Nanoscale structures in ceria and gadolinia-doped ceria

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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.

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

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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.