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**Date: September 18, 2007**

**Time: 1:00 pm – 2:30 pm**

**Room: ET 137**

**Everyone is invited**

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## **Development and Characterization of Catalysts Used in Proton Exchange Membrane Fuel Cells**

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**Abstract.** Development of new catalysts with low cost, high efficiency and durability is critical to fuel cell technology advancement. Platinum and its alloys are widely used as catalysts for oxygen electrode in proton exchange membrane (PEM) fuel cells; however, the oxygen reduction reactions (ORR) on Pt are much slower compared to hydrogen oxidation reactions on Pt surfaces. The demands for Pt have exceeded the supplies for the last ten years, which resulted in soaring prices for Pt. Hence, the design and development of novel non-precious metal catalysts with high catalytic efficiency, good stability, good tolerance of impurities and low cost is crucial to the successful commercialization of the PEM fuel cell technology as an energy source.

The Transition metal phthalocyanine macrocycles is a promising class of catalysts as they exhibit good catalytic activity for oxygen reduction reaction. The adsorption of dioxygen is the first step for oxygen reduction. The interaction between metal and the oxygen molecule and its effect in dissociation of O-O bond is important to understand the reaction mechanism. Hence, in this thesis the focus is on the Computation and characterization of transition metal phthalocyanines as catalysts. Simulation of the different reaction pathways is performed using Density Functional Theory to calculate their catalytic activity. Models for the proton interaction with the oxygen have been proposed to simulate the end product in the reaction mechanism. Microscopy Characterization has been done to study the morphology of the membranes.

The knowledge obtained through this study of molecular modeling and molecular Characterization would help design a better non precious metal catalyst for Oxygen reduction reaction which has better durability and efficiency.

**About the Speaker.** Nitia Ramesh is a Master's student and Research Assistant at the Advance Energy Research Laboratory, IUPUI. She received her B. Tech. degree in Mechanical Engineering from Jawaharlal Nehru Technological University, India in (2004).