Dear *Science* Editors:

I am submitting to your editorial office the attached manuscript entitled “Simulation of Chemical Reaction Dynamics on an NMR Quantum Computer” for your consideration as a Report in your highly prestigious journal *Science*. The manuscript is also accompanied by a supplementary file as online supporting material.

In quantum information science, though it has been quite a few years since the discovery of general-purpose quantum algorithms (such as Shor’s factorizing algorithm), experimental progresses on their execution on a quantum computer is slow because they typically requires thousands of qubits to beat classical computers. By sharp contrast, quantum simulations of specific classically hard problems on a quantum simulator can surpass the capacity of current classical computers with a few tens of qubits (about 30-100 qubits). Indeed, successful quantum simulations of significant and challenging problems in some particular areas will offer a conceivable key milestone for quantum information science and for quantum physics. As a matter of fact, in the strategic report of quantum computation of European Union (<http://www.qurope.net>), it is hoped to realize quantum simulation that cannot be simulated classically within the following 5 years.

The quantum simulation of chemical reaction dynamics, which belongs to one of the most computationally challenging problems in physical sciences, is now demonstrated for the first time in our experiment. The submitted manuscript reports the first NMR-based quantum simulation of a laser-driven chemical reaction process. Our experimental results of the continuous reactant-to-product transformation agree remarkably well with theory, thus offering the first evidence that quantum simulation of chemical reaction dynamics is feasible in practice, even on a rather small quantum computer. Our cross-disciplinary experiment will motivate substantial future studies of quantum simulation of quantum chemistry problems and will attract interests from many research fields including quantum chemistry, chemical physics, quantum information, and quantum computation.

For these reasons, we trust that that the submitted manuscript is of sufficient interest to the broad audience of *Science*. Thank you for your kind consideration of this submission. For your convenience, in a separate file we have also provided a list of possible referees. The suggested referees are renowned international leaders in various research fields closely related to our work.

Looking forward to hearing from you soon.

Sincerely,

Jiangfeng Du

Professor of Physics