MAR15-2014-020019

Abstract for an Invited Paper
for the MAR15 Meeting of
the American Physical Society

Segmental Interactions between Polymers and Small Molecules in Batteries and Biofuel Purification

NITASH BALSARA, UC Berkeley

Polymers such as poly(ethylene oxide) (PEO) and poly(dimethyl siloxane) (PDMS) have the potential to play an important role in the emerging clean energy landscape. Mixtures of PEO and lithium salts are the most widely studied non-flammable electrolyte for rechargeable lithium batteries. PDMS membranes are ideally suited for purifying bioethanol and biobutanol from fermentation broths. The ability of PEO and PDMS to function in these applications depends on segmental interactions between the polymeric host and small molecule guests. One experimental approach for studying these interactions is X-ray absorption spectroscopy (XAS). Models for interpreting XAS spectra of amorphous mixtures and charged species such as salts must quantify the effect of segmental interactions on the electronic structure of the atoms of interest (e.g. sulfur). This combination of experiment and theory is used to determine the species formed in during charging and discharging lithium-sulfur batteries; the theoretical specific energy of lithium-sulfur batteries is a factor of four larger than that of current lithium-ion batteries. Selective transport of alcohols in PDMS-containing membranes is controlled by the size, shape, and connectivity of sub-nanometer cavities or free volume that form and disappear spontaneously as the chain segments undergo Brownian motion. We demonstrate that self-assembly of PDMS-containing block copolymers can be used to control segmental relaxation, which, in turn, affects free volume. Positron annihilation was used to determine the size distribution of free volume cavities in the PDMS-containing block copolymers. The effect of this artificial free volume on selective permeation of alcohols formed by fermentation of sugars derived from lignocellulosic biomass is studied. Molecular dynamics simulations are needed to understand the relationship between self-assembly, free volume, and transport in block copolymers.