Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

First-principles study of interstitial hydrogen in yttria-stabilized zirconia.[1] APOSTOLOS MARINOPOULOS, CEMDRX, Physics Department, University of Coimbra, CEMDRX, PHYSICS DEPARTMENT, UNIVERSITY OF COIMBRA TEAM — Hydrogen is a common impurity in oxides and has been known to exhibit a dual behavior: either by being a dopant or alternatively an amphoteric impurity with the transition (pinning) level, E(+/-), lying inside the gap [1]. By means of calculations based on density-functional theory (DFT) and a hybrid-functional scheme (Heyd-Scuseria-Ernzerhof) we have studied the incorporation of hydrogen in yttria-stabilized zirconia. Equilibrium sites and formation energies were determined and the role of intrinsic oxygen vacancies needed to stabilize the cubic phase of the oxide was particularly examined. Whereas, in its positively-charged state, H^+, hydrogen was found exclusively to form a dative-type bond with O ions, the neutral paramagnetic H^0 displayed a coexistence with deep interstitial configurations with minimal lattice relaxation of the host lattice. A number of atomic-level mechanisms and migration paths were explored in order to understand this site interplay and the dynamics of neutral H^0 in a way that is consistent with the existing experimental data. [1] C.G. Van de Walle and J. Neugebauer, Nature **423**, 626 (2003).

[1]This work was supported by the program COMPETE: FCOMP-01-0124-FEDER-010450 and by the Portuguese Fundação para a Ciência e a Tecnologia (FCT) under the Ciência 2007 and PTDC/FIS/102722/2008 programs.

Apostolos Marinopoulos
CEMDRX, Physics Department, University of Coimbra, Portugal.

Date submitted: 11 Nov 2011 Electronic form version 1.4