

- CHEM371: Physical Chemistry 1
- CHEM472: Physical Chemistry 2
- Lock Haven University
 - CHEM101: Chemistry in the Environment
 - CHEM105: Forensic Chemistry
 - CHEM120: Principles of Chemistry 1 (Lecture and Laboratory)
 - CHEM121: Principles of Chemistry 2 (Laboratory)
 - CHEM205: Introduction to Organic Chemistry (Laboratory)
 - CHEM221: Organic Chemistry 2 (Laboratory)
 - CHEM302: Introduction to Computational Chemistry
 - CHEM320: Thermochemistry and Kinetics
 - CHEM321: Quantum Chemistry and Spectroscopy
 - CHEM328: Science Seminar — “Bridging the two cultures”
 - CHEM328: Science Seminar — “Genius and madness”
 - *Chemistry for bioethanol production*, a non-credit, continuing education course for BioEnergy, LLC at the Clearfield Campus
- Macalester College
 - CHEM111-L: General Chemistry I Laboratory
 - CHEM 222: Analytical Chemistry
 - CHEM 222-L: Analytical Chemistry Laboratory

Course development

- CHEM321: Quantum Chemistry and Spectroscopy
- CHEM302: Introduction to Computational Chemistry
- CHEM105: Forensic Chemistry
- CHEM328: Science Seminar
 - Bridging the two cultures.
 - Genius and madness.
 - * Revised to add Global Awareness and Citizenship - Ethics general education objectives Fall 2016

Grants

- “Molecular simulation at Lock Haven University”, **2020** CHE200017: Extreme Science and Engineering Discovery Environment (XSEDE). 2,000 GPU hours on SDSC Comet.
- “Molecular simulation at Lock Haven University”, **2016–2018** TG-CHE160011: Extreme Science and Engineering Discovery Environment (XSEDE). 50,000 Service Units.
- “Molecular simulation at Lock Haven University”, **2016–2018** TG-CHE160011: Extreme Science and Engineering Discovery Environment (XSEDE). 50,000 Service Units.
- Alternative Workload Leave to be a Visiting Scholar at the Integrative Proteomics Research at Rutgers University, **Spring 2016**.
- “Computational Chemistry Projects at LHUP”, **2011–2012** TG-CHE080050: Extreme Science and Engineering Discovery Environment (XSEDE). 60,000 Service Units.
- “Enhancing the use of Computational Chemistry at LHUP”, **2011** LHUP Academic Computing and Technology Grant. \$12,495.
- “Computational Chemistry Projects at LHUP”, **2010–2011** TG-CHE080050: Tera-Grid. 60,000 Service Units.
- “Computational Chemistry Projects at LHUP”, **2009–2010** TG-CHE080051T: Tera-Grid. 30,000 Service Units; TG-CHE080050: NCSA Abe, LONI QueenBee. 10,000 Service Units.
- “Computational Chemistry Projects at LHUP”, **2008–2009** TG-CHE080051T, Tera-Grid, 30,000 Service Units.
- “Computer Simulations in Support of Studies of Photosystem II and Ab Initio Investigations of 1,3 Sigmatropic Rearrangements in Triazenes”, **2007–2008** TG-CHE070063N, Pittsburgh Supercomputer Center, 10,000 Service Units.

Independent Studies

- “Inorganic Laboratory Development”. Carter Rhoades. Spring 2023–Fall 2024.
- “Investigating the importance of a mild detergent in the activation of a psychrophilic lipase using molecular dynamic simulations”. Zachary Knepp. Spring 2020.
- “1,3-sigmatropic rearrangements in triazene and its carbon analogs”. Kayla Elliot. Spring 2019–Spring 2020.
- “Simulations towards and understanding of the Spinach RNA aptamer”. Isabella Bieker. Fall 2016.
- “1,3-sigmatropic rearrangements in triazene and its carbon analogs”. Aminesh Chavan and Benjamin Rood. Spring 2015.

- “Proton affinity of ethenone and related molecules”. Melissa Semken. Fall 2013–Spring 2014.
- “1,3-sigmatropic rearrangements in triazene and its carbon analogs”. Sun-Young Park, Fall 2013–Fall 2015.
- “1,3-sigmatropic rearrangements in triazene and its carbon analogs”. Miranda Striluk. Spring 2013.
- “Proton affinity of ethenone and related molecules”. Brittni Blust. Spring 2013.
- “Simulation of functionalized gold nanoparticles”. Morgan Olsen. Spring 2013.
- “Hydrogen bonding in substituted benzoates”. Damen Gee. Fall 2012–Spring 2013.
- “Evaluation of software for simulation of nanostructures”. Morgan Olsen. Fall 2012.
- “Heat of formation of ethenone and related molecules”. Julia Tiaw. Spring 2011.
- “Parallelization of semi-numerical Hessian calculation in GAMESS”. Stefjord Todolli. Fall 2010, Spring 2011.
- “A docking study of some tetraazaperylenediones with telomere tetraplex models”. Terry Bartholomew. Spring 2009.
- “Fourier transform infrared spectroscopy/Principal components analysis for identification of microorganisms”. Yayra Hiamey, Dr. Barrie Overton. Spring 2009.
- “A computational investigation of some tetraazaperylenediones”. Terry Bartholomew. Fall 2008.
- “Electronic structure of metallo-carbohedrynes”. Broc Smith. Spring 2008.
- “Fourier transform infrared spectroscopy/Principal components analysis for identification of actinomycetes”. Elizabeth Shive, Dr. Barrie Overton. Spring 2008.
- “1,3 Sigmatropic Rearrangement of a Methyl Group in a Three Carbon System and in Triazene”. Steve Uzupis. Fall 2007.
- “Fourier transform infrared spectroscopy/Principal components analysis for identification of actinomycetes”. Elizabeth Shive, Dr. Barrie Overton, Fall 2007.
- “Electron energy analysis”. Amber Struble. Fall 2006.
- “1,3 hydrogen and methyl migrations in triazenes and their carbon analogs”. Amber Struble. Spring 2006.

Publications

- Range, K. *Forensic Chemistry Laboratory Manual*, Lock Haven University of Pennsylvania: Lock Haven, PA, **2008–2018**.
- Moser A.; Range, K.; York, D. M. “Accurate Proton Affinity and Gas-Phase Basicity Values for Molecules Important in Biocatalysis”, *J. Phys. Chem. B* **2010**, *114*, 13911–13921.
- McCracken, J.; Vassiliev, I.; Yang, E.; Range, K.; Barry, B. A. “ESEEM Studies of Peptide Nitrogen Hyperfine Coupling in Tyrosyl Radicals and Model Peptides”, *J. Phys. Chem. B* **2007**, *111*, 6586–6592.
- Sibert, R.; Josowicz, M.; Porcelli, F.; Veglia, G.; Range, K.; Barry, B. A. “Proton-coupled electron transfer in a biomimetic peptide as a model of enzyme regulatory mechanisms”, *J. Am. Chem. Soc.* **2007**, *129*, 4393–4400.
- Range, K.; López, C. S.; Moser, A.; York, D. “Multi-level and density functional electronic structure calculations of proton affinities and gas-phase basicities involved in biological phosphoryl transfer”, *J. Phys. Chem. A* **2006**, *110*, 791–797.
- Range, K.; Ayala, I.; York, D.; Barry, B. A. “Normal modes of redox-active tyrosine: conformation dependence and comparison to experiment”, *J. Phys. Chem. B.* **2006**, *110*, 10970–10981.
- Giese, T. J.; Gregersen, B. A.; Liu, Y.; Mayaan, E.; Moser, A.; Range, K.; Faza, O. N.; López, C. S.; de Lera, A. R.; Schaftenaar, G.; Lopez, X.; Lee, T.; Karypis, G.; York, D. M. “QCRNA 1.0: A database of Quantum Calculations for RNA catalysis”, *J. Mol. Graph. Model* **2006**, *25*, 423–433.
- Gregersen, B. A.; Giese, T. J.; Liu, Y.; Mayaan, E.; Range, K.; York, D. M. “Simulations of phosphoryl transfer reactions using multiscale quantum models”, *Modeling Molecular Structure and Reactivity in Biological Systems* **2006**, 181–192.
- Range, K. *Application of density functional theory and continuum solvation to reactions and response properties of biological molecules*. Doctoral Thesis. University of Minnesota **2005**.
- Salter, G.; Range, K.; Salter, C. “A virtual instrument panel and serial interface for the Parr 1672 thermometer” *J. Chem. Educ.* **2005**, *82*, 297.
- Range, K.; Riccardi, D; Cui, Q.; Elstner, M.; York, D. “Benchmark calculations of proton affinities and gas-phase basicities of molecules important in the study of biological phosphoryl transfer”, *Phys. Chem. Chem. Phys.* **2005**, *16*, 3070–3079.
- Range, K.; Mayaan, E.; Maher, L. J., III; York, D. “The contribution of phosphate-phosphate repulsions to the free energy of DNA bending”, *Nucleic Acids Research* **2005**, *33*, 1257–1268. (*featured on the cover*)
- Mayaan, E.; Range, K.; York, D. “Structure and binding of Mg(II) ions and di-metal bridge complexes with biological phosphates and phosphoranes” *J. Biol. Inorg. Chem.* **2004**, *9*, 807-817.
- Range, K.; McGrath, M.; Lopez, X.; York, D. “The structure and stability of biological metaphosphate, phosphate and phosphorane compounds in the gas phase and in solution” *J. Am. Chem. Soc.* **2004**, *126*, 1654-1665.

- Ayala, I.; Range, K.; York, D.; Barry, B. A. "Spectroscopic properties of tyrosyl radicals in dipeptides," *J. Am. Chem. Soc.* **2002**, *124*, 5496-5505.
- Salter, C.; Range, K.; Salter, G. "Laser-induced fluorescence of lightsticks," *J. Chem. Educ.* **1999**, *76*, 84-85.
- Range, K. *An ab initio investigation of the hydrogen and methyl migrations of some trans-alkyltriazenes*. Honors Thesis. Moravian College **1998**.

Presentations

- Range, K. "Using WebMO and Gaussian to teach organic chemistry", **2025**, American Chemical Society Fall 2025 National Meeting, Oral.
- Range, K. "Using molecular computation and visualization to teach chemistry", **2024**, Biennial Conference on Chemical Education, Oral.
- Range, K. "Using molecular computation and visualization to teach chemistry", **2024**, Middle Atlantic Regional ACS Meeting, Oral.
- Range, K. "Exploring electron configurations of atoms and ions with WebMO and Gaussian", American Chemical Society Spring 2024 National Meeting, Oral.
- Range, K. "Analyzing infrared and NMR spectra of organic molecules with WebMO and Gaussian", **2022**, Biennial Conference on Chemical Education, Oral.
- Range, K. "Exploring electron configurations of atoms and ions with WebMO and Gaussian", **2022**, Biennial Conference on Chemical Education, Oral.
- May, B. D.; Range, K. "Using R in the Physical Chemistry Laboratory", **2022**, Biennial Conference on Chemical Education, Oral.
- Range, K.; Coval, S. J.; Maresch, M. J.; May, B. D. "Using fragrant molecules to explore chemical structure and spectroscopy", **2020**, 259th ACS National Meeting, Oral. – Canceled due to pandemic
- Range, K. "3D printing workflow for chemical education with free software", **2019**, Moravian College, invited speaker.
- Range, K.; Bieker, I.; York, D. "Towards understanding the chemical physics of the spinach fluorogenic RNA aptamer", **2017**, 253rd ACS National Meeting, Poster.
- Range, K. "Going beyond 'Add trendline': least squares and error analysis throughout the curriculum", **2016**, 251st ACS National Meeting, Oral.
- Range, K. "Molecular visualization and computation early, often, and as an upper-level elective", **2016**, 251st ACS National Meeting, Oral.
- Range, K. "Computational chemistry throughout the curriculum", **2015**, 249th ACS National Meeting, Oral.
- Park, S.; Range, K. "1,3-sigmatropic rearrangements in triazene and its carbon analogs", **2014**, Central PA ACS Local Section Undergraduate Research Poster Session, Penn State University.
- Range, K.; Tiaw, J. "Heat of formation of ethenone", **2013**, 245th ACS National Meeting, Poster.

- Olsen, M.; Range K. "Simulation of functionalized gold nanoparticles", **2013**, 245th ACS National Meeting, Poster.
- Gee, D.; Range, K. "Hydrogen bonding in substituted benzoates", **2013**, 245th ACS National Meeting, Poster.
- Range, K. "Molecular Computation and Visualization in Introductory Chemistry Courses". **2012**, 46th Annual Meeting of the Middle-Atlantic Association of Liberal Arts Chemistry Teachers. Invited speaker.
- Tiaw J.; Range, K. "Heat of formation of ethenone and related molecules", **2011**, Lock Haven University of Pennsylvania, COS Poster.
- Todolli, S.; Range, K. "Parallelization of semi-numerical Hessian calculation in GAMESS", **2011**, Lock Haven University of Pennsylvania, COS Poster.
- Todolli, S.; Range, K. "Parallelization of semi-numerical Hessian calculation in GAMESS", **2010**, Central PA ACS Local Section Undergraduate Research Poster Session, Penn State University.
- Bartholomew, T; Range, K. "A docking study of some tetraazaperylenediones with telomere tetraplex models". **2009**, Lock Haven University of Pennsylvania, COS Poster.
- Range, K.; Salter, O. C.; MacKay, J. A. "Vinyl boronate esters as dienophiles", **2010**, 239th ACS National Meeting, Poster.
- Range, K. "Computational chemistry in pharmaceutical research", **2009**, Rotary Meeting guest speaker.
- Hiamey, Y.; Overton, B.; Range, K. "FTIR/PCA for identification of microorganisms", **2009**, Lock Haven University of Pennsylvania, COS Poster.
- Range, K. "Benchmark calculations of ammonium and nitrate ions in aqueous solution", **2009**, 237th ACS National Meeting, Poster.
- May, B.; Whiting, J.; Range, K. "Teaching physical chemistry using the primary literature", **2008**, Biennial Conference on Chemical Education, Poster.
- Shive, E.; Overton, B.; Range, K. "FTIR/PCA for identification of Actinomycetes", **2008**, Lock Haven University of Pennsylvania, COS Poster.
- Smith, B.; Gerardi, A.; May, B.; Range, K. "Synthesis and Electronic Structure of Metallocarbohedryne Materials", **2008**, Lock Haven University of Pennsylvania, COS Poster.
- Uzupis, S.; Range, K. "1,3 hydrogen and methyl migrations in triazenes and their carbon analogs: The search for a pure DFT solution", **2007**, Lock Haven University of Pennsylvania, Chemistry Research Poster Session.
- Shive, E.; Overton, B.; Range, K. "FTIR/PCA identification of microbes", **2007**, Lock Haven University of Pennsylvania, Chemistry Research Poster Session.
- Salter, C.; Hoffman, G.; Range, K. "Computing Chemical Answers: Effects of Solvation", **2007**, 41st Annual Meeting of the Middle-Atlantic Association of Liberal Arts Chemistry Teachers.

- Range, K. “1,3 hydrogen and methyl migrations in triazenes and their carbon analogs: Do the Woodward-Hoffman rules apply to nitrogen systems?”, **2007**, Lock Haven University of Pennsylvania, COS, Provost’s Colloquium.
- Struble, A.; Libby, D.; Salter, C.; Range, K. “Exploration of Electron Energy Analysis as a method of evaluating reaction pathways”, **2007**, Lock Haven University of Pennsylvania, COS Poster.
- Struble, A.; Range, K. “1,3 sigmatropic rearrangements in triazene and their carbon analogs”, **2006**, Lock Haven University of Pennsylvania, Chemistry Research Poster Session.
- Range, K.; York, D. M. “Accurate proton affinity and gas-phase basicity values of molecules important in biocatalysis”, **2006**, 231st ACS National Meeting, Poster.
- Howell, C.; Range, K.; Tzolov, M. “International issues in scientific research”, **2006**, Antonio de Nebrija University, Madrid, Spain.
- Range, K.; Mayaan, E.; Maher, L. J., III; York, D. “Electrostatics and DNA bending: A COSMO and Monte-Carlo study”, **2004**, Computational Chemical Dynamics from Gas-Phase to Condensed-Phase Systems, Poster.
- Range, K.; Ayala, I.; York, D.; Barry, B. A. “A DFT study of the IR spectra of tyrosinate, tyrosyl radical, and some of their isotopologues,” **2003**, 225th ACS National Meeting, Poster.
- Range, K.; York, D. “Recent developments towards a new DFT-based many-body molecular simulation force field,” **2001**, 222nd ACS National Meeting, Poster.

Publications in Preparation

- Range, K. “Using electronic structure calculations to understand electron configurations of atoms”
- Salter, O. C.; Range, K. “Using electronic structure calculations to understand the helium spectrum”
- Range, K.; Elliott, K.; Struble, A.; Uzipis, S.; Striluk, M.; Foresman, J.; Salter, O. C. “1,3 hydrogen and methyl migrations in triazenes and their carbon analogs”
- Range, K.; Tiaw, J.; Blust, B.; Semken, M. “Heat of formation of ethenone and related molecules”

Service

- Commonwealth University APSCUF Meet and Discuss team, 2022–present
- Physical and Environmental Sciences Department Assistant Chair, 2024–present.
- Biochemistry, Chemistry, Engineering, and Physics Department Assistant Chair, 2023–2024
- Program co-chair, Middle Atlantic Regional Meeting of the American Chemical Society, 2024.
- LHU APSCUF Meet and Discuss team, 2020–2022
- Chemistry Department Chair. 2017–2022

- University Promotions Committee. 2011–2013, 2016–2022
UPC chair 2017–2018 and 2021–2022
- Lock Haven APSCUF Executive Council, Member-at-Large 2011–2013, 2016–present
- Co-advisor of Student Affiliates Chapter of the American Chemical Society at Lock Haven University of Pennsylvania (2006–present)
- Peer reviewer for *Journal of Chemical Education*, *Journal of Physical Chemistry*, *Journal of Molecular Structure: THEOCHEM*, and *Energy & Fuels*
- STEM Integration subgroup. 2020–2021
- Chemistry Integration sub-subgroup. 2020–2021
- Tenure and Promotion Policy and Procedures Integration subgroup. 2020–2021
- Taskforce on Promotion Policy and Procedures, Chair. 2019–2021
- Molecular Computation and Visualization in Undergraduate Education (MoleCVUE) Program Chair 2009, 2013, 2015, 2023
- Summer School Meet and Discuss Committee 2007–2013, Chair 2009–2013
- Academic Technology and Computing Committee 2009–2013, Chair 2011–2013
- APSCUF Nominations and Elections Committee 2009–2013
- Central PA Local Section of the American Chemical Society. Chair 2011
- Moravian College external Honors reviewer 2008

Awards

- Kolthoff Fellowship (1998)
- ACS - Leigh Valley Division Chemistry Award (1998)
- Stuart S. Kulp Senior Chemistry Award (1998)
- John Amos Comenius Scholar (1994-1998)
- Council on Undergraduate Research Fellowship (1997)
- Freshmen Chemistry Achievement Award (1994)
- Boy Scouts of America - Eagle Scout (1992)

Professional Memberships

- American Chemical Society (ACS)
- Molecular Computation and Visualization in Undergraduate Education (MoleCVUE)