Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Ab initio study of {In,Ru,Ir}-doped CeO2[1] ROBERTO NUNEZ-GONZALEZ, Universidad de Sonora, RICARDO RANGEL, Universidad Michoacana de San Nicolas Hidalgo, DONALD H. GALVAN, Centro de Nanociencias y Nanotecnologia. UNAM., ALVARO POSADA-AMARILLAS, Universidad de Sonora — Structural and electronic properties of ceria doped with Indium, Ruthenium and Iridium were calculated using the Full-Potential Augmented Plane Waves with local orbital Method (APW+lo), within the Density Functional Theory. DFT calculations were performed for 1x1x2 and 2x2x2 supercells using GGA and hybrid exchange-correlation potentials. For each cell the atoms were relaxed by minimizing forces. Geometric and band structure results are examined and a comparison with pure ceria structural and electronic properties is performed.

[1]R.N.G. acknowledge support from DCEN13-PI06 project. R.N.G. acknowledge computational support from ACARUS-UNISON.

Roberto Nunez-Gonzalez
Universidad de Sonora

Date submitted: 15 Nov 2013 Electronic form version 1.4