

Enhanced Oxygen Evolution Activity of V and Fe Co-doped Ni(OH)₂

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The oxygen evolution reaction (OER) is an important research topic because it is the core reaction in electrochemical water splitting, rechargeable metal-air batteries, etc. OER is known to follow a complicated four-electron process, where the slow reaction rate is the challenge to be overcome. Herein, we investigated the effect of V and/or Fe doping in Ni(OH)₂ for the development of efficient OER catalyst via density functional theory calculations. By calculating the Gibbs free energy of OER mechanism, we found that V dopant as an active site of (1 0 0) edge significantly lowered the overpotential to drive water oxidation, thus could enhance the catalytic activity. However, edge formation energetics showed that V doping destabilized the edge system, indicating that V ion is not readily exposed on the edge. On the other hand, Fe doping largely increased relaxation energy resulting in the stable edge system. Promisingly, in the V and Fe co-doped system, the two independent characteristics of the doping elements worked synergistically; Fe stabilized the co-doped edge system allowing V to be exposed as a highly active site for OER.