Hybrid Theory Simulation for Polymer Batteries

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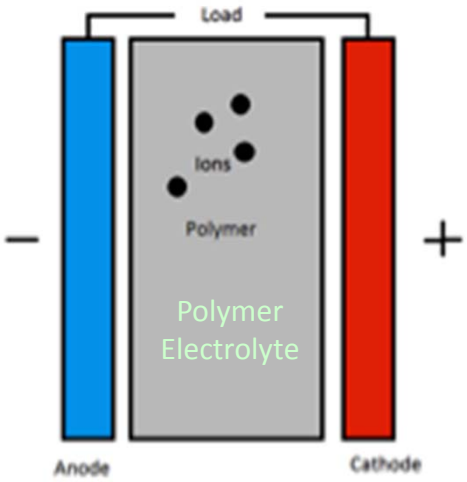
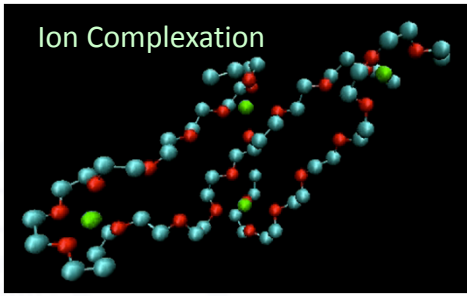
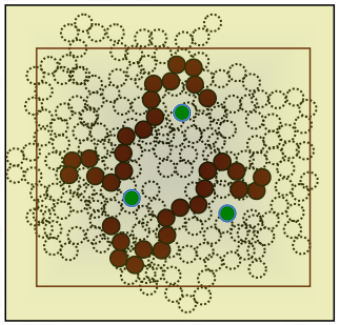


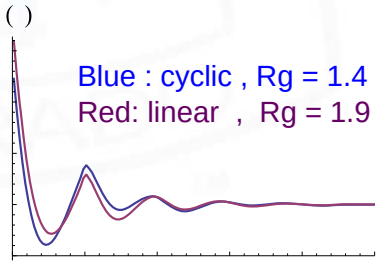
Polymer batteries are of great interest due to their high energy density, stability, and material properties, but suffer from low ionic conductivity, controlled by the complexation of ion by polymer. The ionic conductivity is a challenge for both heory and simulation due to need for capturing ion binding as well as the long times and lengths associated with polymers.





Hybrid theory-simulation

We are developing new efficient **hybrid theory-simulation methodologies** that capture the complexity of ion binding by atomistic simulation of just a few molecules (brown & green in figure), while accounting for the many surrounding polymers (white) by statistical mechanical theory. We have tested our methodology on the surface profiles of blends of linear and cyclic polymers, analogs of the binding regions on the polymer, and have found linear polymers to be enhanced at the surface, in agreement with experiment and in contradiction with previous theory. We are extending our calculations to more realistic models of the polymer chain and ion complex.



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