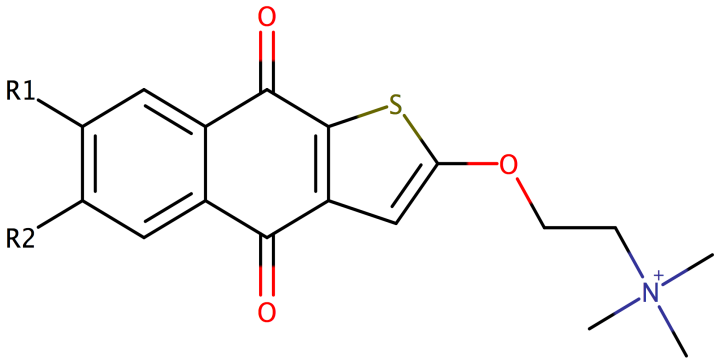
Computational Screening for High Performance Aqueous Redox Flow Battery Materials

Richard Phillips, Joshua Schrier
Department of Chemistry, Haverford College
370 Lancaster Ave, Haverford PA

Redox flow batteries using water-soluble quinone derivatives have significant potential as a means of environmentally clean and cost-effective energy storage. However, to maximize energy density, there must be a larger range of half-cell potentials and improvements must be made to solubility, to increase power density, and cost before redox flow batteries become a viable means of energy storage. Reduction potentials for affordable and synthetically feasible thiophenoquinone derivative frameworks were calculated with model chemistry B3LYP/6-311+G(d,p) for thermochemical calculations (using the SMD solvation model). Our previous work shows that this estimates the redox potential to within +/- 0.03 V. Reduction potentials for the same molecules were calculated with an attached quaternary ammonium tail. Calculations assert that the addition of the quaternary ammonium tail greatly reduces the ΔG of solvation (predicted difference of ~240 kJ/mol for each species). Among the molecules tested, a notable minimum voltage was naphtho(2,3-b)thiophene-4,9-dione with an attached quaternary ammonium tail (NAP) with a predicted reduction potential of 0.15 V.



Calculations were made for the redox potentials for NAP with 9 different functional groups (-NCH_3CH_3, -$NHCH_3$, -NH_2, -CCH, -$CCCH_3$, -SH, -OH, -OCH_3, -SCH_3) each tested in two different positions. From this data, eight molecules are predicted to have lower voltages than NAP, including a molecule with a calculated reduction potential of -0.02 V.