**A diagram of a molecule and a diagram of a computer

Description automatically generatedM.Sc. Project:   
Simulating Water Molecules on a Quantum Computer**

Computer simulations of aqueous systems are used in many research fields, ranging from biological systems to catalytic materials for water electrolysis. To accurately describe such chemical systems, a quantum-mechanical treatment of the molecular electronic structure is required. On classical computers, however, quantum-chemical simulations are very time-consuming due to the fast growth of the molecular Hilbert space with the number of electrons, restricting accurate calculations to small molecular systems. On the contrary, quantum computers are by design well adapted to the simulation of quantum systems, making them highly attractive for applications in quantum chemistry.

This M.Sc. project will take first steps towards the simulation of aqueous chemical processes by quantum computation (QC). To this end, the M.Sc. student will develop a method for calculating the electronic ground state of water molecules on a quantum computer [1]. Adapting a hybrid quantum-classical algorithm recently developed in the Orth group at Saarland University [2], the goal of the project is to investigate properties of the ground state of a many-body Hamiltonian describing the electronic structure of the water molecule. This will be investigated using a quantum Krylov subspace method that uses a quantum-circuit ansatz implemented within the IBM Qiskit framework. Different mappings of the problem onto quantum hardware will be compared. This project will explore the foundations of accurate and effective simulations of water on quantum hardware. The M.Sc. student will be jointly supervised by Prof. Peter P. Orth from Saarland University and Dr. Tobias Binninger from the Institute for Theory and Computation of Energy Materials (IET-3) at Forschungszentrum Jülich.

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**References**

[1] Y. Nam *et al.*, Ground-state energy estimation of the water molecule on a trapped-ion quantum computer, *npj Quantum Inf* **6**, 33 (2020).

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[2] J. C. Getelina *et al.*, Quantum subspace expansion in the presence of hardware noise,   
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See also: *arXiv*:2404.09132 (2024). <https://doi.org/10.48550/arXiv.2404.09132>