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Modulating the reactivity of Pt-based catalysts for PEMFC: A First Principles Study HAI-YAN SU, XIN-HE BAO, WEI-XUE LI, Dalian Institute of Chemical Physics, CAS, Dalian, China — Low-temperature Polymer electrolyte membrane fuel cells (PEMFCs) have been regarded as one of the most promising candidates to produce heat and electricity, especially for electric vehicles or residential co-generation systems. However, the CO poison at the anode and the slow kinetics of the ORR at the cathode for Pt based-catalysts limit its widespread application, which motivated extensive research for more effective catalysts with CO tolerant, highly active and lower Pt loading, and/or highly selective for CO PROX. Density functional theory calculations have been used to screen Pt-based catalysts for PEMFC. It is found that the direct contact with Pt catalysts (so-called Pt-skin) is essential. The reactivity of Pt-skin catalysts towards the oxygen reduction reaction (ORR) and the hydrogen evolution reaction (HER) can be modulated by stepwise increase of Ni contents, which are accomplished by the modification of the reactivity through ligand and geometrical effects. The overall reactivity is however balanced by effective adsorption and desorption of adsorbates. Our calculations show that among various Pt_xNi_y with Pt-skin, Pt_3Ni is the catalyst with the highest overall reactivity. The present work indicates that it may be a good candidate for CO preferential oxidation (PROX) in excess of the hydrogen.

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