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Simulating Molecular Spectroscopy with Circuit Quantum Electrodynamics LING HU, YUECHI MA, WEITING WANG, YUAN XU, KE LIU, Center for Quantum Information, Institute for Interdisciplinary Information Sciences, Tsinghua University, Beijing 100084, China, MANHONG YUNG, Department of Physics, South University of Science and Technology of China, Shenzhen, Guangdong, 518055, China, LUYAN SUN, Center for Quantum Information, Institute for Interdisciplinary Information Sciences, Tsinghua University, Beijing 100084, China — Quantum simulation represents a powerful and promising means to overcome the bottleneck for simulating physical and chemical systems with classical computers. One of the major applications for quantum simulation is to solve molecular problems. However, the molecular simulation experiments performed so far are all confined to the study of static properties of molecules. In this talk, we present a method for simulating the dynamics and the absorption spectrum of molecules, and report the experimental results of its implementation using a superconducting device with a 3D circuit quantum electrodynamics architecture. We simulate the spectra for a variety of scenarios, in particular, for molecules with different Huang-Rhys parameters, which depend on the electron-phonon coupling strength for real molecules. Our simulation results show that our method can be achieved experimentally with high fidelity.

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