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Hydrogen configurations at a high-angle grain boundary in yttria-stabilized zirconia[1] APOSTOLOS MARINOPOULOS, CEMDRX and Physics Department, University of Coimbra — Hydrogen is a common impurity in many technologically-relevant semiconductors and oxides. Being mobile and reactive it can form defect complexes with native defects or other extrinsic point defects. Ab initio calculations based on density-functional theory (DFT) have so far been instrumental in elucidating the tendency of hydrogen to form stable complexes with oxygen vacancies and acceptor dopants. The interaction of hydrogen with internal extended defects, such as grain boundaries, needs also to be addressed given the fact that metal oxides are commonly used in polycrystalline or nanocrystalline forms. The present DFT study aims to determine the type of hydrogen configurations that can exist at the core of a high-angle tilt grain boundary in yttria-stabilized zirconia (YSZ). The core is characterized by strong distortions for both anion and cation sublattices and lower ionic density and coordination numbers that lead to larger interstitial spaces at the interface with respect to the bulk. Formation energies and charge transition levels are determined and compared to those in the bulk YSZ where hydrogen was found to incorporate either at hydroxide-bond configurations or at interstitial sites with strong atomic character.

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Apostolos Marinopoulos
CEMDRX and Physics Department, University of Coimbra

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