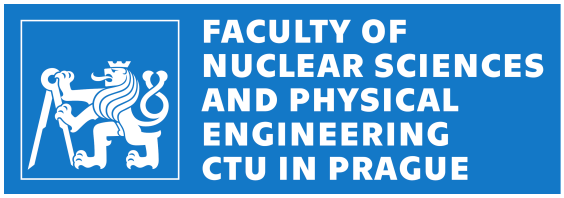

Contribution ID: **31** Type: **Poster**

Applications of quantum computers in quantum chemistry

Wednesday, 25 May 2022 16:10 (20 minutes)

Quantum computing has received a lot of attention recently, and specifically its application in quantum chemistry looks very promising. This research project summarizes the most important methods used in calculating the electronic structure of a chemical system on quantum computers. This includes the formulation of the problem in first and second quantization and the use of classical computational methods of quantum chemistry, starting with the Born-Oppenheimer approximation.
In particular, attention is paid to the Hartree-Fock method, from which more advanced approaches follow. Next, methods for mapping fermions to qubits are discussed and extra space is given to the Bravyi-Kitaev transform. This is then exploited in two quantum algorithms suitable for determining the ground state.
The first is an algorithm for phase estimation. Within this, two methods for simulating the Hamiltonian are described, namely the so-called Trotterization and qubitization. The second is a variational algorithm for energy estimation suitable already for NISQ computers.
Finally, the aim of the research project will be to demonstrate the derived methods on examples of simple molecules.

Primary authors: CIGNA, Ludvík (FNSPE, CTU in Prague); ŠTEFAŇÁK, Martin (CTU FNSPE)

Session Classification: Poster