## **Quantum Computing Seminar**



Monday, 28. August 2023 at 14:15 Auditorium 1, Department of Chemistry Universitetsparken 5, 2100 København Ø

> **Prof. Artur Izmaylov** University of Toronto

## **QUANTUM COMPUTING FOR QUANTUM CHEMISTRY: HOW TO BRING QUANTUM ADVANTAGE SOONER?**

Abstract: Quantum chemistry problem is one of the attractive targets for demonstrating quantum advantage of quantum computing technology. Having strongly correlated systems as the main target, I would like to discuss what new classical computing techniques need to be developed to help quantum computing algorithms to solve the electronic structure problem. Encoding the electronic Hamiltonian in the second quantized form on a quantum computer is not a trivial problem, and its efficiency can become a bottleneck for the entire quantum solution. Dealing with this Hamiltonian can be facilitated by partitioning it into a sum of fragments diagonalizable using rotations from either small Lie groups or the Clifford group. These fragments are convenient for performing various algebraic manipulations required in circuit compiling and quantum measurement. I will illustrate how the Hamiltonian partitioning can be used to improve performance of several quantum algorithms for quantum chemistry (e.g. Variational Quantum Eigensolver and Quantum Phase Estimation).

Meeting URL: https://ucph-ku.zoom.us/j/62210998470?pwd=RnNwOFBSYIhIaXdXRG9SUEVtT3FSdz09

Meeting ID: 622 1099 8470 Passcode: 407250