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Modification Mechanism of La-doped Ti/SnO_2 Electrodes from a micro-perspective: Electrochemical Analysis Compared with Theoretical Calculations

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Elemental doping can effectively improve the catalytic oxidation performance of titanium-based electrodes. To investigate the modification mechanism of La doping of Ti-based SnO_2 electrodes, the electrochemical behaviour of the electrodes was tested using anodic polarization curve, electrochemical impedance spectroscopy (EIS), linear sweep voltammetry (LSV), and the Mott-Schottky (M-S) techniques. The change in the SnO_2 internal lattice structure after La doping is the main reason for the improved performance. Therefore, theoretical calculations are used as an aid in the electrochemical analysis to study the underlying doping mechanism. The electronic structure and the density of SnO_2 lattice states in the electrode coating were calculated using first-principles calculations. Electrochemical tests and theoretical calculations are consistently shown that the doped La mainly improves the electrode performance through three aspects: 1) The band gap of the tin dioxide lattice was reduced, and the electrical conductivity of the electrode was improved; 2) The carrier of the tin dioxide lattice was increased, so that the electrode active site was increased; 3) The density of the tin dioxide lattice was changed, thereby changing the cyclic voltammetry and polarization characteristics of the electrode. The electrode performance is best as the La doping content gives the ratio Sn: Sb: La=100:10:1.5 and that the modification mechanism of the doping is revealed from a microscopic point of view.

Keywords: Modification mechanism; Electrochemical analysis; First-principles calculations; Ti/SnO_2 electrode

FULL TEXT