Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Bandgap Modulation of CeO2 Nanoparticles by Codoping of Y and Co Impurities T.S. WU, C.H. LAI, H.T. JENG, S.L. CHANG, Y.L. SOO, National Tsing Hua University — Interplay of trivalent and divalent dopants in (Y, Co) codoped CeO2 nanoparticles with dominantly tetravalent host cations has been investigated using a variety of structural and optical techniques. The nanoparticle samples were prepared by a Polyol method. As revealed by the x-ray diffraction (XRD) data, all nanocrystal samples under investigation have similar average particle size. The concentration of O vacancies in the samples was found to increase with Y doping level as indicated by the Raman spectroscopy, extended x-ray absorption fine structure (EXAFS), and x-ray absorption near edge structure (XANES) data. As determined from diffuse reflectance spectra, the bandgap of the sample appears to decrease with increasing Y concentration. However, a series of Co-free samples measured for comparison show no dependence of bandgap on Y concentration. We have proposed a theoretical model and performed numerical simulation using the Vienna ab initio simulation package (VASP) to explain such bandgap modulation effect.

Yun-Liang Soo
National Tsing Hua University

Date submitted: 14 Nov 2013 Electronic form version 1.4