AEROSPACE & MECHANICAL ENGINEERING

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INFORMAL COFFEE PERIOD BEFORE THE SEMINAR IN ROOM 365 FITZPATRICK HALL

UNIVERSITY OF NOTRE DAME, NOTRE DAME, INDIANA 46556

SPEAKER: **Professor Jianmin Qu**
Department of Civil and Environmental Engineering
Department of Mechanical Engineering
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Evanston, Illinois

TOPIC: **A COUPLED ELECTRO-CHEMO-MECHANICAL FRAMEWORK FOR DIFFUSION AND DEFORMATION IN SOLIDS**

DATE: Tuesday, March 6, 2012

TIME: 3:30 p.m.

PLACE: 138 DeBartolo Hall

ABSTRACT

Solid materials used in energy conversion and storage devices are often subjected to multiple driving forces (electrical, chemical, radiological, thermal, mechanical, etc.). The interactions among these different driving forces often impact the efficiency, reliability and durability of the devices. Understanding of how the different driving forces interact requires theories and models that are capable of accounting for the coupling of multi-physics processes.

In this talk, a framework is presented that couples the mechanical and chemical (or electrochemical) fields in solids via the use of stress-dependent chemical potentials. To illustrate the development and applications of this coupled electro-chemo-mechanical theory, two examples of practical interest will be discussed, namely, solid oxide fuel cells and lithium ion batteries. Our interest is to understand how solid diffusion generates mechanical stresses, and how such mechanical stresses affect the diffusion. The first example is concerned with the interactions between mechanical stresses and ionic transport in the electrolyte of a solid oxide fuel cell. It is found that the non-uniform oxygen vacancy concentration in the electrolyte can generate significant stresses whose amplitude is comparable to the thermal mismatch induced stress in the cell stack. More importantly, significant stress concentration near processing defects (voids and microcracks) occurs due to the presence of ionic fluxes. The second example is on the insertion of lithium into silicon in silicon anodes in lithium batteries. Using input from *ab initio* and molecular dynamic simulations, we investigated the mechanisms of lithium insertion and how the process is affected by mechanical stresses.

NOTE: ***If you are interested in meeting individually with Prof. Qu, please contact Evelyn at 631-5431***