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 four-year scholarship with a monthly salary of 3’500 PLN for the first two years, and a raise to 4000 PLN for the last two years.

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) Construction of an ML infrastructure and its incorporation into the PyBEST software package to construct pCCD-ready molecular orbitals to accelerate orbital optimization (OO).
(b) Benchmarking of the derived ML-OO procedure to model ground- and excited-state properties of closed- and open-shell systems using pCCD-based methods.
(c) Large-scale modeling of (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.boguslaswski@umk.pl before August 25, 2026.