Alex M. Maldonado, PhD

Researcher and Educator in Computational Chemistry and Biology

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Teaching Experience

University of Pittsburgh

Pittsburgh, PA

Computational Biology (BIOSC 1540) — Spring 2024 – Present

- Designed and delivered an undergraduate course introducing foundational computational biology concepts, incorporating **bioinformatics and computational structural biology**.
- Engaged **approximately 73 students** through interactive lectures and **hands-on computational projects**, including genome assembly and annotation, protein structure prediction, and computer-aided drug design.
- Developed and facilitated (optional) **Programming+ recitations to support advanced coding challenges**, fostering collaborative problem-solving and deeper engagement with computational biology concepts.

Computational Biology Seminar (BIOSC 1630) — Fall 2023, 2024

- Designed a curriculum that immerses **approximately 21 students** in cutting-edge computational biology through **critical reading of primary research articles**.
- Supervised **student-authored perspective articles** through structured assignments, providing detailed feedback to enhance argumentation, clarity, and scientific rigor.
- Emphasized **effective communication** with figure analysis, data interpretation, and group presentations.

Fundamentals of Thermodynamics (CHE 2101) — Spring 2021, 2022

- Worked closely with **Dr. Karl Johnson** to **design, refine, and evaluate homework assignments, exams, and projects**, ensuring they aligned with course objectives and enhanced student learning outcomes.
- **Prepared and delivered lectures on advanced non-local composition models**, integrating theoretical concepts with computational frameworks and Python demonstrations to reinforce understanding.
- Guided students in molecular dynamics and Monte Carlo simulations using LAMMPS and RASPA and developed Python programs for Peng-Robinson thermodynamic calculations, emphasizing **computational problem-solving and coding best practices**.

Reactive Process Engineering (CHE 0400) — Summer 2020

- Worked with **Dr. Joaquin Rodriguez** to incorporate an **innovative bioprocess module** in the curriculum. This module included bioenergetics, metabolic pathways, bioreactors, enzyme kinetics, fermentation, immobilized enzyme reactors, and antibody production.

INVESTING NOW — Summer 2019

- INVESTING NOW is a comprehensive college preparatory program at the University of Pittsburgh that provides academic enrichment, mentoring, and STEAM-focused opportunities to **historically underrepresented pre-college students**.
- Co-created a **five-week educational enrichment program** with modules on alternative **energy sources, circuits, and sustainability**.
- Fostered teamwork, critical thinking, and creativity through **hands-on activities** including designing water filtration systems, building photovoltaic cells, and cardboard wind turbines.

Education

University of Pittsburgh

Aug 2018 – May 2023

I completed a **Ph.D. in Chemical Engineering**, integrating rigorous core engineering coursework with advanced computational and theoretical chemistry studies. Beyond traditional chemical engineering fundamentals (i.e., **transport phenomena, reaction engineering, and thermodynamics**), I pursued interdisciplinary training in **statistical mechanics, quantum chemistry, biophysics, and computational structural biology**. My research under **Dr. John Keith** tackled complex chemical problems at the intersection of theory and applications, particularly in understanding solvated reaction mechanisms through **computational chemistry, software development, and machine learning approaches**.

Western Michigan University

Aug 2013 – Apr 2018

I obtained a **B.S.E in Chemical Engineering** specializing in **bioprocess engineering** with combined **traditional chemical engineering coursework with advanced life sciences studies**, including molecular biology, genetics, human physiology, and microbiology. This interdisciplinary approach gave me a comprehensive understanding of engineering principles and biological systems. Under **Dr. Brian Young's** mentorship, I researched **novel immunobiosensor design**, focusing on developing solutions that balanced technical performance with practical cost considerations, robustness, and scalability. This experience culminated in a **senior design project where I developed a comprehensive facility design** for large-scale immunobiosensor production.

Professional Experience

Postdoctoral Associate

May 2023 – Present

I am currently a postdoctoral associate working with **Dr. Jacob Durrant** in the **Department of Biological Sciences** at the **University of Pittsburgh**. I focus on **applying computational methods to understand and engineer biological systems**. My core responsibilities include:

- Performing molecular simulations to investigate protein dynamics and protein-ligand interactions.
- Developing and implementing reproducible frameworks for force field parameterization.
- Contributing to collaborative projects spanning structural biology, drug design, and gene therapy.
- Creating and maintaining research software tools using Python, TypeScript, and Rust.
- Supporting and mentoring graduate and undergraduate students in computational methods.

Graduate Student Researcher

Aug 2018 – Apr 2023

I was a graduate student researcher under **Dr. John Keith** in the **Department of Chemical and Petroleum Engineering** at the **University of Pittsburgh**. I specialized in **computational chemistry with an emphasis on understanding chemical reactions in solution**. My primary responsibilities included:

- Designing and implementing machine learning approaches for modeling molecular systems.
- Conducting detailed investigations of various solvation modeling techniques.
- Managed research data and established documentation practices for the group.
- Training new group members in computational methods and software tools.

Publications

† denotes equal contributions.

Biomolecular Simulations

11. Rosenbaum, J. C.; Maldonado, A. M.; Durrant, J. D.; Carlson, A. E. Sensitive and ratiometric copper detection using a fluorescent protein. *In preparation*.

    Led the computational investigation of roGFP2 conformational dynamics through extensive molecular dynamics simulations, providing crucial atomic-level insights into the Cu(I)-binding mechanism. Developed and implemented comprehensive analysis workflows while managing all computational data in an open-access framework, ensuring full reproducibility through a public GitHub repository (github.com/oasci/metalflare). Authored the computational methodology sections and created associated figures while collaborating on mechanism proposals that integrated experimental and computational findings.

Computer-Aided Drug Design

10. Kochnev, Y.; Ahmed, M.; Maldonado, A. M.; Durrant, J. D. MolModa: Accessible and secure molecular docking in a web browser. *Nucleic Acids Res.* **2024**, *52* (W1), W498–W506. DOI: 10.1093/nar/gkae406

    Led the development of comprehensive user documentation and tutorials for MolModa, creating detailed technical guides that enable both expert and novice users to utilize the platform's molecular docking capabilities effectively. Authored extensive online materials covering all aspects of the software's functionality, from basic operations to advanced workflows, ensuring the platform's accessibility to researchers across experience levels.

9. Ahmed, M.; † Maldonado, A. M.; † Durrant, J. D. From byte to bench to bedside: Molecular dynamics simulations and drug discovery. *BMC Biology* **2023**, *21* (1), 299. DOI: 10.1186/s12915-023-01791-z

    Provided expert guidance on advanced molecular dynamics techniques as a co-first author, with specific contributions focusing on enhanced sampling methods, machine learning applications in quantum chemistry calculations, and alchemical free energy methods. Served as a technical reviewer and editor, helping to refine and strengthen the manuscript's scientific accuracy and clarity, particularly in sections discussing force fields and computational chemistry approaches.

Force Fields

8. Maldonado, A. M.; Vassilev-Galindo, V.; Poltavsky, I.; Tkatchenko, A.; Keith, J. A. Modeling molecular ensembles with gradient-domain machine learning force fields. *Digital Discovery*. **2023**, *2* (3), 871–880.DOI: 10.1039/D3DD00011G

    Led all aspects of this pioneering research project, including developing custom open-source Python software for calculations and data management, implementing and training multiple machine learning potentials, and creating comprehensive data visualizations. Authored the complete manuscript and supplementary information and associated the GitHub repository with complete documentation and testing frameworks (github.com/keithgroup/mbGDML).

Quantum Chemistry

7. Eikey, E. A.; Maldonado, A. M.; Griego, C. D.; Von Rudorff, G. F.; Keith, J. A. Quantum alchemy beyond singlets: Bonding in diatomic molecules with hydrogen. *J. Chem. Phys.* **2022**, *156* (20), 204111. DOI: 10.1063/5.0079487

    I executed and analyzed the quantum chemistry calculations to assess how well both manual quantum alchemy and Taylor series methods could reproduce molecular geometries and electronic properties. I developed reproducible workflows by establishing a GitHub repository (github.com/

keithgroup/qa-atoms-dimers and github.com/keithgroup/qa-dimers-data) containing all analysis code and archived the complete dataset on Zenodo to ensure transparency and reusability. This work provided key methodological insights for applying quantum alchemy to molecular systems, moving beyond previous atomic-level studies to address the challenges of predicting molecular geometries and bonding.

6. Eikey, E. A.; Maldonado, A. M.; Griego, C. D.; Von Rudorff, G. F.; Keith, J. A. Evaluating quantum alchemy of atoms with thermodynamic cycles: Beyond ground electronic states. *J. Chem. Phys.* **2022**, *156* (6), 064106. DOI: 10.1063/5.0079483

   I led the computational investigation and implementation aspects of this study examining quantum alchemy methods for atomic systems. I developed and executed all quantum chemistry calculations, created the data visualization figures, and established reproducible workflows by creating the GitHub repository (github.com/keithgroup/qa-atoms-dimers and github.com/keithgroup/qa-atoms-data) and archiving the data on Zenodo. This work laid the necessary groundwork for understanding how quantum alchemy methods perform when predicting the electronic properties of atoms, which has implications for accelerating materials discovery through computational screening.

5. Griego, C. D.; † Maldonado, A. M.; † Zhao, L.; et al. Computationally guided searches for efficient catalysts through chemical/materials space: Progress and outlook. *J. Phys. Chem. C* **2021**, *125* (16), 6495–6507. DOI: 10.1021/acs.jpcc.0c11345

   As co-first author, **I led the development and writing of multiple key sections focusing on computational modeling approaches for chemical reactions and environments, including mechanistic understanding, solvent modeling, and machine learning applications.** I created and refined most of the figures, translating complex technical concepts into clear visual representations while integrating contributions from other authors. Additionally, I synthesized findings from our lab's previous publications into a cohesive narrative that advanced the field's understanding of computational catalysis methods.

Solvation Modeling

4. Maldonado, A. M.; Hagiwara, S.; Choi, T. H.; et al. Quantifying uncertainties in solvation procedures for modeling aqueous phase reaction mechanisms. *J. Phys. Chem. A* **2021**, *125* (1), 154–164. DOI: 10.1021/acs.jpca.0c08961

   Led all aspects of this comprehensive computational chemistry study, including **performing implicit and mixed solvation model calculations, managing blind analysis with collaborators, and assisted with QM/MM simulations.** Solely responsible for experimental design, data analysis, figure creation, and manuscript preparation. Created and maintained a complete open-source repository containing all data, analysis scripts, and documentation to ensure the reproducibility of the research.

3. Maldonado, A. M.; Basdogan, Y.; Berryman, J. T.; Rempe, S. B.; Keith, J. A. First principles modeling of chemistry in mixed solvents: Where to go from here? *J. Chem. Phys.* **2020**, *152* (13), 130902. DOI: 10.1063/1.5143207

   Led the development and writing of this perspective article examining computational approaches for modeling electrochemical reactions in mixed solvent environments. Conducted **comprehensive literature analysis** to **identify key challenges and opportunities in the field**, synthesized findings into a clear framework, and **proposed novel approaches combining quasi-chemical theory with machine learning techniques**. Managed the complete manuscript preparation process, including creating all figures, incorporating co-author feedback, and addressing reviewer comments to shape the paper's final form and impact.

2. Basdogan, Y.; Maldonado, A. M.; Keith, J. A. Advances and challenges in modeling solvated reaction mechanisms for fuels and renewable chemicals. *WIREs Comput. Mol. Sci.* **2020**, *10* (2), e1446. DOI: 10.1002/wcms.1446

    Contributed to this comprehensive review article by **conducting extensive literature analysis**, **synthesizing key findings** from across the field of computational solvation modeling, and **developing clear visualizations** to explain complex concepts.

1. Maldonado, A. M.; Keith, J. A.; Schwarz, K.; Sundararaman, R. Solvation effects in first-principles calculations for catalysis. In *Computational catalysis*, 2nd ed.; Janik, M. J., Asthagiri, A., Eds.; Royal Society of Chemistry. *In press*.

    I contributed **fundamental methodological explanations** and guidance for **modeling solvation effects in chemical reactions**, covering both theoretical frameworks and practical implementation approaches for computational studies of solvated systems. Additionally, I **developed and presented a detailed case study analyzing CO2 reduction mechanisms** demonstrated the comparative strengths and limitations of different solvation modeling techniques while providing concrete examples of their application.

Honors and Awards

University of Pittsburgh

Chancellor's Undergraduate Teaching Fellowship — Spring 2025

Co-awarded the **Chancellor's Undergraduate Teaching Fellowship** with **César Guerra-Solano** aimed at **making computational biology more accessible**. The mentorship involves guiding César in developing **'Computational Bytes' (CBytes)**—a series of tiered programming modules that enhance student engagement with computational biology concepts through hands-on Python.

Provost's Dissertation Completion Fellowship — 2022 – 2023

Competitive fellowship awarded to **support final-year doctoral students completing their dissertation**, providing full tuition/fees, medical insurance, and one-year stipend. Selected based on research significance, completion timeline, and demonstrated commitment to diversity in academia.

R. K. Mellon Graduate Fellowship — 2020 – 2022

Prestigious fellowship providing **full tuition and stipend for graduate studies in energy-related research**, established through a major gift from the R.K. Mellon foundation to advance excellence in energy education and research.

STRIVE Scholar Fellowship — 2018 – 2020

NSF-funded fellowship supporting underrepresented minority doctoral students in engineering, providing mentorship and professional development through the STRIVE program. Selected based on academic excellence and commitment to increasing diversity in STEM academia and **provides partial funding for two years**.

National Science Foundation

GRFP Honorable mention — 2018

Received national recognition from the National Science Foundation for proposed graduate research, placing among the top 25% of over 12,000 applications across all fields.

Western Michigan University

Louis Stokes Alliance for Minority Participation (LSAMP) 2017 – 2018

NSF-funded program supporting underrepresented minority students in STEM fields through research opportunities, mentoring, and academic support. Selected based on academic excellence and commitment to increasing diversity in STEM.

Skills and Technical Expertise

Software development

- Proficient in **Python, TypeScript, Rust, and JavaScript**, with extensive experience creating robust and efficient computational chemistry and biology tools.
- Expert in **scientific computing libraries such as NumPy, pandas, Polars, and PyArrow**.
- Integrate pipelines with **distributed computing frameworks like Apache Spark and Ray** to handle computationally intensive workflows across clusters, significantly improving scalability and performance.
- Deploy **scalable workflows on Google Cloud**, optimizing resource allocation and cost for terabyte-scale data processing and high-throughput simulations.
- Develop **containerized pipelines using Docker** for portability and consistency across environments.
- Optimize molecular dynamics simulations and protein modeling pipelines using **MPI for distributed computing and CUDA for GPU acceleration**.

Molecular Modeling and Simulation

- Extensive experience with molecular simulation packages such as **Amber, OpenMM, and the Atomic Simulation Environment** along with **quantum mechanics/molecular mechanics (QM/MM)** simulations.
- Perform **alchemical free energy calculations** to predict binding affinities and solvation-free energies.
- Apply advanced sampling methods, including **umbrella sampling, metadynamics, Gaussian accelerated molecular dynamics (GaMD), nudged elastic band (NEB), and growing string methods**, to explore challenging conformational landscapes and reaction pathways.
- Develop and refine **custom force fields for non-standard residues, small molecules, and cofactors** to improve the accuracy of molecular simulations.
- Skilled in **quantum chemistry tools** such as **ORCA, xTB, Psi4**, and **PySCF** for electronic structure calculations and reaction mechanism modeling.

Bioinformatics

- **Analyze and clean DNA sequencing data** using tools like **FastQC** and **Fastp** to remove low-quality reads, adapters, and contaminants.
- Implement **genome assembly pipelines using SPAdes and annotate genomes with Prokka**, generating functionally annotated genomic datasets for downstream analysis.
- Quantify **gene expression from RNA-Seq data using Salmon and statistical modeling** to analyze differential gene expression.

Machine Learning and Data Science

- Apply traditional machine learning methods (e.g., **random forests, SVMs, and ensemble methods**) and advanced deep learning techniques, including **transformer architectures** and **graph neural networks**.
- Design and implement custom architectures for biological applications using **PyTorch**, **scikit-learn**, and the **Deep Graph Library**.
- Analyze and visualize high-dimensional datasets using **UMAP** and **PCA**.
- Process and engineer features from noisy, large-scale biological data, with expertise in **cleaning and preprocessing** techniques.

Scientific Visualization and Communication

- Create clear and impactful visualizations for molecular systems using tools such as **Inkscape, Blender, Adobe Illustrator, and GIMP**.
- Proficient in specialized tools like **PyMOL, ChimeraX, and VMD** to produce detailed representations of biomolecular systems.
- Design engaging, interactive visualizations using **web-based frameworks like p5.js and Reveal.js**, tailoring content for diverse audiences, from researchers to the general public.
- Create insightful and aesthetically compelling plots and figures using Python libraries (e.g., **Matplotlib, Plotly, Seaborn**) and integrate them with static and interactive visualization platforms.

Mentorship and Student Development

Graduate Mentorship

I have provided **extensive technical and professional development mentoring to graduate students** throughout my academic career, focusing on both computational expertise and essential academic skills. My mentorship focuses on fostering well-rounded research capabilities by developing:

Technical Skills

- Training in computational chemistry and structural biology.
- Expertise in high-performance computing and best practices for scientific computing.
- Programming skills with a focus on scientific Python applications.

Professional Development

- Academic writing and oral presentation skill development.
- Project planning and research strategy guidance.

During graduate school, I mentored students in developing foundational computational skills while navigating the challenges of graduate studies. This included one-on-one training in quantum chemistry methods and software development, complemented by guidance in scientific communication skills. As a postdoctoral associate, I have increased mentoring responsibilities with students by providing comprehensive guidance across technical and professional domains. This expanded role allows me to support students through all aspects of their graduate research journey, from computational methods to research communication.

Mentees: Sanjana Parimi (Fall 2023 - Present), May Ahmed (Spring 2023 - Present), Mitch Lesko (Summer 2023 - Spring 2024), Dominick Filonowich (Fall 2022 - Spring 2023), Lingyan Zhao (Spring 2020 - Fall 2023), Emily Eikey (Fall 2020 - Fall 2021)

Undergraduate Mentorship

I have mentored undergraduate students across diverse computational chemistry and biology projects, developing a structured yet adaptable mentoring approach. My mentoring philosophy centers on providing **clear initial objectives while maintaining flexibility** to adjust based on student progress. This approach has proven successful across technical research projects and professional development mentoring.

My technical mentorship spans multiple domains, including quantum chemistry calculations, machine learning applications, protein-ligand docking, and software development. For each student, I establish **structured weekly check-ins** complemented by **continuous availability through email or in-person discussions**, ensuring consistent progress while maintaining independence.

Professional development has been a key focus of my mentoring. I've successfully guided students toward various career paths, including:

- Supporting Eesha Mukherjee through her successful PhD applications and program selection;
- Helping Elizabeth Taylor navigate and gain acceptance to MS programs;
- Assisting Wyatt Kriebel in building computational biology expertise to strengthen his graduate applications.

My approach to mentoring goes well beyond just guiding research—I help students navigate everything from crafting effective statements and selecting the right programs to mapping out their career paths. While I tailor my support to each student's unique situation, I never compromise on academic rigor. When COVID-19 hit, I smoothly pivoted to remote mentoring by establishing virtual daily check-ins and clear communication structures. Understanding the varied demands on students' time, particularly those balancing work and studies, I maintain flexibility in scheduling our meetings. I provide comprehensive support for REU students through twice-weekly meetings, focusing intensively on developing their scientific writing and presentation abilities.

Mentees: Jay Grimsdall (Spring 2025 - Present), Wyatt Kriebel (Spring 2024 - Present), Corleigh Forrester (Summer 2024), Rushali Patel (Spring 2024 - Summer 2024), Elizabeth Taylor (Fall 2024 - Summer 2024), Eesha Mukherjee (Fall 2023 - Spring 2024), Margarita Prifti (Summer 2022), Estela Millan (Summer 2021), Eli Lipsman (Summer 2020), Peter Fatouros (Summer 2019)

Teaching Assistants

I am building a comprehensive teaching assistant (TA) development program that combines teaching experience, professional development, and personalized mentorship.

- TAs attend all lectures and conduct weekly office hours in pairs or small groups, fostering collaborative teaching approaches. This structured exposure to different teaching formats helps them develop their teaching style while ensuring consistent support for current students.
- Through weekly team meetings, TAs gain experience in curriculum development and pedagogical planning. They provide critical feedback on course materials and teaching approaches, particularly on integrating Python programming with biological concepts. Their insights have directly shaped course improvements, such as restructuring computational content to serve student needs better.
- I provide personalized mentorship in lecture preparation and delivery, pedagogical theory, computational biology research, and graduate school preparation. This tailored approach ensures each TA develops according to their career aspirations.

TAs: Priyam Chauhan (Spring 2025), César Guerra-Solano (Spring 2025), Jay Grimsdall (Spring 2025), Caelyn Peppler (Spring 2025), Mariska Goswami (Spring 2025), Justine Denby (Fall 2024 - Spring 2025), Rushali Patel (Spring 2024, 2025), Reya Kundu (Spring 2024 - Fall 2024), James Liu (Spring 2024), Gabe Medeiros (Spring 2024)

Service and Outreach

Open Educational Resources

I am dedicated to making computational biology more accessible by developing comprehensive, open-source educational resources. This commitment led me to found **O**pen **A**cademic **Sci**ence (OASCI), an initiative creating **freely available educational content across scientific computing**. Specifically, I maintain the Breadcrumb series (crumblearn.org), a comprehensive collection of educational websites covering essential computational biology topics. These resources are licensed under **CC BY-NC-SA 4.0**, allowing free use with non-commercial attribution. Materials span:

- Core computational methods (Python, Software Engineering, High-Performance Computing);
- Biological applications (Biophysics, Computer-Aided Drug Design, Molecular Dynamics);
- Data analysis (Statistics, Supervised Learning, Unsupervised Learning);
- Specialized topics (Quantum Chemistry, Bioinformatics, Computational Structural Biology).

Student Organizations

As the **faculty advisor** to the **Computational Health Sciences Club** since Fall 2024, I have supported **comprehensive initiatives to enrich computational biology students' educational experience and career preparedness** at the University of Pittsburgh. My contributions have focused on creating sustainable resources and hands-on opportunities:

- Established a **seminar series** featuring academic researchers and industry professionals, helping students understand career trajectories and current challenges in computational health sciences.
- Developed and coordinated a **drug discovery competition** with monetary prizes, providing students with real-world experience applying computational methods to pharmaceutical research.
- Created lasting digital resources through a **comprehensive website and handbook**, including a curated directory of all computational biology research labs in Pittsburgh, serving as a valuable reference for students exploring research opportunities.
- Designed and led **hands-on computational biology projects**, which is tailored to students' interests and gives them practical experience with industry-standard tools and methodologies.

Open-Source Software

`povme` (github.com/durrantlab/povme)

Led comprehensive modernization of this widely-used protein pocket analysis tool by reimplementing its core framework in modern Python. Enhanced the software's capabilities through **parallel processing optimizations, robust data validation with Pydantic, and improved testing coverage**. Initially developed for structure-based drug discovery, POVME enables researchers to analyze binding pocket shapes and volumes from molecular simulations, supporting critical applications in drug design and protein-ligand interactions.

`wisp` (github.com/durrantlab/wisp)

Improved the stability and reliability of this established tool for analyzing **allosteric pathways in molecular dynamics simulations** through comprehensive code modernization. Enhanced the software with automated testing infrastructure, bug fixes, and improved documentation while maintaining its core capability to identify communication pathways between protein regions.

`subpex` (github.com/durrantlab/subpex)

Led **modernization of this protein sampling tool** by rewriting its implementation with modern software engineering practices. The software uses **weighted ensemble path sampling to explore protein pocket conformations for ensemble docking**, leveraging WESTPA for enhanced sampling. Enhanced with automated testing, continuous integration, and improved documentation while maintaining its core capabilities to generate diverse protein conformational ensembles. The framework supports multiple MD engines (AMBER, NAMD) and progress coordinates for flexibility in sampling strategies.

`vaxstats` (github.com/oasci/vaxstats)

Developed an open-source **statistical framework for vaccine research** in collaboration with the **Dr. Reed in the Center for Vaccine Research at the University of Pittsburgh**. The software provides specialized tools for analyzing and forecasting vaccine-related data through a modular architecture supporting data preparation, statistical modeling, and scientific visualization.

`simlify` (github.com/oasci/simlify)

Created an open-source **Python** framework that simplifies the development and execution of molecular simulations. The software provides a **modular architecture for building customizable simulation workflows**, enabling researchers to focus on scientific objectives rather than technical implementation.

`atomea` (github.com/oasci/atomea)

Developed an open-source **Python** framework that **standardizes atomistic simulation workflows through extensible schema definitions.** The software leverages Pydantic for robust data validation and Jinja2 for automated input file generation, enabling **reproducible computational chemistry and biology research**. Features include automated file preparation, flexible data storage (Zarr integration), and standardized output parsing.

`citator` (github.com/oasci/citator)

Created an **open-source reference management plugin for Obsidian** that streamlines academic citation workflows. The software enables seamless integration of BibTeX references into note-taking through automated literature note creation, customizable citation templates, and Pandoc-style citation support. Built with **TypeScript** and maintains high code quality through comprehensive testing and automated documentation generation, making scholarly note-taking more efficient for researchers and academics.

`reptar` (github.com/oasci/reptar)

Developed an open-source **Python** framework for **computational chemistry and biology that streamlines data management for research projects**. The software enables **flexible storage and analysis of large-scale computational results through a unified interface** supporting multiple file formats (exdir, zarr, JSON, npz), automated data parsing, and standardized export to common molecular formats (ASE, GAP, PDB, SchNetPack). Framework emphasizes reproducibility and FAIR data principles through version-controlled data storage and automated documentation. **Note: `reptar` has been superseeded by `atomea`.**

`mbgdml` (github.com/oasci/mbgdml)

Developed an open-source **Python** framework that enables **size-transferable machine learning potentials by combining gradient-domain machine learning with many-body expansions**. The software provides tools for training quantum-mechanical force fields, performing molecular dynamics simulations, and analyzing molecular ensembles with high accuracy.

`cclib` (github.com/oasci/cclib)

Contributed improvements to this foundational **Python** library for computational chemistry by **implementing bug fixes and expanding the test suite**. The software serves as a **universal parser for quantum chemistry calculations**, supporting 15+ major computational packages (including Gaussian, ORCA, Q-Chem) and enabling standardized access to electronic structure data.