Quantum computing applied to calculations of molecular energies

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Quantum chemical calculations achieved a huge success in the last decades, particularly due to the enormous progress in computer technology. They became an indispensable part of basic as well as applied chemical research. The situation is however far from ideal. Exact solution of the Schrödinger equation within a finite one-particle basis set (full configuration interaction, FCI) is limited only to the smallest systems (diatomics, triatomics) because of the exponential scaling of its computational cost. Computational quantum chemistry is therefore based on *approximate* methods with polynomial scaling (e.g. DFT, MP2, CCSD, etc.), which can be applied to larger systems, but whose accuracy is often not high enough.

Quantum computers are appealing for their ability to solve some tasks much faster than their classical counterparts. To be more precise, there exist polynomially scaling algorithms to solve tasks, for which only algorithms with an exponential scaling on classical computers are known. The most prominent example is the famous Shor's algorithm for factoring integers, with potentially far-reaching consequences for cryptography. For quantum chemistry, the Abrams's and Lloyd's polynomially scaling algorithm for solving the many-body Hamiltonian eigenvalue problem [1] is of central importance. It has been estimated, that a quantum computer with mere 64 qubits would outperform largest classical supercomputers in FCI [2].

Our work represents a continuation of the pioneering work by Aspuru-Guzik et al. [2]. We will present in detail, how the "quantum diagonalization" algorithm [1] can be used for molecular Hamiltonians. We have developed our own software for simulation of a quantum computer. Its first applications are simulations of quantum FCI (QFCI) calculations of the dissociation of hydrogen molecule.

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[1] Abrams, D. S.; Lloyd, S. *Phys.Rev.Lett.* **1999,** *83,* 5162-5165.
[2] Aspuru-Guzik, A.; Dutoi, A. D.; Love, P. J.; Head-Gordon, M. *Science* **2005,** *309,* 1704-1707.

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