Plasma-Modulated Trimetallic Mn-Ni-Co Phosphides for Complementary Water Splitting

Kholoud E. Salem[1,2], Amina A. Saleh[1], Ghada E. Khedr[1], Basamat S. Shaheen[1], Nageh K. Allam[1]

[1]Energy Materials Laboratory, School of Sciences and Engineering, The American University in Cairo, New Cairo

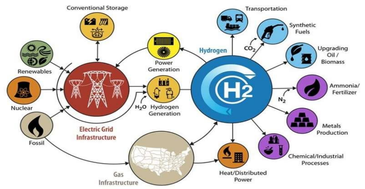
[2]Department of Chemical Engineering, McMaster University, Hamilton, Ontario L8S 4L7, Canada

جامعة الملك عبدالله للعلوم والتقنية
King Abdullah University of Science and Technology | Clean Combustion Research Center

KAUST Research Conference: Hydrogen-Based Mobility and Power

Introduction

Inspiration: Split Water into sustainable hydrogen fuel, which remains a grand challenge

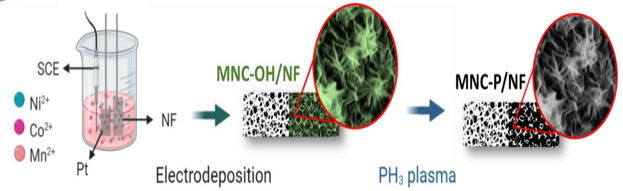


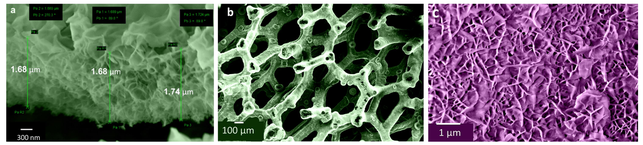
Benefits of Bifunctional Transition Metal Phosphides:

- Low cost and high abundance
- Environmentally benign approach
- Low overpotentials for HER/OER
- Low overpotential for the overall water splitting
- Tunable electronic structure
- High electric conductivity

Schematic illustration of the H_2@Scale concept. Credit: National Renewable Energy Laboratory

Methodology





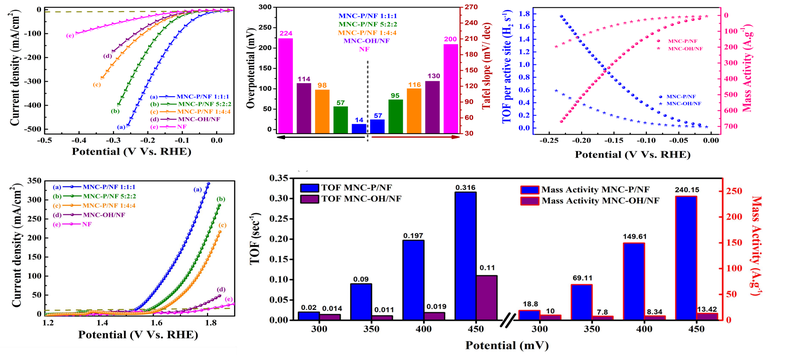
- Quaternary metallic Mn-Ni-Co-P films prepared by electrodeposition on flexible Ni foam substrate
- phosphidation *via* PH_3 plasma treatment

K. E. Salem, A. A. Saleh, G. E. Khedr, B. S. Shaheen, N. K. Allam, ENERGY Environ. Mater. 2022, 0, 1-13.

Results

Electrochemical measurements

1 M KOH; 5 mV s^{-1} (N_2 sat'd); iR-corrected LSV; background corrected; (overpotential + Tafel values) at −10 mA cm^{-2}

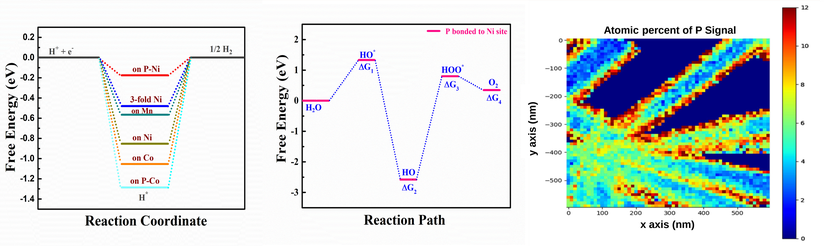


- Mn-Ni-Co-P/ NF shows small overpotentials of (-14 mV) and (289 mV) vs. RHE for HER and OER, respectively
- Lower Tafel slopes/ High mass activity and Turnover frequency values

K. E. Salem, A. A. Saleh, G. E. Khedr, B. S. Shaheen, N. K. Allam, ENERGY Environ. Mater. 2022, 0, 1-13..

Density Functional Theory

The details of the calculations based on the standard Cambridge Serial Total Energy Package (CASTEP)

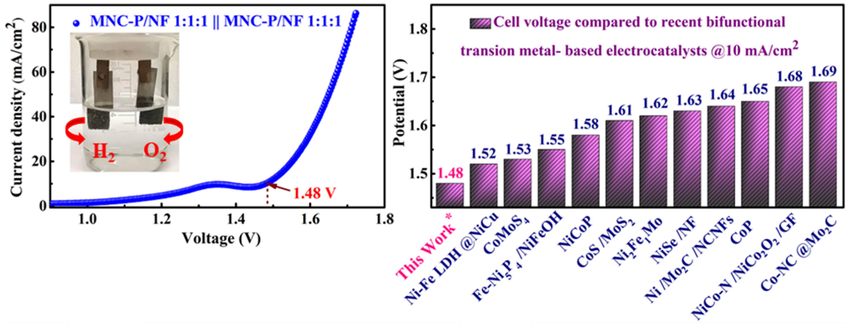


- DFT indicates that the top of P bonded to the Ni site of MnNiCoP is the optimum site for hydrogen adsorption with ΔG_H^* of −0.17 eV
- The best performance was provoked for the metal-Ni site with the rate-determining step being the third step of OER (O* to OOH*)

K. E. Salem, A. A. Saleh, G. E. Khedr, B. S. Shaheen, N. K. Allam, ENERGY Environ. Mater. 2022, 0, 1-13.

Overall device configuration

1 M KOH; iR-corrected LSV, 1mV s^{-1} (N_2 sat'd); background corrected; cell voltage at −10 mA cm^{-2}

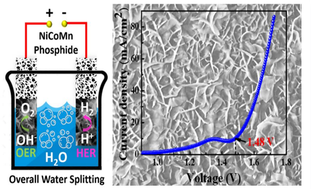


- A full single water alkaline-electrolyzer system was constructed using the bifunctional MNC-P/NF 1:1:1 as both the anode and cathode
- Very low cell voltage of 1.48 V vs. RHE o attain a current density of 10 mA cm^{-2}

K. E. Salem, A. A. Saleh, G. E. Khedr, B. S. Shaheen, N. K. Allam, ENERGY Environ. Mater. 2022, 0, 1-13.DOI 10.1002/eem2.12324.

Summary

- Active plasma-treated MnNiCo phosphide catalysts integrated into a full water electrolyzer
- The activity is ascribed to the uniform porous structure of the catalyst, metal like conductivity and optimized composition
- The simultaneous metal-phosphide bonds completely modified the electronic structure of the catalyst



Acknowledgment

The financial support of this work by the American University in Cairo is highly valued.

Kholoud Abousalem
Email: abousalk@mcmaster.ca

THE AMERICAN UNIVERSITY IN CAIRO 100 YEARS

EML Energy Materials Laboratory