

Editorial: Quantum Computing for Chemistry



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Quantum computing is an emerging technology with the potential to revolutionize computational studies in chemistry and materials science. Unlike conventional classical computers, quantum computers can harness the power of quantum superpositions and entangled states to achieve a quantum advantage in various challenging computational chemistry problems. In recent years, there has been a growing interest in exploring new ways to apply quantum computing to chemistry. This is reflected in the increasing number of manuscripts published in *The Journal of Chemical Theory and Computation* (JCTC) on this topic.

This **Virtual Issue** on “Quantum Computing for Chemistry” highlights recent articles published by *The Journal of Chemical Theory and Computation* (JCTC) on this exciting and rapidly evolving field. The selection of papers reflects the abundance of open problems in quantum computing simulations for chemistry. Most of these papers report new quantum algorithms for predicting the electronic structure of molecules^{1–7} and simulating chemical dynamics.^{8,9} For example, ref 1 presents a new quantum algorithm that produces wave functions for quantum chemistry problems that are systematically improvable. Reference 6 introduces low-cost wave functions based on coupled-cluster with paired double excitations, which are optimal wave function ansätze for variational quantum algorithms. Other papers in this **Virtual Issue** seek to reduce quantum resource requirements using Hamiltonian downfolding^{10–12} and encoding of operators.^{13–15} One paper presents an approach to estimating quantum resources needed for practical applications of quantum computation in chemistry.¹⁶ Another paper describes the realization of quantum computers with molecular electronics,¹⁷ and one paper introduces software for emulating quantum algorithms for quantum chemistry.¹⁸ This impressive selection of papers highlights only a small fraction of the cutting-edge research at the interface of theoretical chemistry and quantum computing. Quantum computing has also been applied to solve challenging classical problems that arise in chemistry, such as molecular docking and molecular search in databases. We hope the highlighted articles will inspire researchers to further develop this field, as the JCTC is committed to publishing highly impactful manuscripts in this broad area of chemical theory and quantum computation.

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Notes

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