HERBERT DANIEL LUDOWIEG

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EDUCATION

University at Buffalo, The State University of New York April 2023
Doctor of Philosophy in Chemistry
Thesis: *Spin-orbit coupling and vibronic effects on spectroscopic properties of metal complexes*

University at Buffalo, The State University of New York June 2018
Bachelor of Science in Physics | Bachelor of Arts in Chemistry | Minor in Mathematics

EXPERIENCE

RESEARCH ASSISTANT August 2018 – May 2023
University at Buffalo, Buffalo, NY

Performed novel research in the field of computational chemistry by computing vibronic effects as numerical derivatives via the central finite difference method. Created a Python library using cutting-edge mathematical models, increasing the understanding of the origins of vibronic effects.

- Optimized existing implementations to calculate the vibronic effects of molecules, significantly reducing the computational time tenfold.
- Published in the prestigious journal *Science Advances* for the first quantitative comparison of theory and experiment in magneto-chiral dichroism.
- Added a parameter to a quantum chemistry package, causing a sign flip resulting in a relative accuracy of 2.
- Analyzed data generated by proof-of-concept calculations, ensuring correct behavior of code implementations.
- Presented theoretical research findings to an audience of theoreticians and experimentalists.
- Contributed to five separate scientific publications as a co-first author or first author.

TEACHING ASSISTANT August 2018 – May 2021
University at Buffalo, Buffalo, NY

- Graded homework and exams for a class of over 50 students.
- Oversaw classes, going over relevant course material and homework corrections.
- Mentored students during office hours on class material.

UNDERGRADUATE RESEARCH ASSISTANT May 2016 – August 2018
University at Buffalo, Buffalo, NY

- Designed a graphical user interface for the Kramers-Kronig transformation to make it more user-friendly.
- Implemented a visualizer for NMR shielding tensors in 3D space for Exatomic. The back-end is coded in Python, and the front-end is coded in JavaScript.

SKILLS

- **Programming languages**: Python, Bash, Latex, slurm, FORTRAN, C++, Markdown, HTML, JavaScript
- **Data analysis**: Pandas, SQL/MySQL
- **Version control**: Git, Apache Subversion
- **Libraries**: NumPy, Pandas, matplotlib, Numba, SciPy, pytest
- **Operating Systems**: Linux, Windows
- **Visualization**: matplotlib, Tableau

CODING PROJECTS

VIBRAV (https://github.com/herbertludowieg/vibrav)

- Compute vibronic effects of molecules with a central finite difference numerical differentiation scheme.
- Advanced the field of computational chemistry as it provides a robust and intuitive interface from state-of-the-art quantum chemistry packages for calculating vibronic effects.
- Built CI/CD pipeline with GitHub actions. Code coverage and quality checks are accomplished with Codacy. Code is automatically deployed to PyPi.

- Led to numerous scientific publications in influential journals, such as Science Advances.
- Implemented a new model to approximate derivatives with a multi-point differentiation scheme.

Exatomic (https://github.com/exa-analytics/exatomic)
- Added visualization of a 3x3 matrix in 3D space to an existing GUI embedded in a Jupyter notebook.
- Coordinated with original developers, increasing coverage of edge cases through unit tests.
- Created new parsers to organize unstructured data into data frames for analysis.
- Assisted with developing GitHub actions workflows for code coverage and quality checks by Codacy.

MCD-Molcas (https://github.com/jautschbach/mcd-molcas)
- Generated CI pipeline of FORTRAN code with GitHub actions for GCC and Intel oneAPI compilers.
- Unit testing includes analyzing unstructured standard outputs with a Python script.

PUBLICATIONS

- **Ludowieg, H D**; Srebro-Hooper, M; Crassous, J; Autschbach, J. *ChemistryOpen* **2022** 11 e202200020. DOI: https://chemistry-europe.onlinelibrary.wiley.com/doi/10.1002/open.202200020
- Morgante, P; **Ludowieg, H D**; Autschbach, J. *The Journal of Physical Chemistry* **2022** 126 (19) 2909 – 2927. DOI: https://pubs.acs.org/doi/10.1021/acs.jpca.2c00951
- Atzori, M; **Ludowieg, H D**; et al. *Science Advances* **2021** 7 (17) eabg2859. DOI: https://www.science.org/doi/10.1126/sciadv.abg2859
- Ganguly, G; **Ludowieg, H D**; Autschbach, J. *Journal of Chemical Theory and Computation* **2020** 16 (8) 5189 – 5202. DOI: https://pubs.acs.org/doi/abs/10.1021/acs.jctc.0c00386
- Abella, L; **Ludowieg, H D**; Autschbach, J. *Chirality* **2020** 32 (6) 741 – 752. DOI: https://onlinelibrary.wiley.com/doi/abs/10.1002/chir.23194

ACHIEVEMENTS

GRADUATE RESEARCH HIGHLIGHT June 2021
- Received award for contributions to research publications in the *Journal of Chemical Theory and Computation* and *Science Advances*.

PUBLIC PRESENTATIONS

SEEDS4CD (Twitter) May 2021
- Technical presentation on original research performed on transition metal complexes that led to two publications. Contributions included the development of necessary tools in collaboration with lab members.

RESEARCH PROJECTS

VIBRONIC COUPLING
- Created code to calculate vibronic coupling effects of spin-forbidden transitions.
- Read over two hundred output files performing mathematical operations with complex data types.
- Led to publication in the Journal of Chemical Theory and Computation for the qualitative study of a multi-reference ground state molecule, $[U(Cl)_6]^{2-}$ and $[U(Br)_6]^{2-}$.
- Led to publication in Science Advances for the first qualitative comparison of theory and experiment for the vibrationally resolved magneto-chiral dichroism spectrum of $[Ni(en)_3]^{2+}$.

VIBRATIONAL RAMAN OPTICAL ACTIVITY
- Implemented code into the VIBRAV Python program package to calculate the Vibrational Raman Optical Activity of molecules.
- Led to publication in Chirality for a comparative study on the $[Co(en)_3]^{3+}$ and $[Rh(en)_3]^{3+}$ molecules.