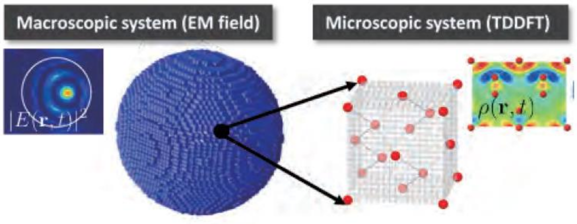
Division of Quantum Condensed Matter Physics

Chief: YABANA Kazuhiro, Professor, Ph.D., Deputy Director of CCS

The matter that exists around us is made up of atoms, which are composed of nuclei and electrons. This matter exhibits a variety of properties depending on its composition and structure, and their use supports much of science and technology today. In our division, we consider diverse types of matter, such as quantum many-body systems coupled by Coulomb interactions, and use computers to solve quantum mechanics equations. We aim to obtain the knowledge that will become the basis for the next generation of technology by understanding the various properties of matter, utilizing the quantum information of matter, and searching for matter with new functions.

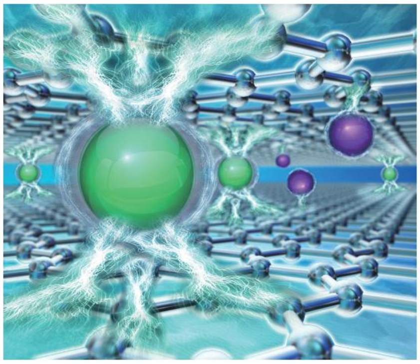
Interaction of light and matter

Light has given us the means to precisely measure the properties of matter. In recent years, the use of intense and very short pulses of light in optical science has led to real-time measurements of ultrafast electron motion and manipulation of electron motion by light. In collaboration with computer scientists and researchers from other institutions, we are investigating the interaction between light and matter using first-principles computational methods such as time-dependent density functional theory and developing the first-principles code **SALMON** (Scalable Ab initio Light-Matter simulator for Optics and Nanoscience), which works on massively parallel computations. SALMON was developed as an open-source software and can be downloaded at https://salmon-tddft.jp.



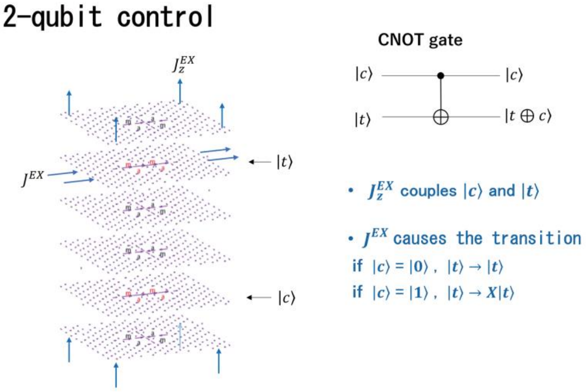
"SALMON" can be downloaded !
open-source software
SALMON (Scalable Ab initio Light-Matter simulator for Optics and Nanoscience)

First-principles simulation of chemical reactions at the solid–liquid interface



With the growing concern for environmental issues, there is a need to significantly improve the performance and durability of energy-related devices such as fuel cells and storage batteries. We run simulations of chemical reactions that occur in these devices at the microscale to understand the reaction mechanisms from a quantum mechanics perspective. The simulation results are used in the design of devices and development of materials to improve device performance. We are also developing computational methods and programs for the simulations, and the code for these has been released in the form of open-source software used widely by researchers both in Japan and abroad.

Emergent gauge field matter



In superconductors, magnetic materials, strongly correlated matter, and topological matter, an emergent gauge field—which differs from an electromagnetic field—is introduced in the mathematical form known as the Berry connection. When considering the function of such matter and their responses to external fields, it is necessary to incorporate the emergent gauge field into the calculations. We are developing such a method and using it to perform material science quantum calculations. Emergent gauge fields give rise to "topological quantum states," and it is possible to build a quantum computer using the quantum information in these states. The realization of such a computer is also a part of our work. Additionally, we are studying ultrafast dynamics in strongly correlated matter and topological matter irradiated by intense laser beams and electronic state control via laser beams through simulations using theoretical models.