# First-principles Study of Surface Reactivity of Transition Metals-doped $Sr_{1-x}Y_xTiO_3$ for Solid Oxide Fuel Cell Applications

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In recent years, the yttria-doped strontium titanium oxide (Sr0.92Y0.08TiO3-δ; SYT) has received much attention as an alternative anode material for solid oxide fuel cell (SOFC) due to its high sulfur/carbon resistance, good electronic/ionic conductivity and phase stability in typical SOFC anode operating conditions. However, SYT has exhibited the poor electro-catalytic activity toward fuel (i.e. H2 or hydrocarbon) oxidation. Thus, it is very essential to understand the factors controlling the reactivity of SYT toward SOFC anode reactions for developing effective SYT-based anode materials.
In this talk, using spin-polarized density functional theory calculations, we will present some recent theoretical results we have on the role of oxygen vacancy formation energy in determining the reactivity of H2 oxidation.
This work hints the importance of knowing how to properly tailor the surface reactivity of oxide-based anode materials for achieving wanted electro-catalytic activity for SOFC application.