Samuel Bekoe

Department of Chemistry & Biochemistry
University of California, Los Angeles
United States
+1 (949) 317 8557
sbekoe@ucla.edu, sbekoe@uci.edu, sambek419@gmail.com

Education

2018 – 2023 **University of California Irvine**
Graduate Studies, PhD in Computational and Theoretical Chemistry.
Thesis title: *Structure-Preserving Methods for Molecular Response Calculations*.
Advisor: Professor Filipp Furche

2013 – 2017 **B.Sc. Kwame Nkrumah University of Science and Technology** in Chemistry, First Class (Honors).
Thesis title: *DFT Studies of the Ring Opening Reaction of Dialkoxy-Methylenecylcopropanes to Trimethylenemethanes and Follow-up reactions*.
Advisors: Professor Evans Adei and Dr. Richard Tia

Publications

Journal Articles (peer-reviewed)

1. Bekoe, Samuel, Rappoport, D., Moussa, J., & Furche, F. (2023). Structure-preserving methods for response calculations. *Manuscript under preparation*.

2. Rappoport, D., Bekoe, Samuel, Mohanam, L. N., Le, S., George, N., Shen, Z., & Furche, F. (2023). Libkrylov: A modular open-source software library for extremely large on-the-fly matrix computations. *J. Comput. Chem.*, *44*(11), 1105–1118. Contribution: (I) Contributed to discussion and design of library interface. (II) Implemented preconditioner types. (III) Implemented some of the global and linear algebra utility functions in the library. (IV) Contributed to testing library functions. (V) Wrote user guide and gitlab wiki. doi:https://doi.org/10.1002/jcc.27068

3. Goodwin, C. A. P., Ciccone, S. R., Bekoe, Samuel, Majumdar, S., Scott, B. L., Ziller, J. W., … Evans, W. J. (2022). 2.2.2-cryptand complexes of neptunium(iii) and plutonium(iii). *Chem. Commun.*, *58*, 997–1000. Contributions: Ran all electronic structure calculations and related analysis, presenting and discussing results with other authors. Contributed to manuscript and wrote computational details section of supporting information. doi:10.1039/D1CC05904A

4. Jenkins, T. F., Bekoe, Samuel, Ziller, J. W., Furche, F., & Evans, W. J. (2021). Synthesis of a Heteroleptic Pentamethylcyclopentadienyl Yttrium(II) Complex, [K(2.2.2-Cryptand)](C5Me5)2YII[N(SiMe3)2], and Its C–H Bond Activated Y(III) Derivative. *Organometallics*, *40*(23), 3917–3925. Contributions: Ran all electronic structure calculations and related analysis, presenting and discussing results with other authors. Contributed to manuscript and wrote computational details section of supporting information. doi:10.1021/acs.organomet.1c00482

5. Wedal, J. C., Samuel Bekoe, Ziller, J. W., Furche, F., & Evans, W. J. (2020). C–H Bond Activation via U(II) in the Reduction of Heteroleptic Bis(trimethylsilyl)amide U(III) Complexes. *Organometallics*, *39*, 3425–3432. Contributions: Ran all electronic structure calculations and related analysis, presenting and discussing results with other authors. Contributed to manuscript and wrote computational details section of supporting information. doi:10.1021/acs.organomet.0c00496

6. Huh, D. N., Ciccone, S. R., Bekoe, Samuel, Roy, S., Ziller, J. W., Furche, F., & Evans, W. J. (2020). Synthesis of Ln(II)-in-Cryptand Complexes by Chemical Reduction of Ln(III)-in-Cryptand Precursors: Isolation of a Nd(II)-in-Cryptand Complex. *Angew. Chem. Int. Ed.*, *59*(37), 16141–16146. Contributions: Ran all electronic structure calculations and related analysis, presenting and discussing results with other authors. Contributed to manuscript and wrote computational details section of supporting information. doi:10.1002/anie.202006393

7. Wedal, J. C., Bekoe, Samuel, Ziller, J. W., Furche, F., & Evans, W. J. (2019). In Search of Tris(trimethylsilylcyclopentadienyl) Thorium. *Dalton Trans.*, *48*, 16633–16640. Contributions: Ran all electronic structure calculations and related analysis, presenting and discussing results with other authors. Contributed to manuscript and wrote computational details section of supporting information. doi:10.1039/C9DT03674A

8. Bekoe, Samuel, Osei, M. K., Tia, R., & Adei, E. (2017). Density Functional Theory Studies on the Generation of Trimethylenemethanes from the Ring Opening of Dialkoxymethylenecyclopropanes and Methylenecyclopropanethioacetals and Follow-up Reactions. *J. Mol. Model.*, *24*(1), 24. Contributions: Suggested and ran geometry optimization and transition state search calculations for the mechanistic studies. Contributed to 70% of manuscript writing. doi:10.1007/s00894-017-3558-7

Software

1. Rappoport, D., Bekoe, Samuel, Mohanam, L. N., & Furche, F. (2022). Libkrylov, a Modular Open-Source Software Library for Extremely Large Eigenvalue and Linear Problems. Version 1.0.0. Contribution: (I) Contributed to discussion and design of library interface. (II) Implemented preconditioner types. (III) Implemented some of the global and linear algebra utility functions in the library. (IV) Contributed to testing library functions. (V) Wrote user guide and gitlab wiki. doi:10.5281/zenodo.5935799

2. Furche, F., & co-workers. (2022). Libkrylov, a Modular Open-Source Software Library for Extremely Large Eigenvalue and Linear Problems. Retrieved from https://gitlab.com/libkrylov/libkrylov-stable

3. Mohanam, L. N., Samuel Bekoe, Shen, Z., George, N., & Furche, F. (2020). Libkrylov, a Modular Open-Source Software Library for Extremely Large Eigenvalue and Linear Problems. Contribution: (I) Contributed to testing library functions (wrote Python codes for testing purposes). (II) Contributed to gitlab wiki. doi:10.5281/zenodo.3974054

Research Experience

2023 – Present

Postdoctoral Scholar, University of California, Los Angeles
Supervisor: Professor Prineha Narang
Project title: "Nonlinear Optical Response Properties in Graphene-based nanosystems"

- Developing first-principle methodologies to analyse the fundamental factors behind the enhancements in resonant harmonic generation in graphene-based nanosystems, as observed in experiments.

Software used: Octopus, Quantum Espresso

Research Experience (continued)

2018 – 2023 **Graduate Research Assistant, University of California, Irvine**
Supervisor: Professor Filipp Furche
Project title: "Development of Libkrylov for linear response calculations of time-dependent density functional theory (TDDFT) and time-dependent Hatree-Fock (TDHF)"

- Design and implementation of a modular and open-source library based on the Krylov subspace method for solving on-the-fly large and dense eigenvalue and linear problems that arise in quantum chemistry and other scientific disciplines.

Project title: "Application of electronic structure methods to characterize rare-earth and actinide complexes"

- Descriptioin of novel rare-earth and actinide complexes with density functional methods. Characterization of ground state electronic structure, analyses of vibrational and excited state properties [1 - 5].

Software used and developed: Libkrylov [1], TURBOMOLE

2013 – 2017 **Undergraduate Research Assistant, Kwame Nkrumah University of Science and Technology**,
Supervisors: Professor Evans Adei and Dr. Richard Tia
Project title: "DFT Studies of the Ring Opening Reaction of Dialkoxy-Methylenecylcopropanes to Trimethylenemethanes and Follow-up reactions [6]"

- Mechanistic studies on the ring opening reaction of dialkoxy-Methylenecylcopropanes to trimethylenemethanes.

Software used: Spartan, Gaussian

Teaching

2022 **University of California, Irvine** - Irvine, CA. Undergraduate Chemistry Teacher Assistant

- Teaching general Chemistry lab course Chem 1LC
- Facilitating student-led discussions through Argument Driven Inquiry (ADI)

2018 – 2019 **University of California, Irvine** - Irvine, CA. Undergraduate Chemistry Teacher Assistant

- Taught general Chemistry lecture and lab courses (Chem 5, Chem 1A and Chem 1LC)
- Led discussions and lab sessions for over 200 students

Teaching (continued)

2017 – 2018 **Kwame Nkrumah University of Science and Technology** - Kumasi, Gh. Undergraduate Chemistry Teacher Assistant

- Taught freshman general Chemistry lecture and lab courses (Chem 155/156, 180)
- Taught senior year Chemistry lecture courses (Chem 451/452)
- Led discussions and lab sessions for over 400 students

Posters and Presentations

2023 **ACS Spring 2023**, Indianapolis, Oral.
Libkrylov: A Modular Open-Source Software Library for extremely large on-the-fly matrix computation

2022 **SoCal TheoChem 5**, Riverside, Oral.
Libkrylov: A Modular Open-Source Software Library for extremely large on-the-fly matrix computation

2020 **NSF CSSI PI meeting**, Seattle, Oral and Poster.
Libkrylov: A Modular Open-Source Software Library for extremely large and dense eigenvalue and linear problems

Workshops

May-Oct 2024 **OpenMP Training Series**, Remote.
OpenMP Introduction, Tasking, Optimization for NUMA and SIMD, What Could Possibly Go Wrong Using OpenMP, Introduction to Offloading with OpenMP, Advanced OpenMP Offloading Topics

Apr 2024 **MolSSI Best Practices**, Remote.
Version Control and Sharing Code; Making a Python Package Part; Continuous Integration, Testing and Distribution

Mar 2024 **NERSC FUN Training March 2024: Introduction to Parallel Programming in Fortran**, Remote.
Introduction to parallel programming concepts and models; Performance Profiling with CrayPat; Parallel programming patterns with do concurrent; Parallel programming patterns with OpenMP; Parallel programming patterns with MPI; Parallel programming patterns with Coarrays

Feb 2024 **Winter School on Quantum Information Science for Chemistry**, UCLA.
Introduction to Quantum Information, Classical Quantum Chemistry and QIS applications, Optical Cycling Centers, Quantum Algorithms for Chemistry, Molecular Spin Qubits

NERSC SpinUp Application, Remote.
Database-backed web apps that access project data; Workflow orchestration tools running outside of HPC; API servers for real-time or distributed projects

Service

2023 — **ACS Spring 2023 Session Presider**.
Presided over the Machine Learning session of the ACS Spring 2023.

2021 - 2023 — **Hardware and Software Deputy, Furche Group**.
Periodically evaluates hardware, updates with new developments, and performs tests and maintenance for the Furche group. Manages purchasing of computing hardware and software for group use.

2019 - 2021 — **Furche Group High School Outreach Program**.
Involved with the outreach program organized by the Furche group, which aims to provide high school students from disenfranchised backgrounds with the opportunity to conduct scientific research in chemistry. Worked closely with students to teach concepts in chemistry and application of electronic structure theory to understand chemical systems.

- Elizabeth Bulla, Pacifica High School, Garden Grove, CA. Class of 2020
- Aakrsh Misra, Dana Hills High School, Dana Point, CA. Class of 2022

Awards and Achievements

2022 — **Molecular Sciences Software Institute (MolSSI) 2022 - 2023 Software Fellowship**

Skills

AI Training	Outlier: >1 year AI training in STEM topics (Chemistry, Physics and Mathematics).
Programming	Fortran (2003): 5 years general programming experience and 3 years experience with independent development of parts of code.
	Python: 5 years general programming experience with simple codes for testing and data visualization purposes.
	C++: 3 year experience with interoperating C with Fortran
	MATLAB: 4 year experience with testing small matrix problems
Tools	UNIX environment, bash scripting, git, debugging and profiling tools (GNU debugger), CI/build tools (make and cmake), GPU, HPC, Docker, OpenMP
Electronic Structure Packages	TURBOMOLE, Spartan, Gaussian, Octopus, Quantum Espresso
HPC	UCI HPC and GreenPlanet clusters, NERSC Perlmutter cluster, OLCF Fronteir and Summit clusters, CHPC Lengau cluster