

**Institute of Energy Technology – Professorship of Renewable Energy Carriers*****Invitation to a Seminar***

**Date:** Thursday, July 1, 2010  
**Time:** 16:00-17:00  
**Place:** Maschinenlaboratorium ETH Zürich, ML-J25/26

**Speaker:** **Dr. Mark Allendorf**  
**Sandia National Laboratories**  
**Livermore, CA, USA**

**Title:**  
**Thermodynamic and Kinetic Investigations of Thermochemical  
CO<sub>2</sub> and H<sub>2</sub>O Splitting**

**Abstract** - Production of fuels (CO<sub>2</sub> and/or H<sub>2</sub>) using thermochemical reduction/oxidation cycles is attracting considerable interest as a result of both climate change and economic and political realities. Two materials under serious consideration are metal-substituted ferrites (e.g., CoFe<sub>2</sub>O<sub>4</sub>) and ceria (CeO<sub>2</sub>). A fundamental understanding of both the thermodynamics and kinetics of the chemical reactions involved in gas splitting is essential for the successful implementation of these materials for fuel production. This presentation will summarize recent experimental and computational work at Sandia National Laboratories focused on these two metal-oxide systems. Measurements of CO<sub>2</sub> and H<sub>2</sub>O splitting rates will be described, in which a stagnation-flow reactor equipped with a molecular-beam mass spectrometer was used to detect the formation of CO and H<sub>2</sub>. We also employ a novel platform for the ferrite redox materials, in which nanoscale coatings are deposited by atomic layer deposition. This provides exquisite control over layer thickness and composition. Analytical and thermodynamic modeling, backed by microstructure analysis and high-temperature x-ray diffraction, were used to evaluate potential rate-limiting mechanisms, including diffusion, surface chemistry, and nucleation. The results suggest a common rate-limiting mechanism that is independent of sample morphology. Results of phase-equilibrium modeling will also be described, illustrating the importance of including solid solution phases for accurate prediction of thermal reduction and gas splitting.

**Dr. Mark Allendorf** is a Distinguished Member of the Technical Staff at Sandia National Laboratories in Livermore, CA. He received his PhD in inorganic chemistry from Stanford University in 1986. His current research interests include nanoporous materials for chemical and radiation sensing, metal hydrides for hydrogen storage, and high-temperature chemistry for solar-driven fuels production. Dr. Allendorf is a Fellow of The Electrochemical Society and formerly that organization's president. He is the author of over 120 technical papers and the editor of seven books.