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Investigating computational methods to predict redox potentials for quinones

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Due to an ongoing pursuit to replace fossil fuels with renewable energy sources, there is a high demand for large-scale electrical grid storage. Computational chemistry methods can be used to predict redox potentials of benzoquinones and hydroquinone's; the potentials of which can be tailored by the addition of electron withdrawing groups and electron donating groups. Quinones are an attractive organic material for aqueous flow batteries because they are low cost and undergo a reversible two-electron, two-proton redox reaction. Therefore, these organic species can be stored as chemical energy in electrolyte tanks, and be pumped into a regenerative fuel cell to undergo oxidation and reduction, when electric power is needed. This study has two objectives: 1) find a theory and functional pair that accurately predicts redox potentials, 2) find potential organic species for an aqueous flow battery. This presentation will report geometry optimizations using different theories and functionals, to determine which experimental set up most accurately predicts redox potentials. Quantum chemical calculations were performed using the 2012 MOLPRO software package. Accuracy is measured by the linear correlation between calculated potentials and experimental potentials. Experimental values are from Wedege's 2016 scientific report, *Organic Redox Species in Aqueous Flow Batteries: Redox Potentials, Chemical Stability and Solubility.* Quantum chemical methods can thus aid electrochemists in the effort to make an all organic aqueous flow battery, provided accurate redox potentials are ensured by calculations.

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