Molecular simulation with quantum computers

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Quantum mechanical simulations of molecules provide a sub-atomic understanding of chemical reactions and properties. Due to the exponential scaling of the simulation of many-body systems, these simulations are obtained only as approximations to the electronic Schrodinger equation. Although, in principle one can increase the sophistication of an approximation arbitrarily until a desired accuracy is reached, more sophisticated calculations rapidly become intractable for even the largest supercomputers. Quantum computers provide a promising route to bypass these limitations in molecular simulation. In this talk, I will discuss some of the basic ideas underlying the use of quantum computation for molecular simulation and describe some of the recent work from our group.