Realizing Exited States and Dynamics Simulations on Near-Term Quantum Computers

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Computational chemistry is considered one of the key applications that has the potential of exploiting quantum computers for scientific discovery. Over the years, significant advances have been made developing algorithms and methodologies to make quantum chemistry simulations on quantum computers a reality. I will highlight some of our efforts developing approaches and algorithms to obtain excited states from molecular simulations, and study the dynamics of closed and open quantum systems on quantum computers. To obtain reliable results from NISQ quantum computers, error mitigation, and reduction of computational complexity are essential. Some of our efforts to enable reliable quantum chemistry simulations will be discussed. While progress has been made in hardware, software, and algorithms, much work is still to be done to make scientific quantum computing a reality. I will introduce the AIDE-QC (aide-qc.org) software stack containing high level programming models, quantum compilers, and validation and debugging tools, aimed at providing a software platform to enable the scientific community easier access to quantum computing platforms.