Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Towards Quantum Chemistry on a Quantum Computer ALAN ASPURU-GUZIK, Department of Chemistry and Chemical Biology, Harvard University — The fundamental problem faced in quantum chemistry is the calculation of molecular properties, which are of practical importance in fields ranging from materials science to biochemistry. Recently, an efficient algorithm has been proposed enabling a quantum computer to overcome this problem by achieving only a polynomial resource scaling with system size. Such a tool would therefore provide an extremely powerful tool for new science and technology. Here we present a photonic implementation for the smallest problem: obtaining the energies of H2, the hydrogen molecule in a minimal basis. We perform a key algorithmic step - the iterative phase estimation algorithm - in full, achieving a high level of precision and robustness to error. We implement other algorithmic steps with assistance from a classical computer and explain how this non-scalable approach could be avoided. Finally, we provide new theoretical results which lay the foundations for the next generation of simulation experiments using quantum computers. We have made early experimental progress towards the long-term goal of exploiting quantum information to speed up quantum chemistry calculations.

Alan Aspuru-Guzik
Department of Chemistry and Chemical Biology, Harvard University

Date submitted: 02 Dec 2009 Electronic form version 1.4