CNE Summer School Summary of Teaching Material

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The lectures were segmented between three 1.5-hour lectures provided in a single day.

The morning lecture focused on polymer electrolyte structure and function with a short video on preparative methods for fuel cell membrane electrode assemblies. The morning lecture included an in-class workshop on deriving full fuel cell performance curves using anode and cathode polarization curves including a high-level review of Butler Volmer kinetics. The session concluded with a comparison of classical molecular dynamics contrasted with ab-initio MD applied to polymer electrolytes.

The mid-day session continued discussion of molecular dynamics with an emphasis on correlating MD calculations to infrared spectroscopy. We showed that given any overall ratio of waters to ionomer exchange sites, there exists a distribution of local exchange site ratios. The concept of vibrational spectra as a sum of spectra representing a distribution of waters to exchange sites was introduced.

The final session focused on operando Raman micro-spectroscopy of fuel cell electrode layers. It was demonstrated that when attempting to obtain Raman spectra of black layers, there is an advantage to having the Raman laser focal point above the surface of interest. Background from the focal point is eliminated by sequestering the focal point within a Raman grade CaF_2 window.