Quantum chemistry problems, such as static molecular energy calculation and dynamical chemical reaction simulation, become very intractable on classical computers with the system scaling up. However, quantum simulation is a feasible and effective approach to these problems. Proof-of-principle experiments have been implemented on the calculation of the hydrogen molecular energies and the one-dimensional chemical isomerization reaction dynamics using nuclear magnetic resonance (NMR) quantum simulators. We expect that quantum simulation will surpass the classical computers towards quantum chemistry in the near future.