# Quantum Computing for Chemistry: Scaling up and Accelerating the Quantum-Circuit Simulations with NVIDIA CUDA Quantum

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CUDA quantum is an open-source programming model extending both C++ and Python with quantum kernels intended for compilation and execution on quantum hardware. Along with CUDA quantum, NVIDIA has developed cuQuantum, an optimized library for accelerating quantum computing workflows. With NVIDIA Tensor Core GPUs, developers can use cuQuantum to speed up quantum circuit simulations based on state vector and tensor network methods by orders of magnitude. CUDA Quantum in combination with cuQuantum forms a powerful platform for hybrid algorithm research.

In this talk, I will introduce CUDA quantum and show its advantages in quantum chemistry for hybrid quantum-classical algorithmic research and development. Specifically, I will demonstrate a hybrid application considering the reduction of molecules on a metallic surface. The results will demonstrate quantum programmability, integration of classical and quantum resources, and large-scale quantum circuit simulation on GPU supercomputing architectures.