The Basics of Quantum Computing for Chemists

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Abstract

The rapid and successful strides in quantum chemistry in the past decades can be largely credited to a conspicuous synergy between theoretical and computational advancements. However, the architectural computer archetype that enabled such a progress is approaching a state of more stagnant development. One of the most promising technological avenues for the continuing progress of quantum chemistry is the emerging quantum computing paradigm. This revolutionary proposal comes with several challenges, which span a wide array of disciplines. In chemistry, it implies, among other things, a need to reformulate some of its long established cornerstones in order to adjust to the operational demands and constraints of quantum computers. Due to its relatively recent emergence, much of quantum computing may still seem fairly nebulous and largely unknown to most chemists. It is in this context that here we review and illustrate the basic aspects of quantum information and their relation to quantum computing insofar as enabling simulations of quantum chemistry. We consider some of the most relevant developments in light of these aspects and discuss the current landscape when of relevance to quantum chemical simulations in quantum computers.

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