A Perspective on Quantum Computing in Chemistry

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Chemistry was identified some years ago as a promising area for the early applications of quantum computers.[1] Consultancy firms were discussing the disruptive potential of the emerging quantum technology for the chemical industry in general and for pharma in particular, while Google and Microsoft have also published their more cautious evaluation of the potential benefits.[2,3] More recently, the general applicability of exponential speed-up arguments to problems of quantum chemistry has also been questioned.[4] In this contribution, our own recent results[5] will be presented in the specific case of pharmaceutical applications. While pharmaceutical systems are not typically strongly correlated, and thus are not of the type where quantum advantage is typically anticipated, this choice is motivated by the recent interest of the pharmaceutical industry in quantum computing. Based on a number of assumptions consistent with the current state-of-the-art quantum algorithms, we find that the time required to compute the exact energy within an active space scales polynomially with the number of active space orbitals in the system considered. While this is promising, it remains to be seen what advantage this will yield over CC and DFT approaches once the quantum hardware is available to carry out these calculations. Indeed, quantum benefit defined in terms of gains over established workflows may be at least as hard to achieve as quantum advantage defined in terms of formal criteria.

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