

Seminar Title:
Quantum Computing using Atomic and Molecular Systems

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Centre for Quantum Engineering, Research and Education

TCG CREST

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日時：2026年9月24日(木) 14:00 – 16:00

Date and Time: Thursday, September 24, 2026, 14:00 – 16:00

場所：理学研究科5号館4階401号室

Venue: Room 401, 4th Floor, Bldg. No. 5, Graduate School of Science

Abstract:

Quantum computing is currently one of the most promising areas of science and technology. There have been important advances in the applications of this field to atomic and molecular systems in the past decade. This has been possible due to the development of quantum algorithms that are necessary for performing electronic structure computations on digital quantum computers and quantum annealers. The first such quantum algorithm known as the Variational Quantum Eigensolver (VQE) was applied to some atoms and a relatively large number of molecules. More recently, another algorithm known as the Quantum Selected Configuration Interaction (QSCI)/ Sample based Quantum Diagonalization (SQD) is being increasingly used for computing electronic structure of molecules. Quantum annealing algorithms have also been used to compute atomic and molecular properties.

In my talk, I shall present results of our group's work on properties of atomic and diatomic molecular systems using the VQE, QSCI/SQD and quantum annealing algorithms. I shall discuss the accuracy of these results by comparing with results from classical computations and comment on the prospects of improving them in the future.

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