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Density functional theory study of triple phase boundaries of solid oxide fuel cells ANGELO BONGIORNO, MASSIMO MALAGOLI, Georgia Institute of Technology — In this work, we present a modeling study of triple phase boundary regions of solid oxide fuel cells (SOFCs) based on a density functional theory approach. In particular, we consider the following solid oxide electrolytes, yttrium-doped barium zirconate (BZY) and yttrium-doped barium cerate (BCY), and the following metallic catalysts, palladium, nickel, and copper. Thus, we use density functional theory calculations to construct the energy landscape for a hydrogen species crossing triple phase boundaries based on the materials above. This study focuses, in particular, on the role played by the metal-oxide interface in controlling the proton transfer from the catalyst to the electrolyte component of triple phase boundaries. Our results are discussed in light of the hydrogen spilling process occurring at triple phase boundaries based on nickel and yttria-stabilized zirconia.

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