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Utilizing quantum computing for mechanistic modeling of reactions in hydrogen fuel cells.

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Fuel cells offer an elegant means of harnessing the chemical energy stored within the bonds of hydrogen and oxygen, converting it into electrical energy. However, existing fuel cell technologies suffer by a significant overpotential during the oxygen reduction reaction (ORR) at the cathode.
Given hydrogen's pivotal role as a promising low-carbon and sustainable fuel for the future, there is a growing endeavour to simulate its reactivity under various operational conditions and using diverse catalysts.

In this context, we explore of the cathodic reduction of oxygen employing quantum computing techniques. Our approach involves modelling the reaction pathways and determining energy levels through multiconfigurational methods, all structured within a NISQ-friendly workflow. We adopt a Variational Quantum Eigensolver strategy, leveraging the Unitary Coupled Cluster Singles and Doubles ansatz wavefunction within a compact active orbital space to capture static correlation energy. Subsequently, we measure the expectation value of energy and reduced density matrices enabling us to perform the perturbation expansion necessary for capturing dynamical correlation on a classical computer.

We demonstrate that the catalyst's structure significantly impacts the reaction pathway of the ORR, as well as the electronic wavefunction's nature, which becomes highly correlated when a sublayer of cobalt is introduced beneath the surface of platinum. This scenario presents an ideal opportunity for quantum computers, as they may offer advantages over conventional strongly correlated methodologies.

Abstract category

Quantum Chemistry

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