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Quantum computation for quantum chemistry¹

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Numerically exact simulation of quantum systems on classical computers is in general, an intractable computational problem. Computational chemists have made progress in the development of approximate methods to tackle complex chemical problems. The downside of these approximate methods is that their failure for certain important cases such as long-range charge transfer states in the case of traditional density functional theory. In 1982, Richard Feynman suggested that a quantum device should be able to simulate quantum systems (in our case, molecules) exactly using quantum computers in a tractable fashion. Our group has been working in the development of quantum chemistry algorithms for quantum devices. In this talk, I will describe how quantum computers can be employed to carry out numerically exact quantum chemistry and chemical reaction dynamics calculations, as well as molecular properties. Finally, I will describe our recent experimental quantum computation of the energy of the hydrogen molecule using an optical quantum computer.

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