

Quantum Computing Use Cases in Computational Chemistry

Catalyst Modeling and Synthesis

State of the Art: Simulations and AI have revolutionized the design of custom chemicals and materials, leading to substance designs with specific properties. However, their synthesis requires lab experiments and validation. Improved catalyst modeling (MOFs, Zeolites, etc.) unlock opportunities for clean energy, energy storage, and efficient resource use, which can improve existing refining processes and quality.

Despite quantum mechanics' crucial role in understanding chemical behaviors, traditional computational methods struggle with the complexity of quantum equations. Even top supercomputing centers take weeks to accurately simulate water phase changes. Modeling catalyst formation is challenging due to their indefinite growth and geometric tiling in all directions.

Improving Crude Oil Recovery and Chemical Performance

State of the Art: The use of libraries like LAMMPS for molecular dynamics and psi4 for quantum chemistry improves the computational design of functional materials and chemicals. These tools allow for the application of simplified assumptions like Density-Functional Theory (DFT), enabling the efficient and accurate modeling of complex systems with tradeoffs.

Recent advances in the oil field have seen the application of chemical enhanced oil recovery (EOR) methods, which rely on the injection of chemicals to boost oil recovery. This technique has been found to be effective in recovering bypassed oil and residual oil trapped in the reservoir. Quantum mechanical effects start to dominate when modeling nanometer pores and smaller. The liquid and vapor phase behavior is particularly interesting.

Quantum Opportunities

Catalyst Modeling and Synthesis

Quantum computing offers significantly improved precision and could help in the formulation of mixtures by making possible an improved understanding of the complex molecular-level processes involved. The most effective strategies split the work over classical and quantum computers.

Methods such as embedding, multi-scale, and fragment techniques, are critical for describing complex chemical systems efficiently with limited quantum computational resources. This lowers qubit requirements from millions to hundreds, depending on the size and numbers of unique chemical fragments. More efficient algorithms are possible, such as modeling kinetics with quantum circuits, resulting in a computationally efficient N-Body algorithm.

Improving Crude Oil Recovery and Chemical Performance

Despite quantum mechanics' foundational role in understanding chemical behaviors, traditional computational approaches face significant challenges, largely due to the complexity and computational intensity of quantum mechanical equations. Efficient quantum algorithms for chemistry problems are expected to have run-times and resource requirements that scale polynomially with system size and desired accuracy, opening up the possibility of modeling chemical systems with improved levels of precision.

Current resource estimates suggest that 50,000 qubits are needed for quantum circuits to model molecules like hexane, with 600,000 qubits needed for molecules with 20 carbon atoms.

