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Hydrogen bistability in non-magnetic oxides JACOB GAVARTIN, ALEXANDER SHLUGER, MARSHALL STONEHAM, University College London, U.K., STEVE COX, ISIS Facility, Rutherford Appleton Lab, U.K. — Recent extensive muonium spectroscopy measurements (μSR) [1] suggest a general correlation between stable muonium (Mu) forms in non magnetic oxides and their band gap, E_g: in the materials with Eg<4 eV, Mu is, as a rule, fully ionized; in the oxides with Eg>7 eV, most of the Mu exists in the atomic form, while both ionized and atomic forms of Mu coexist in the oxides with the band gap in the interval 4<Eg<7 eV. Based on the analogy between muonium and hydrogen, we propose a general model which may explain such a correlation and makes important predictions about hydrogen behavior in non-magnetic oxides. As an example, we use ab initio calculations to extract the parameters for this model to explain difference in hydrogen behavior in HfO_2, ZrO_2 films and in their silicates at low hydrogen concentrations [2]. We further discuss the role of hydrogen in mechanisms of tetragonal to a monoclinic phase transformations in ZrO_2 and HfO_2. 1. S.F.J. Cox, J.L. Gavartin, J.S. Lord et al. J. Phys. : Condens. Matter, 2006 (in press). 2. R.P. Pezzi, L. Miotti, K.P. Bastos *et al. Appl. Phys. Lett.* **85** 3540 (2004).

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