Visiting Professors

Visiting Professor
TSUCHIMOCHI, Takashi *(from Shibaura Institute of Technology)*

Theoretical and Computational Chemistry for Degenerate Electronic Structures

Our research focuses on quantum chemistry to compute the electronic structure of materials. We are particularly interested in chemical systems where electrons are strongly correlated, making them notoriously difficult to compute with traditional approaches due to either the inappropriate treatment of quantum entanglement or prohibitively large computational costs. To tackle this conundrum, we have proposed several methodologies based on symmetry-breaking of the underlying wave function as well as its restoration by means of symmetry-projection. While these methods primarily fall within the realm of wave function theory, we are integrating these concepts into the more affordable density functional theory. We have also been extensively exploring the potential of quantum computer to address such challenging electronic structures; recently, we have proposed a novel quantum-classical hybrid algorithm that mitigates the quantum measurement in optimizing the ground state energy. Finally, we actively collaborate with experimental groups to elucidate real chemical systems where quantum mechanical effects become important.

Visiting Professor
FUJII, Keisuke *(from The University of Osaka)*

Theoretical Research on the Fundamentals and Applications of Quantum Computers

Our research explores both theoretical foundations and applications of quantum computing. While recent advances have realized cloud-accessible devices with over 100 qubits, current noisy intermediate-scale quantum computers (NISQ) remain strongly affected by noise. We investigate how such devices can still be applied to meaningful tasks, such as machine learning and quantum many-body simulations, through noise mitigation. In parallel, we study architectures and physical systems for realizing large-scale fault-tolerant quantum computers (FTQC) with quantum error correction and estimate the resources required for practical problems. Recently, we have proposed new protocols for magic state distillation that significantly reduce FTQC resource requirements, and we are investigating how compiler-level optimizations can further reduce overhead.

Visiting Associate Professor
ABE, Minori *(from Tokyo University of Agriculture and Technology)*

Development of Relativistic Quantum Chemistry Software and Its Applications, and Generative AI Models for Chemistry

We have developed relativistic quantum chemistry software to compute molecular electronic structures involving heavy atoms. The CASPT2 method is employed in our program to treat multireference electron correlation effects, and relativistic effects are accurately incorporated by connecting to the DIRAC software. The software is publicly available on GitHub (https://github.com/RQC-HU/dirac_caspt2), and its application to the spectra of UO_2^{2+} has been published in the *Journal of Chemical Theory and Computation*.

In parallel, we have also developed generative machine learning models for chemical tasks based on the Bayesian Flow Network (ChemBFN). This model learns molecular structures from SMILES representations and generates new molecules in SMILES format. Furthermore, it can be fine-tuned for regression and classification tasks, enabling the generation of molecules with desired physical properties (N. Tao and M. Abe, *J. Chem. Inf. Model.* **65(3)**, 1178–1187 (2025)).