3rd Generation Solar Cells for Green H₂ Production by Water Splitting

I. Pinho¹, S. Gonçalves^{1,2}, S. Caspani^{1,2}, J. Couto ^{1,2}, A. Mendes³, J. P. Araújo^{1,2}, A. Apolinário^{1,2*}

¹IFIMUP, Department of Physics and Astronomy, Faculty of Sciences, University of Porto, Rua do Campo Alegre s/n, 4169–007 Porto, Portugal

²LaPMET, Rua do Campo Alegre s/n, 4169-007 Porto, Portugal

³LEPABE, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465

*arlete.apolinário@fc.up.pt

Energy is a constant and primary resource in our lives, global energy demand is increasing yearly and so does the need for clean and renewable sources. Green H2 production through solar water splitting is a promising solution to address the current global energy challenges. Photoelectrochemical (PEC) cells are one of the most promising ways to convert solar energy into hydrogen: traditionally comprising of a photoanode or photocathode (n-type or p-type semiconductor, respectively) and metal counter electrode (CE) both emerged in an aqueous electrolyte, these devices use sunlight to drive electrolysis of water, producing H₂ and O₂ molecules [1]. Tandem PEC cells use both a photoanode and photocathode, discarding the need for a metal CE and allowing for bigger efficiencies than single absorber PEC cells. We carried out numerical simulations using Shockley-Queisser limit that indicate a theoretical STH efficiency of around 21.6% for a bandgap pairing of 1.33 & 1.87 eV of the photoelectrodes, being in agreement with literature [5]. There are several semiconductors that can be used as photoelectrodes, with the most appealing being those that are inexpensive, non-toxic, and composed of abundant materials, including Fe₂O₃, WO₃, and TiO₂ (for n-type) [2,3,4]. Cupric Oxide (CuO) is a p-type semiconductor that is inexpensive, non-toxic, environmentally friendly and abundant material with reported tunable bandgap in the range [1.2-2.6] eV based on preparation conditions [6], making it a suitable candidate for a tandem PEC cell photocathode. Although having an exceptional maximum theoretical current density of -35 mA/cm², reported efficiencies are still far from theoretical value and long-term stability is still a concern and topic of active research. In this work, different cost-effective and scalable fabrication methods of CuO thin films are exploited, mostly relying on electrodeposition and annealing procedures. Several electrodeposition parameters are optimized, including applied voltage, pH and deposition rates. The obtained CuO thin films are characterized in terms of morphology and structure as well as their photoelectrochemical performance by J-V measurements under illumination.

References

- [1] M. Gratzel, Nature 414(6861) p.338-344 (2001)
- [2] Paula Quitério, J. Phys. Chem. C p.12865-13508 (2020)
- [3] Sofia Gonçalves, Applied Materials and Interfaces, p.64389-65740 (2024)
- [4] A. Apolinário, Journal of Materials Chemistry A, p.9067-9078 (2014)
- [5] Mathieu S. Prévot, Kevin Sivula*, Phys. Chem. C p.17879–17893 (2013)
- [6] Linhua Xu, Optik, Volume 158, 382-390 (2018)

Figures

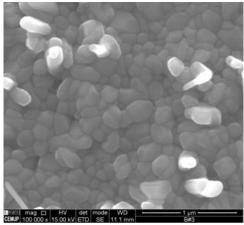


Figure 1: Synthetized CuO by electrodeposition of Cu at pH 2.7 and posterior annealing at 550°C.