



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



**WORKSHOP ON NEW MATERIALS FOR RENEWABLE ENERGY**  
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**PRACTICALITIES OF MOLECULAR COMPUTATIONAL MODELING RELEVANT TO  
RENEWABLE ENERGY TECHNOLOGIES**

**Christopher CRAMER**

Dept. of Chemistry and Supercomputer Institute  
University of Minnesota  
Minneapolis, MN, U.S.A.

ABSTRACT 1:

The computational tools used to predict thermodynamic quantities having special relevance to renewable energy will be discussed with the goal of making more clear the scope and limitations of various models. Properties like  $pK_a$ , standard reduction potential, free energies of activation and reaction in condensed phases, and dye absorption wavelengths will be included.