# PHYSICAL MATHEMATICS SEMINAR

# Charge ordering in Room Temperature Ionic Liquids


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**ABSTRACT:**

Ionic liquids have emerged in recent years as promising candidates for the next generation of electrochemical devices, but due to the strong electrostatic interactions, classical theories of electrolytes fail to explain their observed charge ordering. We show that given the ionic positions extracted from molecular simulations, the ionic charges minimize a "spin-glass" Hamiltonian with remarkable accuracy. The minimization procedure is carried by the powerful Goemans-Williamson Max-Cut algorithm, adapted for a fully-connected graph with Coulombic interactions. We find that our approach works well for a wide range of behaviors, from room-temperature ionic liquids and molten salts with long-ranged charge oscillations to short-range correlations in "water-in-salt" electrolytes. It can be extended to other disordered systems with strong anti-ferromagnetic interactions, such as the two-dimensional vortex patterns found in bacterial turbulence. We demonstrate how the persistent layering structure exists due to positional ordering, which is maximized in ionic solids but gradually disappears with added solvent. As the electrolyte becomes more disordered, geometrical frustrations in the spin-glass ground state reduce correlation lengths.


**TUESDAY, OCTOBER 22, 2019**
**2:30 PM – 3:30 PM**
**Building 2, Room 131**

***Reception following in Building 2, Room 290***
***(Math Dept. Common Room)***

*http://math.mit.edu/seminars/pms/*

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