

Institution:

Nicolaus Copernicus University in Toruń, Poland, Faculty of Chemistry

Research field: Quantum Chemistry

Project title: Accelerating Simplified Coupled Cluster Models by Means of Quantum-Information- and Correlation-Driven Domains and Machine Learning.

Position: Ph.D. student, a three-year scholarship with a monthly salary of 5'000 PLN

Requirements:

The Ph.D. candidate should have basic knowledge of quantum mechanics, quantum chemistry, and computational chemistry. Moreover, the candidate should have primary experience with some well-known quantum chemistry software packages, like, for instance, Amsterdam Density Functional, NWChem, Molpro, Molcas, and Turbomole, and should be aware of conventional quantum chemistry methods and their optimization schemes (like Density Functional Theory calculations or Coupled Cluster calculations). Furthermore, the Ph.D. candidate should have excellent programming skills and fundamental knowledge of common programming languages and libraries (Python, C++, CuPy, and PyTorch) as well as of machine learning. Previous programming experience in PyBEST is highly recommended.

Project description:

- (a) Design and implementation of a domain-based linear algebra factory in PyBEST and its incorporation into the PyBEST ecosystem.
- (b) Profiling a pCCD-based correlation-driven domain construction and, if insufficient, derivation of an ML-assisted domain-construction procedure.
- (c) Implementation of CD domain-based CC models and their EOM extensions for electronically excited, ionized, and electron-attached states.
- (d) Benchmarking of the proposed models against ground- and excited-state properties of closed- and open-shell systems.
- (e) Quantum-chemical modeling of (the building blocks of) organic electronics

Selection Process/Required documents:

- Curriculum vitae
- statement of the candidate's research interests, experience, and skills (in English)

**Documents should be submitted to Prof. Katharina Boguslawski:
k.boguslawski@umk.pl before August 25, 2026.**