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Quantum computing in chemistry, molecular biology, and materials science

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Abstract

Many problems in molecular science and condensed-phase systems, which are both governed by the dynamics of electrons and atomic nuclei, demand an explicit quantum mechanical description. In such quantum problems, the representation of wave functions grows exponentially with system size, which poses a severe restriction on traditional approaches. However, such quantum problems should naturally benefit from digital quantum simulation on a number of logical qubits, as this would scale only linearly with system size. In recent years, we have considered quantum computing applications in molecular biology, catalysis, and physical chemistry in general, with a focus on how and where to establish a quantum advantage in these areas (see list of references below). In my talk, I will elaborate on the potential benefits of quantum computing in these application areas, especially when compared to state-of-the-art traditional approaches.

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