

# 3D-printed monolith metallic Ni-Mo Electrodes for Ultrahigh Current Hydrogen Evolution

Yanran Xun<sup>1</sup>, Hongmei Jin<sup>2</sup>, Yuemeng Li<sup>1</sup>, Shixiang Zhou<sup>1</sup>, Kaixi Zhang<sup>1</sup>, Xi Xu<sup>3</sup>, Win Jonhson<sup>1</sup>, Shuai Chang<sup>4</sup>, Teck Leong Tan<sup>2</sup>, and Jun Ding<sup>1</sup>

<sup>1</sup>National University of Singapore

<sup>2</sup>Institute of High Performance Computing

<sup>3</sup>Northwestern Polytechnical University

<sup>4</sup>Harbin Institute of Technology

November 1, 2023

## Abstract

In this work, we reported a series of monolithic 3D-printed Ni-Mo alloy electrodes for highly efficient water splitting at high current density (1500 mA cm<sup>-2</sup>) with excellent stability, which provides a solution to scale up Ni-Mo catalysts for HER to industry use. All possible Ni-Mo metal/alloy phases were achieved by tuning the atomic composition and heat treatment procedure, and they were investigated through both experiment and simulation, and the optimal NiMo phase shows the best performance. Density functional theory (DFT) calculations elucidate that the NiMo phase has the lowest H<sub>2</sub>O dissociation energy, which further explains the exceptional performance of NiMo. In addition, the microporosity was modulated via controlled thermal treatment, indicating that the 1100 °C sintered sample has the best catalytic performance, which is attributed to the high electrochemical surface area (ECSA). Finally, the 4 different macrostructures were achieved by 3D printing, and they further improved the catalytic performance. The gyroid structure exhibits the best catalytic performance of driving 500 mA cm<sup>-2</sup> at a low overpotential of 228 mV and 1500 mA cm<sup>-2</sup> at 325 mV as it maximizes the efficient bubble removal from the electrode surface, which offers the great potential for high current density water splitting.

## Hosted file

Manuscript of NiMo electrode for HER.docx available at <https://authorea.com/users/694822/articles/683740-3d-printed-monolith-metallic-ni-mo-electrodes-for-ultrahigh-current-hydrogen-evolution>