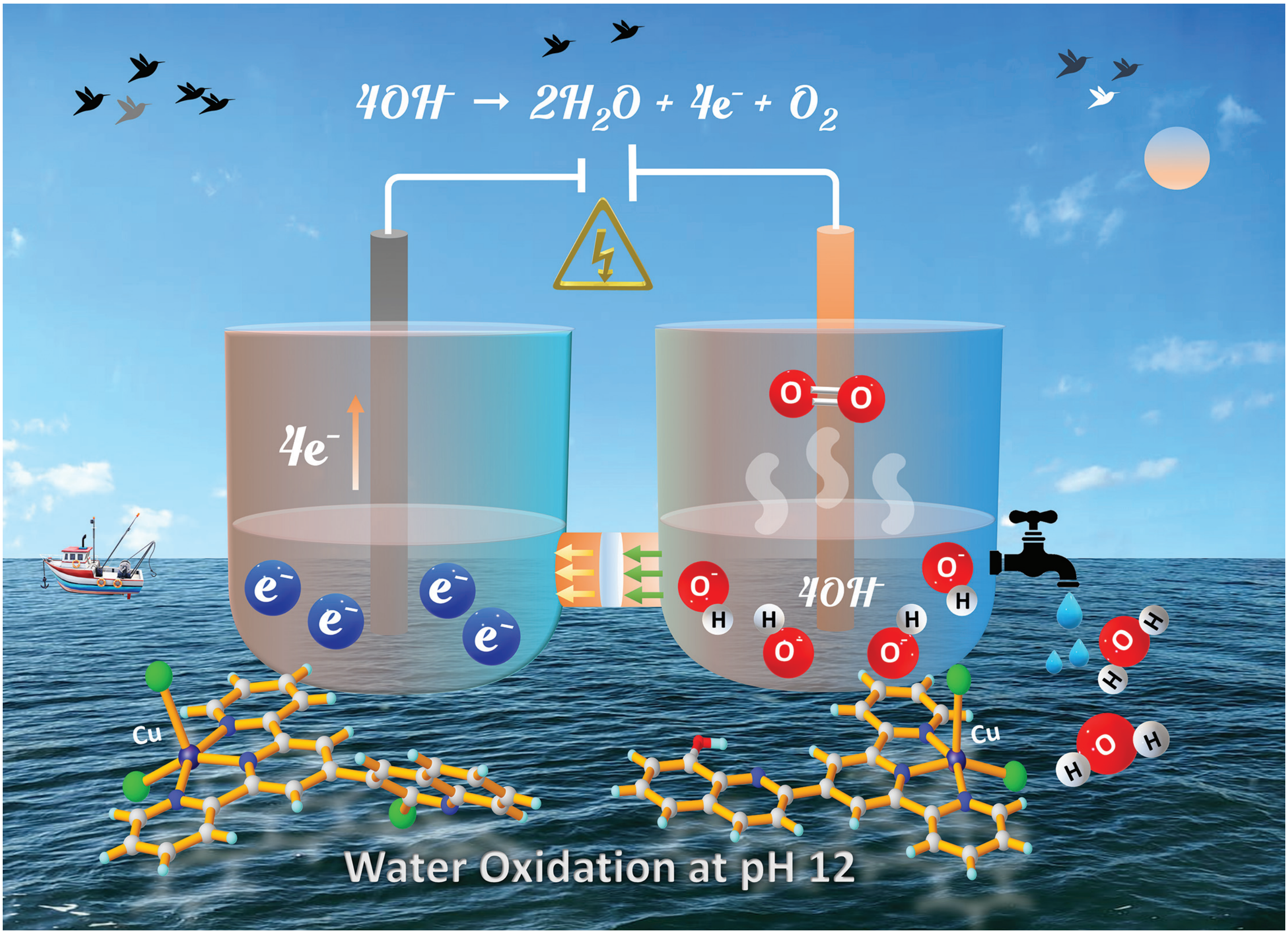

Showcasing research from Professor Sumanta Kumar Padhi's laboratory, Department of Chemistry and Chemical Biology, IIT(ISM) Dhanbad, Jharkhand, INDIA.

Electrochemical water oxidation using single-site Cu(II) molecular complexes: a mechanism elucidated by computational studies

Two penta-coordinated Cu(II) complexes were investigated as electrocatalysts for water oxidation in phosphate buffer (pH 12): [Cu(QCl-Tpy)Cl_2] (QCl-Tpy = 3-([2,2′:6′,2″-terpyridin]-4′-yl)-2-chloroquinoline) and [Cu(8HQ-Tpy)Cl_2] (8HQ-Tpy = 2-([2,2′:6′,2″-terpyridin]-4′-yl)quinolin-8-ol). Both follow a Water Nucleophilic Attack (WNA) pathway with first-order kinetics, where O–O bond formation is made possible by buffer-assisted proton transfer. TOF_{max} values of 10 000 s^{-1} and 15 000 s^{-1} were found using Foot of the Wave Analysis; Tafel plots verified the latter's higher activity. According to theoretical research, WNA is supported, and oxygen evolution is more advantageous in alkaline environments because of hydroxide nucleophilicity.

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As featured in:


Volume 54
Number 37
7 October 2025
Pages 13793-14228

Dalton Transactions

An international journal of inorganic chemistry

rsc.li/dalton

ISSN 1477-9226

ROYAL SOCIETY OF CHEMISTRY

PAPER
Manabu Hagiwara *et al.*
Improving the dielectric temperature stability of Bi_2SiO_5-based ceramics through the spontaneous formation of paraelectric–ferroelectric nanocomposite structures

See Sumanta Kumar Padhi *et al.*,
Dalton Trans., 2025, **54**, 13894.

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