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A Joint Paper on Prediction of Optical Properties of OLED Materials was Published in a Nature Research Journal
– The World-First Calculation of the Excited States of OLED Materials on Quantum Computers –

Mitsubishi Chemical Corporation
IBM Japan, Ltd.
JSR Corporation
Keio University

Mitsubishi Chemical Corporation (headquartered in Chiyoda, Tokyo, President & CEO Masayuki Waga), IBM Japan, Ltd. (headquartered in Chuo, Tokyo, General Manager Akio Yamaguchi), JSR Corporation (headquartered in Minato, Tokyo, CEO Eric Johnson) and Keio University (headquartered in Minato, Tokyo, President Akira Haseyama) are pleased to announce that a paper describing the research results of "Predicting Optical Properties of OLED Materials on Quantum Computers," a joint project from IBM Quantum Network Hub at Keio University,* has been published in "npj Computational Materials," a world-renowned Nature Research Journal.

Scientist at Mitsubishi Chemical and IBM initiated a joint research project with collaborators at JSR and Keio University to calculate the excited states of thermally activated delayed fluorescence (TADF) emitters which are applied to the fabrication of efficient OLEDs. The parties have developed a new scheme to mitigate the error from current noisy quantum computers and succeeded in improving the calculation accuracy. This is the world-first research case of applying quantum computers to excited states calculations of commercial materials.

We expect the proposed error mitigation scheme, together with the improvements of the performance of quantum computers will provide ever more accurate quantum chemistry calculation results for designing OLED emitters with high quantum efficiency in the near term.

We continue research in the area of using quantum computers to accelerate the development of a wide range of new materials.

*About the IBM Quantum Network Hub at Keio University

Opened in May 2018 by Keio University and IBM Japan on the Yagami Campus of the university's Faculty of Science and Technology, the IBM Quantum Network Hub at Keio University brings together academia and industry, with Mitsubishi Chemical and JSR as founding members. It is also the first IBM Quantum Hub in Asia leveraging IBM Quantum Systems, the most advanced quantum computers developed by IBM and delivered via the cloud.

For further information, please contact:
Communication Division, Mitsubishi Chemical Corporation Tel: [+81] (0)3-6748-7161
External Relations, IBM Japan, Ltd. Tel: [+81] (0)3-3808-5120
Corporate Communications Dept., JSR Corporation Tel: [+81] (0)3-6218-3517
Office of Communications and Public Relations, Keio University Tel: [+81] (0)3-5427-1541

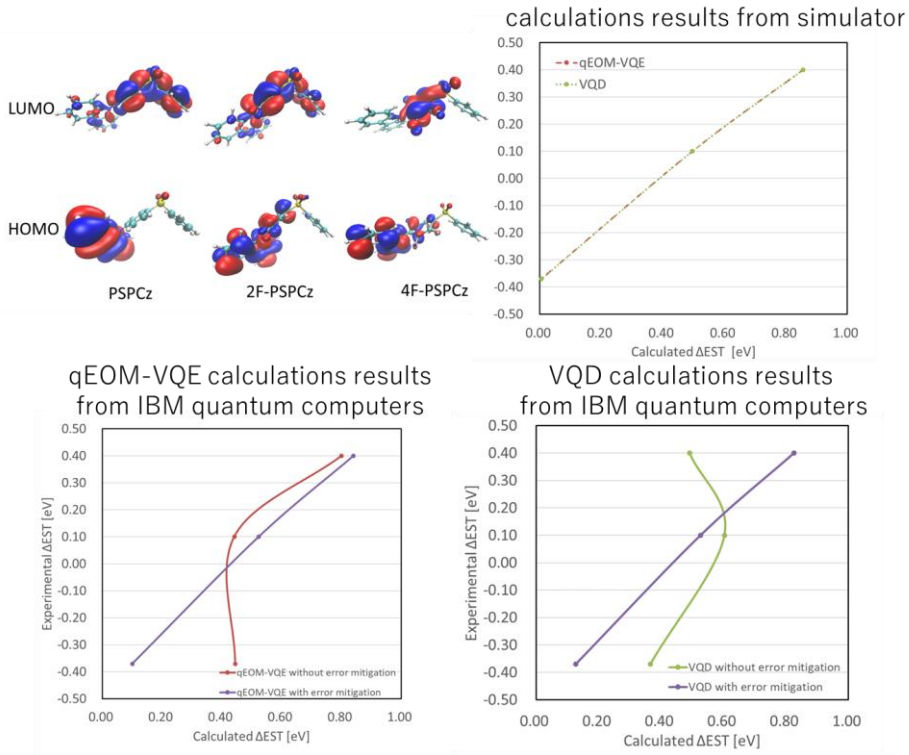
Reference

[Content of this research project]

The *ab initio* calculation of excited states of large size molecules on classical computer is rather demanding as far as computer time is concerned. In recent year, some quantum algorithms for exponential speedup of excited state calculations with the use of quantum computers have been proposed. These algorithms are expected to be useful to perform calculations of large systems that have not been possible on classical computers. On the other hand, most benchmark calculation for the validation of these algorithms in the literature were only applied to simple molecular systems such as H2, LiH and for the complicated chemical systems few surveys of the ability of these algorithms has been carried out. Moreover, due to the error in quantum computer, it is difficult to achieve chemical accuracy for the calculations on current device.

The goal of the work is to use two quantum algorithms (qEOM-VQE and VQD algorithms) to reliably predict excited states energies of TADF materials which is used as a kind of OLED emitters. The feature of TADF materials is that the first triplet state (T1) is sufficiently close to the first singlet state (S1) in energy (normally within several kcal/mol) that non-emissive T1 excitons can be thermally excited to an emissive S1 state. The mechanism enables the performance of TADF emitters for OLED device with potentially 100% internal quantum efficiency, in contrast to the OLED device using conventional fluorophores which efficiency is inherently limited to 25%. Thus, theoretical approaches to accurately predict S1 and T1 states can make a contribution to the development of TADF materials.

In this work, three TADF molecules (PSPCz, 2F-PSPCz, and 4F-PSPCZ) were selected from Mitsubishi Chemical's patent and their molecular orbitals of HOMO and LUMO (Fig. 1) were used as an active space to calculate the S1 and T1 excited states on noise-free quantum computer simulator and IBM quantum computers. Excellent agreement (correlation coefficient of 0.99) between S1-T1 gap predicted by calculations on simulator and spectra experiments were found, as shown in Fig 1. Fig 1 also indicates that the calculations on IBM quantum computers can not accurately calculate the S1 and T1 states, suggesting the noise from quantum computers is the main culprit of deviation of S1-T1 gap from the experimental data. To mitigate the error from the noisy quantum computers, a new error mitigation scheme using quantum tomography techniques was proposed. In the scheme, the corresponding quantum state of the calculation result is firstly measured by quantum tomography techniques. The measured quantum state is then used to estimate the error of the calculation and finally correct the calculation results. By utilizing the scheme, a maximum difference of 88 mHa from quantum computers to the exact eigenvalues was improved to approximately 4 mHa. Consequently, good agreement was achieved between calculations on quantum computers and experiment data. Going forward, we plan to extend the proposed approach to much larger size systems so that quantum computers can be utilized for the applications of the development of a wider range of new commercial materials.



IBM Quantum Computer

Fig. 1:Molecular structures and orbitals of TADF materials (PSPCz, 2F-PSPCz, and 4F-PSPCZ) and correlations between calculation results and experiment data

<Co-authors>

- Qi Gao, Takao Kobayashi, and Eriko Watanabe, Mitsubishi Chemical Corporation Science & Innovation Center
- Hajime Nakamura, IBM Research-Tokyo
- Gavin O. Jones and Mario Motta, IBM Research-Almaden
- Yu-ya Ohnishi, JSR Corporation
- Michihiko Sugawara, Hiroshi Watanabe, and Naoki Yamamoto, Keio University