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ACCEPTED MANUSCRIPT

Bridging the Gap between Macroscopic Electrochemical Measurements and Microscopic Molecular Dynamic Simulations: Porous Carbon Supercapacitor with Ionic Liquids

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Abstract

We apply a combination of experimental measurements and molecular dynamic (MD) simulations to describe imidazolium ionic liquids with porous carbon electrode. On the experiment's side, electrochemical measurements are conducted on two types of porous carbon electrodes prepared from different pore size distributions. The general trend of variations for impedance are identified at various temperatures and electrode geometries in Nyquist plots. On the simulation's side, fundamental geometries including slit and cylindrical pores are modeled to determine the ions' behaviours during charging and discharging process. By examining the local charges variations, the electrode charging or polarization are correlated with ion dynamics or relaxation, particularly in the vicinity of electrode. In one-to-one correspondence to experiments, linear segment of impedance for individual pores gives rise to the constant phase element in fitting of porous electrode's equivalent circuit. Our MD simulations explored the path of implementing the techniques of cyclic voltammetry and electrochemical impedance spectroscopy.

1. Introduction

The ionic-liquids based supercapacitor system remains the subject of extensive experimental and theoretical studies. MD simulations have studied

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