

Joint CQSE & NCTS Special Seminar

2024
Nov. 25, Monday

Time: Nov. 25, 14:20 ~ 15:20

Title: Bridging Quantum Computation and the Fragment Molecular Orbital Method

Speaker: Dr. Kenji SUGISAKI (Project Associate Professor, Keio University)

Place: NCTS Physics Lecture Hall, 4F, Chee-Chun Leung Cosmology Hall, NTU

Online Link:

<https://nationaltaiwanuniversity-zbh.my.webex.com/nationaltaiwanuniversity-zbh.my/j.php?MTID=m892333ef8a4f21d92f3f6bdb3b756533>

Abstract:

Quantum chemical calculations of atoms and molecules are one of the most important applications of quantum computers. Quantum phase estimation (QPE) and variational quantum eigensolver (VQE) are two major approaches and they have been extensively studied both theoretically and experimentally. Although quantum computers are expected to perform quantum chemical calculations with lower computational cost compared to classical computers, further reduction of the computational cost is very important to apply these methods to larger molecules. In this study we combined the fragment molecular orbital (FMO) method with quantum computations (VQE with the unitary coupled cluster singles and doubles (UCCSD) ansatz and QPE). In the FMO method, the energy of a dimer consisting of two monomers separated by a large distance should be equal to twice the energy of a monomer, known as size consistency, is essential. From the definitions, both the VQE-UCCSD and the QPE should satisfy the size consistency. However, we numerically prove that the Trotter decomposition introduced to construct the quantum circuit can break the size consistency [1,2].

[1] K. Sugisaki, T. Nakano, Y. Mochizuki, J. Comp. Chem., 45, 2204 (2024).

[2] K. Sugisaki, AIP Adv., 14, 095021 (2024).

Biography:

2006 Ph.D. in Chemistry (Osaka City University)

2006-2008 Research Associate at Osaka City University

2008-2013 Postdoctoral Researcher at Osaka City University

2013-2016 Specially Appointed Assistant Professor at Osaka City University
2016-2022 Specially Appointed Lecturer at Osaka City University
2020-Present Visiting Associate Professor at the Centre for Quantum Engineering,
Research and Education (CQuERE), TCG Centres for Research and Education in Science
and Technology (TCG-Crest), India
2022-2023 Specially Appointed Lecturer at Osaka Metropolitan University
(On 2022 April the name of the university has changed by uniting Osaka City
University and Osaka Prefecture University)
2019-2023 JST PRESTO researcher
2023-Present Project Associate Professor at Keio University_

