

Engineering of a highly stable metal-organic Co-film for efficient electrocatalytic water oxidation in acidic media

Summary

Water oxidation is traditionally performed over IrO₂ and RuO₂ owing to their high stability at low pH compared to molecular O₂ evolution catalysts. The low stability of molecular complexes in acids limits their industrial exploitation as anodes in water-splitting devices, where high current densities and proton conductivity are required. Herein, an existing Co(1,10-phenanthroline)₂ complex film is engineered to improve its pH-stability *via* extra OH substituents on the ligand, *i.e.* 1,10-phenanthroline-4,7-diol. This novel Co(1,10-phenanthroline-4,7-diol)₂ complex film is active for water oxidation at low overpotentials and stable at low pH. Since the calculated water oxidation overpotentials of both complexes are similar, the difference in water oxidation activity is attributed to a smaller charge transfer resistance, which originates from a different anchoring style to the electrode *via* the OH groups of the ligand. This result is supported by electrochemical impedance measurements. The catalyst film displayed high catalytic current and excellent stability in both neutral and strongly acidic conditions (0.1 M H₃PO₄). This is opposed to cobalt-phosphate (Co-Pi) or Co oxide catalysts, which degrade immediately under strongly acidic conditions. The supreme pH-stability of the Co(1,10-phenanthroline-4,7-diol)₂ film is computationally rationalized by a high crystal formation energy observed in DFT calculations. In summary, an acid-stable and active cobalt-based metal-organic film is reported that competes well with most reported earth-abundant catalysts for water oxidation under similar conditions.

Published in: *Materials Today Energy* (2020), 17, 100437.