presenter at Doherty Library Seminar Series - Delivered invited talk: "Scientific Modeling and Strategies for Evaluation," exploring types of scientific models (empirical, computational, statistical) and frameworks for evaluating reliability, falsifiability, and applicability in research and policy.

Professional Conferences - Applied new knowledge to course redesign, lab innovation, and student research mentoring. - Spring 2025 - ACS National Meeting in San Diego - Summer 2024 - Gordon Research Conference on Chemical Dynamics

Publications

Smith GK, Ke Z, Hengge AC, Xu D, Guo H. Active-site dynamics of SpvC virulence factor from *Salmonella typhimurium* and density functional theory study of phosphothreonine lyase catalysis. *The Journal of Physical Chemistry B*. 2009; 113(46):15327-33.

Smith GK, Lin S, Lai W, Datye A, Xie D, Guo H. Initial steps in methanol steam reforming on PdZn and ZnO surfaces: Density functional theory studies. *Surface Science*. 2011;605(7-8):750-759.

Smith GK, Ke Z, Hengge AC, Guo H. Insights into the phosphoryl transfer mechanism of cyclin-dependent protein kinases from ab-initio QM/MM free-energy Studies. *The Journal of Physical Chemistry B*. 2011;115(46):13713-22.

Smith CR, **Smith GK**, Yang Z, Xu D, Guo H. Quantum mechanical/molecular mechanical study of anthrax lethal factor catalysis. *Theoretical Chemistry Accounts*. 2010;128(1):83-90.

Lin S, Johnson RS, **Smith GK**, Xie D, Guo H. Pathways for methanol steam reforming involving adsorbed formaldehyde and hydroxyl intermediates on Cu(111): density functional theory studies. *Physical Chemistry Chemical Physics*. 2011;13(20):9622-31.

Ke Z, **Smith GK**, Yingkai Z, Guo H. Molecular Mechanism for Eliminylation, a Newly Discovered Post-Translational Modification. *Journal of the American Chemical Society*. 2011; 133(29):11103-05

Johnson RS, DeLaRiva A, Ashbacher V, Halevi B, Villanueva CJ, **Smith GK**, Lin S, Datye AK, and Guo H. The CO oxidation mechanism and reactivity on PdZn alloys. *Physical Chemistry Chemical Physics*. 2013; 15: 7768-7776

Awards / Scholarships / Fellowships

1994 Carl S. Ell Scholarship Academic Achievement

1994 NSF REU University of New Mexico

1995 NSF REU MIT Haystack Observatory

1996 NSF REU Northeastern University

2008 Clark-Person-Graham Endowment Teaching Assistant Award

2008-2010 NSF IGERT Fellowship Interdisciplinary Study and Research

2009 NSF EAPSI Fellowship Research Abroad in Nanjing, China

2010 Hillard L. Smith / Dow Fellowship Research Award

2011 NSF IGERT Poster Competition Finalist