

# Towards Quantum Chemical Calculations Using Quantum Computers with a Balanced Shot Budget

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In recent years, there has been a growing interest in algorithms that hybridise quantum and classical computing, as a new approach to electronic structure theory. One of the main challenges in the application of quantum-classical hybrid algorithms in quantum chemistry, exemplified by variational quantum algorithms, is the enormous sampling cost. In this talk, I will discuss approaches that consider the balance of shot budgets in quantum-classical hybrid algorithms. First, I will show that attempts to reduce shot budgets using unbiased estimators, such as Fermionic Shadows, may not be the optimal approach [1]. Then the algorithms we have developed to perform electronic state calculations within realistic shot budgets, including Computational Basis Sampling (CBS) [2] and Quantum Selected Configuration Interaction (QSCI) [3,4], will be presented. Finally, I will describe our proposed approaches for incorporating dynamic electron correlation into practical quantum chemical computations by integrating methods such as CBS and QSCI with existing techniques such as coupled cluster theory [5].

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[3] Keita Kanno, Masaya Kohda, Ryosuke Imai, Sho Koh, Kosuke Mitarai, Wataru Mizukami, Yuya O. Nakagawa, "Quantum-Selected Configuration Interaction: Classical Diagonalization of Hamiltonians in Subspaces Selected by Quantum Computers," arXiv:2302.11320 (2023).

[4] Yuya O. Nakagawa, Masahiko Kamoshita, Wataru Mizukami, Shotaro Sudo, Yu-ya Ohnishi, "ADAPT-QSCI: Adaptive Construction of Input State for Quantum-Selected Configuration Interaction," arXiv:2311.01105 (2023).

[5] Luca Erhart, Yuichiro Yoshida, Viktor Khinevich, Wataru Mizukami, "Coupled Cluster Method Tailored with Quantum Computing," arXiv:2312.11012 (2023).