

Nanoscale structures in ceria and gadolinia-doped ceria

A. N. Cormack

Kazuo Inamori School of Engineering

New York State College of Ceramics

Alfred University

Abstract:

Ceria is a fascinating material, with a number of important technological applications, ranging from SOFC electrolytes to catalysis. In almost all cases, it is the atomic scale structural features which underlie its usefulness. An appropriate way to approach this is to consider its point defect chemistry, particularly from the point of view of defect aggregation which is observed to occur in doped systems.

In this presentation, we will discuss the aggregation into nano-domains, of the dopants and compensating oxygen vacancies, in gadolinia-doped ceria, using atomistic computer simulations to model the structure and energetics of the doped systems. We approach this from both the viewpoint of the possible structures which can arise from increasing the size of the dopant aggregates and by considering the energetics of strings of oxygen vacancies. We will argue that phase separation is the equilibrium condition, suggesting that the nano-domain structures are only kinetically stable.

In addition, we will discuss briefly some very recent results on defect formation in ceria nano-particles.

Perspectives in the Development of Semiconductor Sensitized Solar Cells

Iván Mora-Seró¹

¹ Grup de dispositius Fotovoltaics i Optoelectrònics, Departament de Física, Universitat Jaume I, 12071 Castelló, Spain.

Abstract:

Semiconductor sensitized solar cells have attracted a growing interests in the last few years. Starting from conversion efficiencies quite low, these have grown very rapidly to values around 4-5%. Further increase in cell performance could arrive from the study and optimization of three aspects of these cells: i) materials, including not only light absorbing material but also electron and hole conductors and counter electrodes; ii) Control of recombination and band alignment by surface treatments; and iii) development of absorbing nanocomposites with enhanced light harvesting and collecting properties. In addition a clear model of the device is needed and will help in the development of these systems. We will analyze these three topics that could promote real breakthroughs in the design and development of semiconductor sensitized solar cells.

Sunlight to Fuel Generation: The spectroscopy of electron transfers between light absorber, catalyst, and reactants

Tanja Cuk

Lawrence Berkeley National Laboratory, USA

Abstract:

The principal challenge for artificial photosynthesis is to design units that complete the two necessary half reactions—the oxidation of water and the reduction of carbon dioxide—efficiently in visible, rather than UV, light. In so doing, the reaction will need to proceed close to the thermodynamic potential of the generated fuels. Therefore, the system should be designed to exploit the inherent efficiency determined by the time scale, molecular configuration, and electronic potential of electrons transfers between the light absorber, catalyst, and reactants. Many of these electron transfer rates, and the electronic and structural configuration in which they occur, are not currently known for water oxidation, let alone for carbon dioxide reduction. In this talk, I will introduce three techniques—time resolved optical spectroscopy, photoemission, and time resolved x-ray spectroscopy—with which to identify the electronic and structural configuration of the important electron transfers.