Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Proton diffusion at the wet yttria stabilized zirconia surface: an ab-initio study CLOTILDE CUCINOTTA, STEFANO SANVITO, Trinity College Dublin, MARCO BERNASCONI, University of Milano Bicocca — It is known that in humid environment yttria stabilized zirconia (YSZ) powders display protonic conduction in a thin layer of water adsorbed on the oxide. The conductivity depends strongly on temperature which affects the thickness of the water layers and the presence of surface defects. Different models have been proposed to explain surface conductivity on the wet YSZ surface but the microscopic details of proton diffusion have not been fully elucidated. On the basis of ab-initio simulations, we here address the study of the structure of the wet YSZ surface and of the possible mechanisms for protonic diffusion at the YSZ surface at different temperatures. We calculate the enthalpies of defects formation and migration and compare protonic surface diffusion in the water layers with the outcome of conductibility and thermogravimetry measurements. This study is of relevance for electrode reactions of SOFCs but it is also of more general interest as the same mechanisms of proton conductivity in adsorbed water layers might take place at the wet surface of other solid oxides.

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Date submitted: 14 Nov 2013 Electronic form version 1.4