Artur Wodyński

Quantum chemistry expert with 10+ years of experience in developing novel computational methods and density functional theory approaches. Specialized in designing human-crafted functionals that minimize the "zero-sum game" and in pioneering neural-network-driven local mixing functions for local hybrids. Extensive expertise in applying broader machine learning techniques to enhance quantum chemical methods. Author of 31 peer-reviewed publications, including groundbreaking contributions to local hybrid functionals and strong-correlation models published in JCP, JCTC and ACR. Experienced mentor, software developer, and interdisciplinary collaborator.

Education

PhD in Chemical Science
University of Warsaw, Poland
2011–2015

- Focused on computational methods for nuclear magnetic resonance of transition metal compounds.

MSc in Chemistry
University of Warsaw, Poland
2006–2011

- Specialization in computational and theoretical chemistry.

Professional Experience

Researcher
Technische Universität Berlin, Germany
2016–Present

- Pioneered neural-network-based local mixing functions for local hybrids, integrating machine learning techniques (Python/TensorFlow) with classical quantum-chemical codes like Turbomole, showcasing the ability to connect modern AI approaches to established quantum-chemical frameworks.
- Developed the LH24n-D4 functional that, in SCF calculations, achieves the lowest errors among rung 4 functionals when benchmarked against the GMTKN55 test suite (WTMAD-2: 3.1 kcal/mol).
- Engaged in ongoing projects utilizing various machine learning techniques to develop local mixing functions (LMFs) optimized for large-scale training datasets.
- Developed cutting-edge range-separated local hybrid functionals minimizing the "zero-sum game" by simultaneously reducing fractional spin and fractional charge errors by at least 50-70%
- Contributed to quantum chemical models for EPR spectra of heavy elements.
- Mentored students, including guiding research on AI-enhanced functional designs.

Research Assistant
Institute of Nuclear Chemistry and Technology, Poland
2013–2014

- Investigated actinide/lanthanide selectivity using advanced theoretical approaches.

PhD Researcher
University of Warsaw, Poland
2011–2015

- Designed computational protocols for transition metal nuclear magnetic resonance.
- Supervised laboratories and mentored graduate students.

Grants and Awards

Mobility Plus Fellowship — Polish Ministry of Science, 2016–2017
Quantum chemical research on iron-sulfur clusters in proteins (Postdoc project in TU Berlin).

Technical Skills

- **Programming:** Python (TensorFlow, scikit-learn, etc.), Fortran, BASH, awk, and others.
- **Software:** Turbomole, PySCF, Gaussian, DIRAC, ADF, and many others.
- **Machine Learning:** Neural networks and basis set expansion for local mixing functions; experience in training, hyperparameter tuning, model evaluation.
- **Other Skills:** HPC (High-Performance Computing), GitHub, version control workflows, and optimizing computational pipelines for large-scale simulations.

Languages

- Polish (Native), English (C1), German (A2)
