

# CHEMICAL, BIOLOGICAL & MATERIALS ENGINEERING

100 E. Boyd, Sarkeys Energy Center, T-301

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The University of Oklahoma

Norman, Oklahoma

PHILLIPS 66 SEMINAR SERIES, 2016 – 2017

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## DR. EDWARD MAGINN

DORINI FAMILY PROFESSOR AND DEPARTMENT CHAIR

CHEMICAL AND BIOMOLECULAR ENGINEERING

UNIVERSITY OF NOTRE DAME

NOTRE DAME, INDIANA

Our seminar

### **“UNRAVELING THE STRUCTURE AND DYNAMICS OF ELECTROLYTES AND IONIC LIQUIDS VIA MOLECULAR SIMULATION”**

Liquids that contain charged species, such as electrolytes and ionic liquids, have many important technological applications in fields such as energy storage, separations, and catalysis. By changing the structure of the molecules or employing mixtures, the properties of these fluids can be altered significantly. The key question is: what should we do to get the properties we want? In other words, how should I change the structure of the molecule or ion? What type of solvent should I add to the mixture to get the behavior I want? To answer this, we use atomistic-level simulations to compute structural, thermodynamic and transport properties of these systems. We are able to provide molecular-level explanations for experimental observations, and we can predict properties of systems that may not yet have even been made in the laboratory.

In this talk, I will focus on recent efforts we have made as a member of the DOE-sponsored Joint Center for Energy Storage Research (JCESR) in computing conductivity, viscosity, and self-diffusivity of ionic liquids mixed with monovalent and divalent cations and diluents such as glycol ethers. Using high throughput computational methods, we have identified several new types of anions that may enable the use of divalent cations such as  $Mg^{2+}$  in rechargeable batteries. We have also helped explain unusual trends observed experimentally in the liquid dynamics of cations with progressively longer alkyl tails. Finally, I will describe how simulations can be coupled with X-ray scattering experiments to provide a detailed picture of the organization of these liquids on the 1-20 nm length scale.

**THURSDAY, APRIL 20, 2017**

**COOKIES AND COFFEE -- 1:30 P.M.**

**SEMINAR -- 1:45 P.M.**

**SARKEYS ENERGY CENTER, M-204**

**THIS IS A REQUIRED SEMINAR FOR CHE 5971**

Accommodations on the basis of disability are available by contacting the office.