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Quantum computing for chemistry

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Abstract

Five years ago, we discussed whether and how quantum computing may contribute to the solution of actual chemical problems that are hard to tackle with traditional means at the example of the nitrogenase enzyme [PNAS 114 (2017) 7555]. We have recently updated that study at another example (a carbon dioxide fixation catalyst), considering latest estimates for hardware timings and algorithmic advances [Phys. Rev. Res. 3 (2021) 033055]. A main result of these efforts, which always target the exact many-particle wave function, has been that quantum computing may indeed become a game changer in the not too distant future. Accordingly, we proceeded to present a more general discussion of a potential quantum advantage in the molecular sciences in a perspective article [arXiv:2102.10081], which ponders the many aspects of a quantum computation in comparison to competing traditional methods (see, e.g., the density matrix renormalization algorithm as an example [J. Chem. Phys. 152 (2020) 040903]). Apart from error-controlled exact-diagonalization solutions, more approximate parametrization obtained, for example, with the variational quantum eigensolver are also advantageous (see, for instance, our contribution to this field regarding vibrational spectroscopy [Chem. Sci. 11 (2020) 6842]). In my talk, I will review our work of the past years and present an outlook to future work.