



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

QUANTUM CHEMICAL CHARACTERIZATION OF HOMOGENEOUS CATALYTIC PROCESSES FOR WATER SPLITTING AND CO₂ REDUCTION

Christopher CRAMER

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

ABSTRACT 1I:

Recent work illustrating the use of molecular modeling to elucidate details of catalytic processes relevant for renewable energy technologies will be presented. The possibilities for synergy between theory and experimental design will be emphasized.