**Electronic transport through the Ni/ZrO2 interface: First-principles calculations**

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Solid oxide fuel cells (SOFC) have advantages of higher energy density, higher conversion efficiency and non-pollution than other types of fuel cells. Although Ni/ZrO2 is a conventional anode material of them and influences their conversion efficiency, the effect of interface orientations on junction conductance has been rarely addressed. In this work, we study the geometric and electronic properties of the Ni/ZrO2 heterostructures from first-principle, based on density functional theory and non-equilibrium Green's function formalism, focusing on the effect of six interface orientations on conduction features. Whereas hydrogen and methane are the common fuels in the usage of SOFC and their open circuit voltages are respectively 1.05 V and 1.15 V, our results suggest that SOFC with the 90o heterostructure would offer better performance among the studied orientations.