

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Morphology-induced low temperature conductivity in ionic liquids.¹ AYKUT ERBAS, MONICA OLVERA DE LA CRUZ, Northwestern University, OLVERA DE LA CRUZ TEAM — Ionic liquids exhibit nano-scale liquid crystalline order depending on the polymeric details of salt molecules. The resulting morphology and temperature behavior are key factors in determining the room temperature conductivity of ionic liquids. Here we discuss the phase behavior and related ionic conductivities of dry ionic liquids with volume fractions close to unity by using extensive molecular dynamics simulations. Temperature dependence, effective persistence length of tails, and excluded volume symmetry of amphiphilic ionic liquid molecules are investigated in large scale systems with short and long-range electrostatics. Our results suggest that by adjusting stiffness of the amphiphilic molecules and excluded volume interactions, lamellar or interconnected 3D phases can be obtained. Resulting phases have significant effects on the conductive properties. If there is no excluded volume asymmetry along the molecules, mostly lamellar phases with anisotropic conductivities emerge. If the excluded volume interactions become asymmetric, lamellar phases are replaced by interconnected phases consist of charged groups. Within temperature ranges that morphological phases are observed, conductivities exhibit low-temperature maxima in accord with experiments of ionic liquid-based liquid

¹Center of Bio-inspired Energy Center (CBES)

Aykut Erbas
Northwestern University

Date submitted: 05 Nov 2015

Electronic form version 1.4