



*The Abdus Salam*  
**International Centre for Theoretical Physics**



**WORKSHOP ON NEW MATERIALS FOR RENEWABLE ENERGY**  
**17 - 21 October 2011, ICTP, Trieste**

**THEORETICAL MODELING OF PROTON-COUPLED ELECTRON TRANSFER  
REACTIONS IN ENERGY RELATED MATERIALS**

**Alexander V. SOUDACKOV and Sharon HAMMES-SCHIFFER**

Dept. of Chemistry, The Pennsylvania State University  
University Park, PA 16802, U.S.A.

**ABSTRACT 1:**

Proton-coupled electron transfer (PCET) reactions play an important role in many energy related processes including natural and artificial photosynthesis, catalytic and electrocatalytic hydrogen and oxygen evolution, and processes in solar cells. This talk will present a broad overview of theoretical developments in the field of PCET with emphasis on calculation of rate constants and kinetic isotope effects of PCET reactions in solution and at electrochemical interfaces. Several applications of the theory to experimentally studied PCET systems will be discussed.