

# Quantum Computing for Quantum Chemistry

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In quantum computing, significant efforts are devoted to developing quantum algorithms with the long-term goal of accessing properties of molecular systems beyond the reach of classical computation. However, current quantum devices remain very noisy and limited, requiring adapted algorithmic strategies.

In this introductory talk, I will present how a molecular physics problem can be formulated for implementation on current quantum computer. More specifically, I will discuss how the electronic structure of a molecule can be mapped onto a collection of qubits. Based on this, I will then discuss a key algorithm for approximating molecular ground states that is tailored to near-term devices: the Variational Quantum Eigensolver.

I will then extend this framework to molecular polaritonic systems, where a molecule is strongly coupled to a photonic environment inside an optical cavity. Simulating *ab initio* polaritonic chemistry requires efficient representations of strongly correlated light-matter states, raising the question of whether qubit-based encodings are optimal or whether alternative paradigms may offer advantages. I will then discuss encoding strategies based on quBits, quDits, and quModes, with an emphasis on higher-dimensional representations.