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 with each other, 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. Recently, we have also been extensively exploring the potential of quantum computer to address such challenging electronic structures; we have proposed novel quantum-classical hybrid algorithms for accurately determining both ground and excited states in fermionic systems.

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

Theoretical Research on the Fundamentals and Applications of Quantum Computers

Our research interests include theoretical foundations and applied research related to quantum computing. The development of quantum computer hardware has made remarkable progress in recent years. Quantum computers with 50 to over 100 qubits have already been realized and quantum computers can be used from the cloud. However, current quantum computers are known as noisy intermediate-scale quantum computers (NISQ), suffering from noise. In the future, it is hoped to realize a larger-scale quantum computer and a fault-tolerant quantum computer (FTQC) with quantum error correction. Our group is investigating how quantum computers of the scale currently realized can be used for useful tasks, such as machine learning and quantum many-body simulations, by mitigating noise. At the same time, we are also analyzing what physical systems can be used to construct a large-scale FTQC and how much resources are needed to solve problems of practical interest.

Visiting Associate Professor
ABE, Minori *(from Hiroshima University)*

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. Our program was used to elucidate the ground and excited electronic states of several actinide compounds, such as UO_2^{2+} and $Cm(phen)_2^{3+}$. Our calculated excitation energies agree with experimental data and previously reported theoretical results. We will make our program publicly available on GitHub.