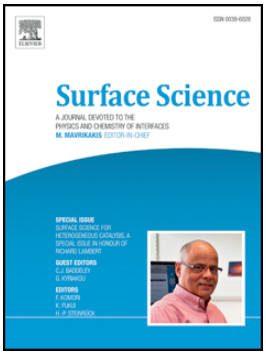

Density functional theory study of the interaction of H_2O, CO_2 and CO with the ZrO_2 (111), Ni/ZrO_2 (111), YSZ (111) and Ni/YSZ (111) surfaces

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Density Functional Theory Study of the Interaction of H_2O, CO_2 and CO with the ZrO_2 (111), Ni/ZrO_2 (111), YSZ (111) and Ni/YSZ (111) Surfaces

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Abstract

The triple phase boundary (TPB), where the gas phase, Ni particles and the yttria-stabilised zirconia (YSZ) surface meet, plays a significant role in the performance of solid oxide fuel cells (SOFC). Indeed, the key reactions take place at the TPB, where molecules such as H_2O, CO_2 and CO interact and react. We have systematically studied the interaction of H_2O, CO_2 and CO with the dominant surfaces of four materials that are relevant to SOFC, i.e. ZrO_2(111), Ni/ZrO_2(111), YSZ(111) and Ni/YSZ(111) of cubic ZrO_2 stabilized with 9% of yttria (Y_2O_3). The study employed spin polarized density functional theory (DFT), taking into account the long-range dispersion forces. We have investigated up to five initial adsorption sites for the three molecules and have identified the geometries and electronic structures of the most stable adsorption configurations. We have also analysed the vibrational modes of the three molecules in the gas phase and compared them with the adsorbed molecules. A decrease of the wavenumbers of the vibrational modes for the three adsorbed molecules was observed, confirming the influence of the surface on the molecules' intra-molecular bonds. These results are in line with the important role of Ni in this system, in particular for the CO adsorption and activation.

Key words: Triple Phase Boundary, yttria-stabilized zirconia, molecule-surface interaction, fuel cell, supported nanoparticles, surface science.