

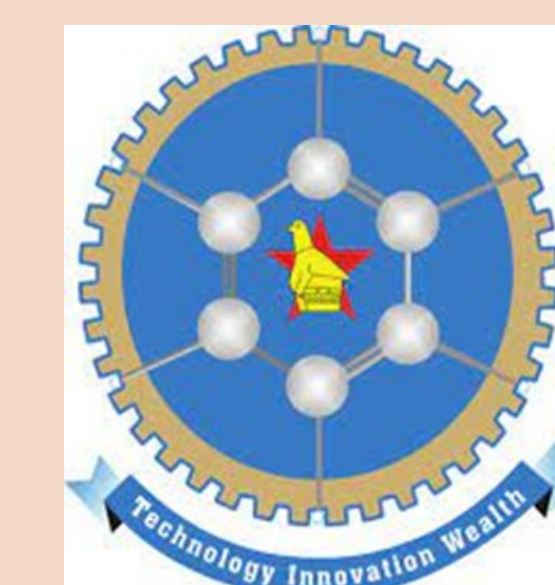
Chiral photoelectrodes for efficient generation of hydrogen through photoelectrocatalytic water-splitting

Rufaro KAWONDERA¹, Wilbert MTANGI¹, Stephen NYONI², Gift MEHLANA³

¹Institute of Materials Science, Processing and Engineering Technology, Chinhoyi University of Technology, Chinhoyi, ZIMBABWE

²Department of Chemistry, School of Natural Sciences and Mathematics, Chinhoyi University of Technology, Chinhoyi, ZIMBABWE

³Department of Chemical Technology, Midlands State University, Gweru, ZIMBABWE



Introduction

- Photoelectrocatalytic water-splitting** is a process which mimics the natural photosynthesis by producing hydrogen using solar energy in the presence of a photoelectrocatalyst.
- Why hydrogen?** It is renewable, non-toxic, by products of combustion are not harmful to humans and has high energy density
- Challenges of photoelectrocatalytic water-splitting** High Oxygen Evolution Barrier, high overpotential and formation of hydrogen peroxide which affects the stability of the photoelectrodes.

Results

- Water splitting experiments have been carried out using: bare electrodes and electrodes coated with chiral and achiral molecules.
- Quantification of hydrogen peroxide by spectrophotometric titration of the electrolytes was carried out.
- Electrolyte obtained from bare photoelectrodes and photoelectrodes coated with achiral molecules showed the presence of hydrogen peroxide by peaking at 436nm.
- For the electrolyte that had chiral molecule coated photoelectrodes, no detectable amount of hydrogen peroxide was observed. The results are as shown if figure 2 below:

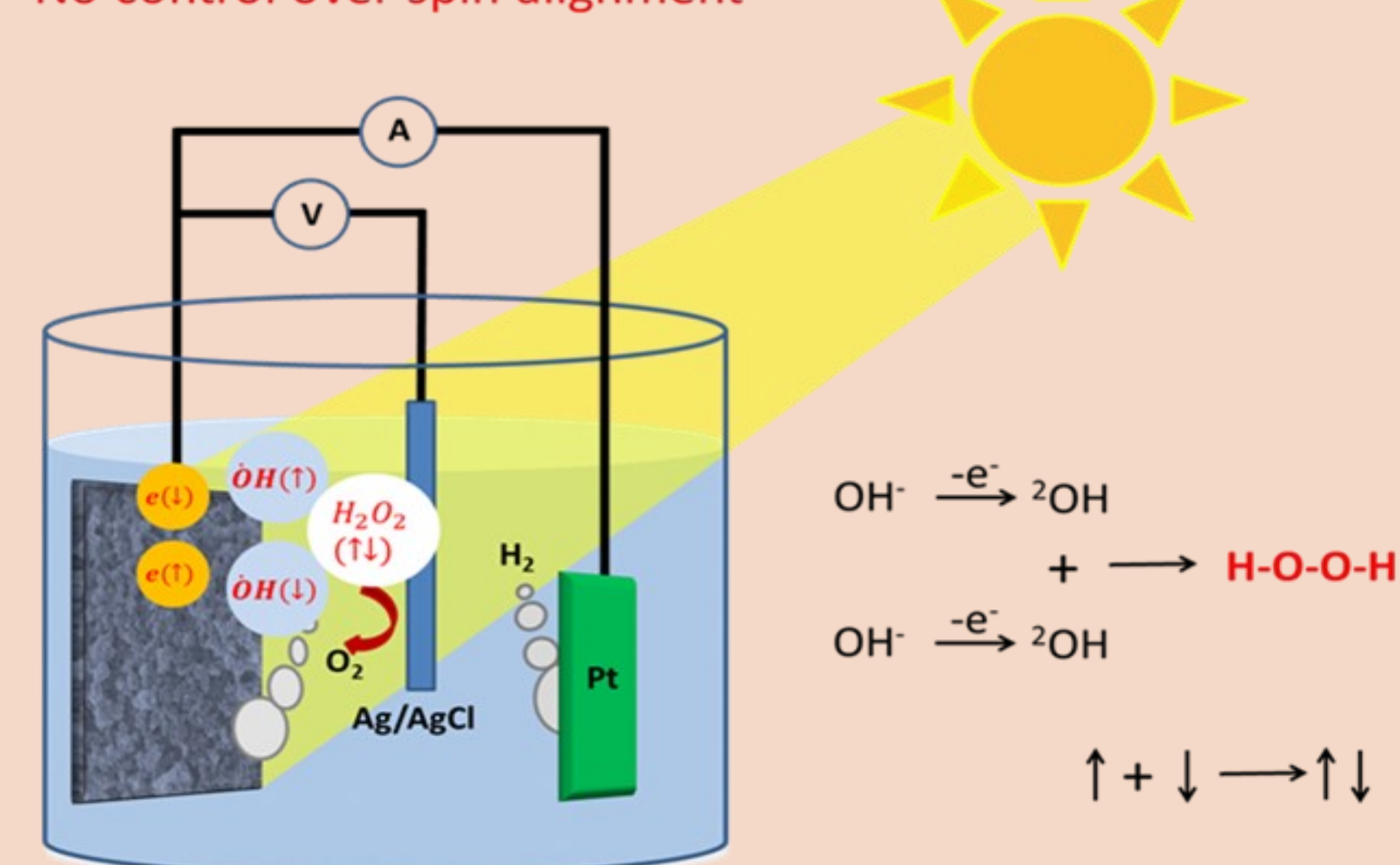
Hypothesis

The high overpotential and peroxide formation associated with the artificial process may be reduced by using chiral based electrodes.

Experimental

The functionalised photoelectrodes are fabricated by prepared coating the electrodes with chiral molecules. To assess performance of the electrodes, water splitting tests are carried out in which chiral molecule coated photoelectrodes, achiral molecule coated photoelectrodes and bare electrodes are used and their performance compared.

No control over spin alignment



Control over spin alignment

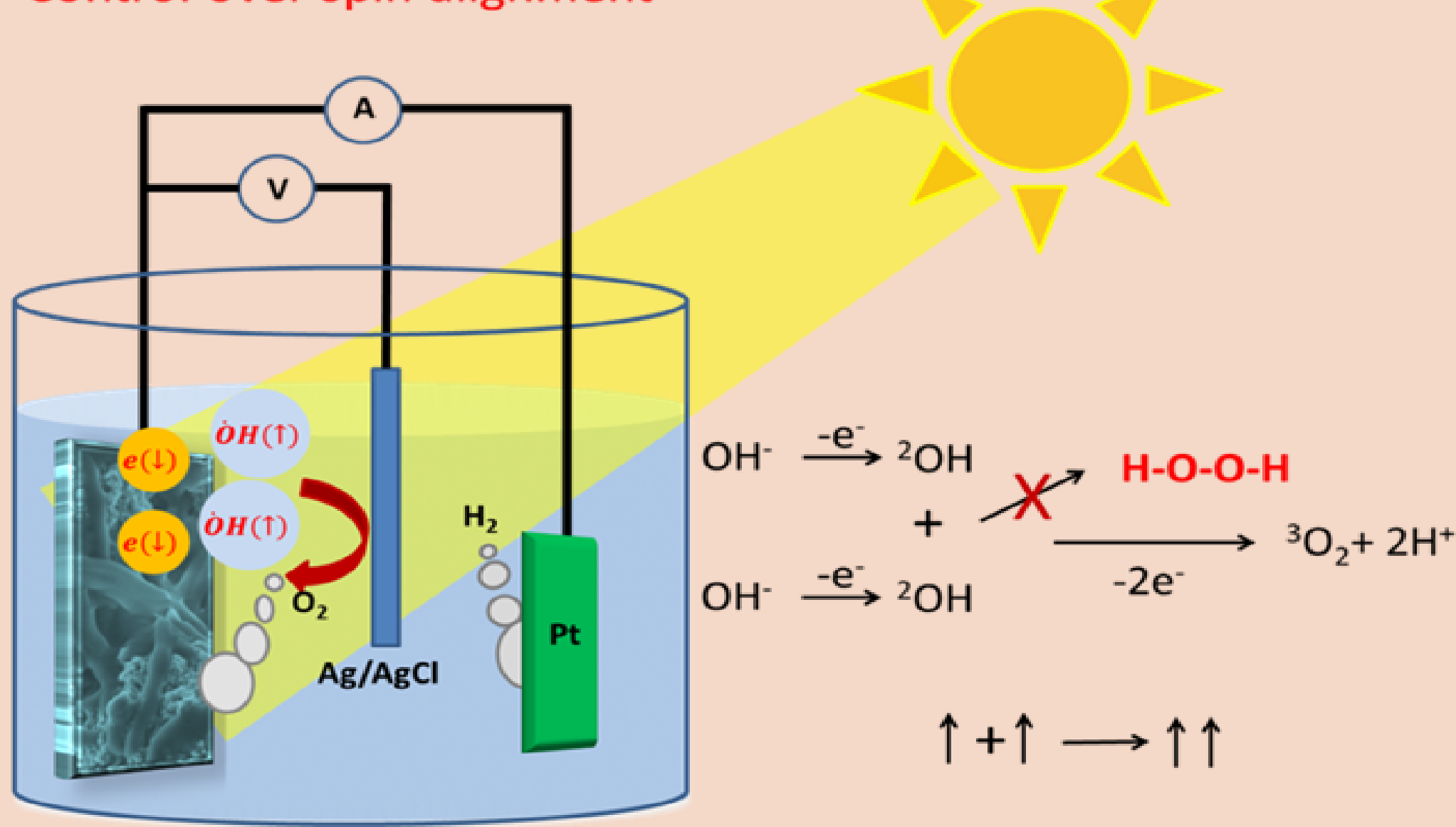


Figure 1 Experimental set up a) bare electrodes b) chiral molecule coated electrodes

With no spin control, H₂O₂ formation is favoured on the singlet surface

By using chiral-molecule coated electrodes spin control of electrons is introduced

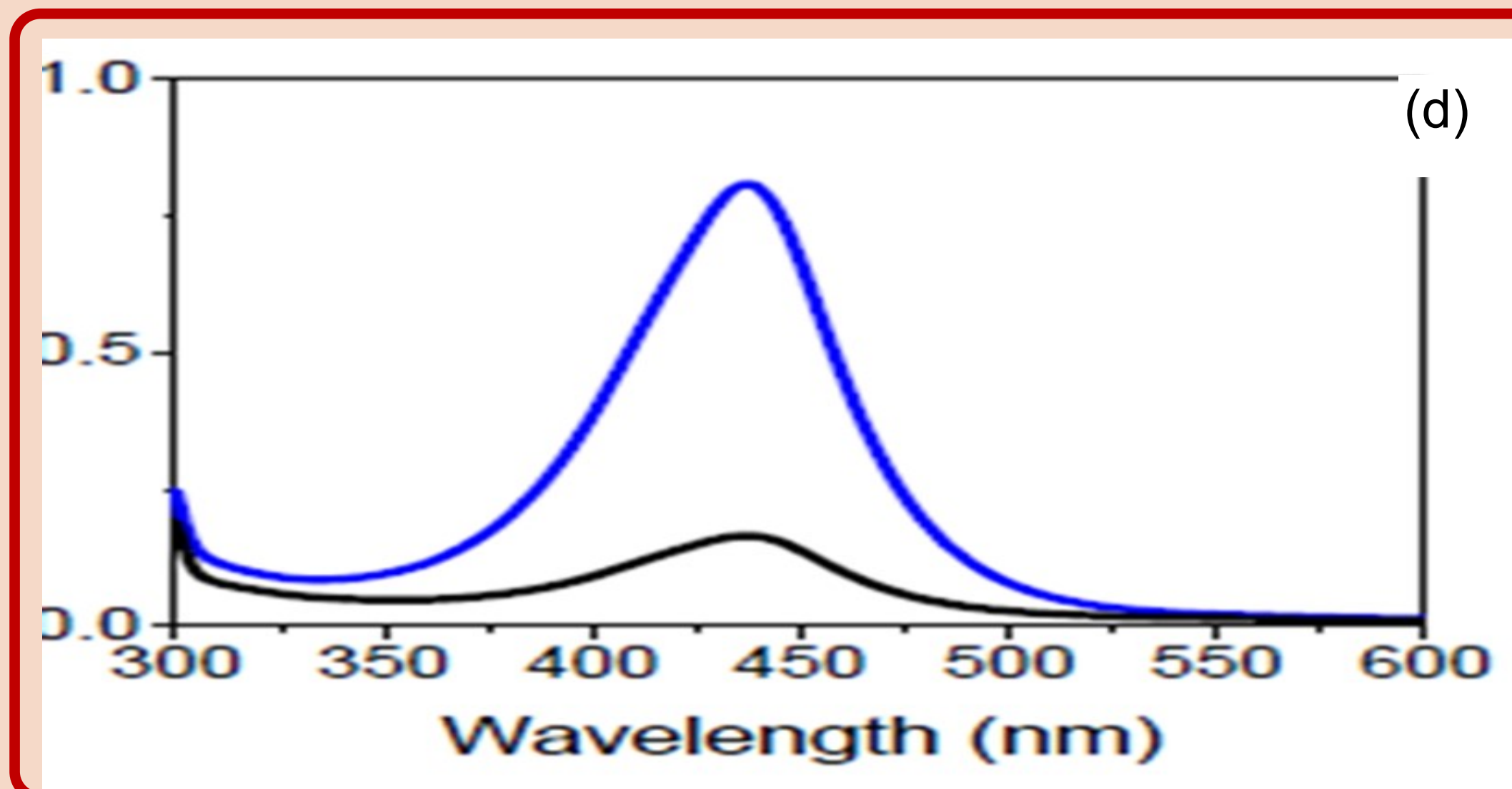
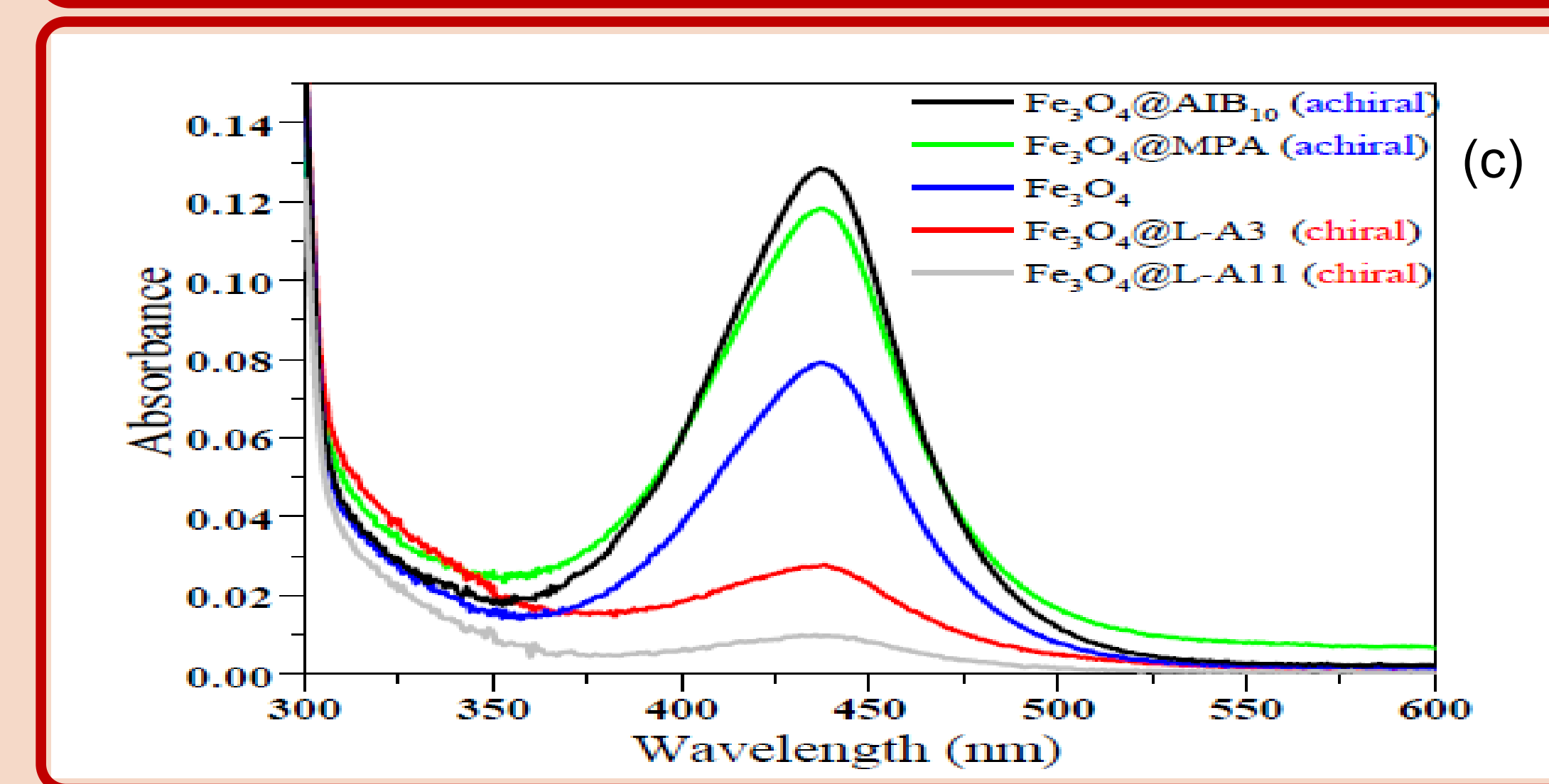
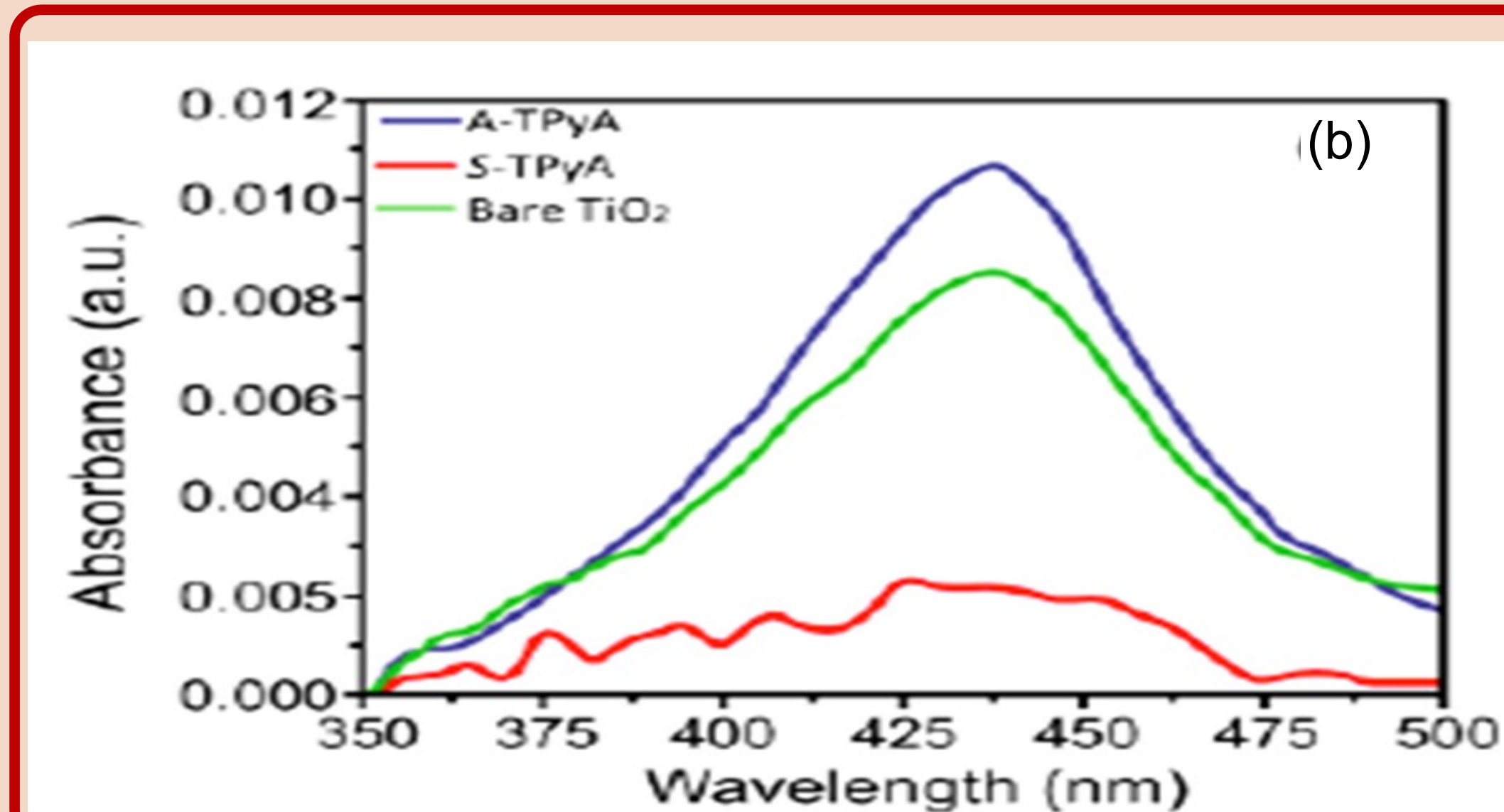
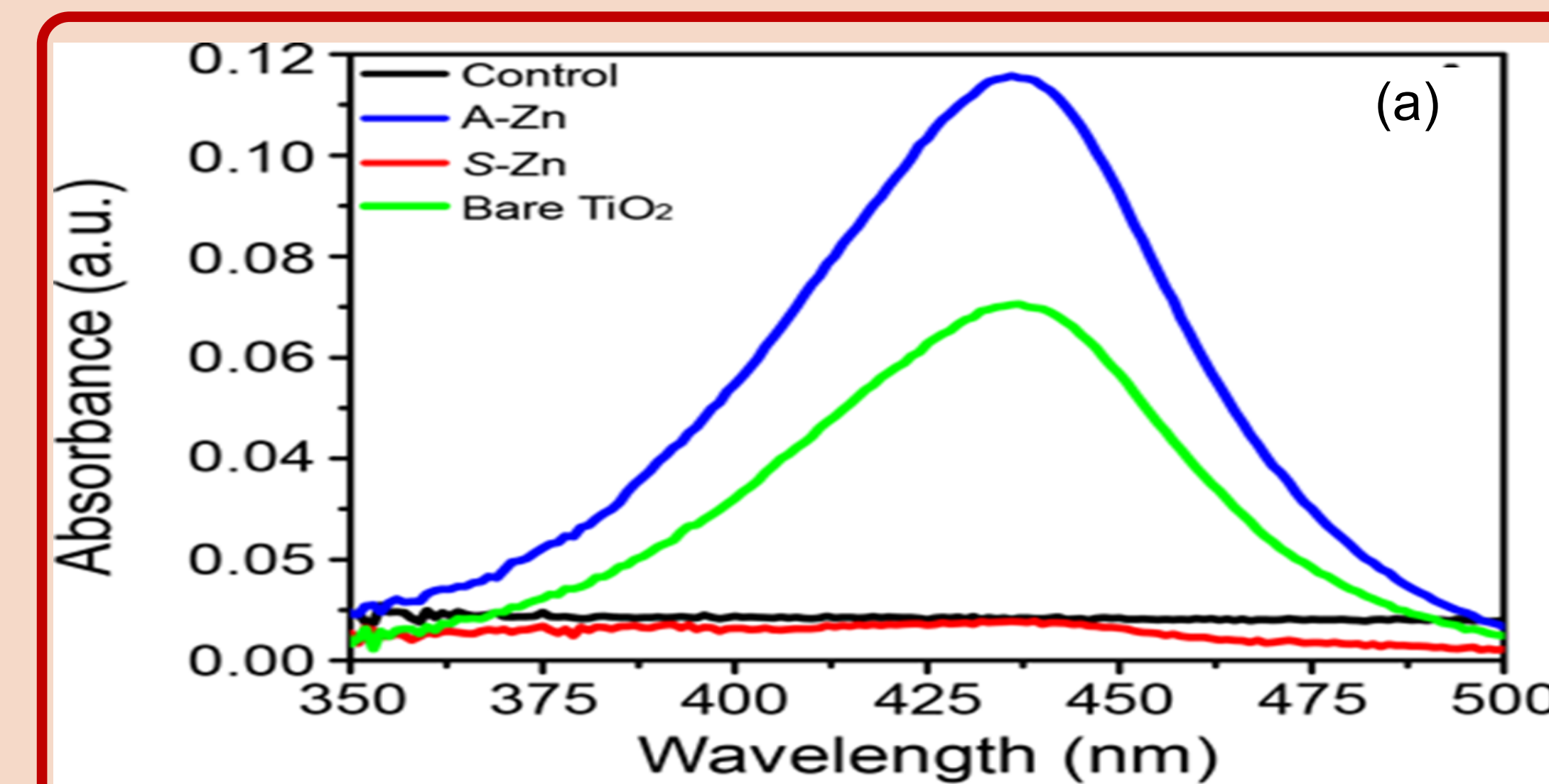


Figure 2: (a) Comparison of H₂O₂ from PECs using Bare TiO₂, achiral Zn porphyrins and chiral Zn porphyrins molecules (b) Comparison of H₂O₂ present from PECs using bare TiO₂, achiral molecule and chiral molecules (c) Comparison of H₂O₂ present in a PEC using bare Fe₃O₄ NPs, Fe₃O₄ NPs coated in achiral molecules and Fe₃O₄ NPs coated in chiral molecules (d) Comparison of H₂O₂ from PECs using L-CoOx (chiral) and meso-CoOx (achiral)

Conclusion

This research highlights the importance of spin on water splitting and how it improves the efficiency of the PEC

References

- Gosh S, Bloom B. P., Lu Y., Lamont D. & Waldeck D. (2020). Increasing the efficiency of Water Splitting through Spin Polarization using Cobalt Oxide Thin Film Catalysts. *J. Phys. Chem.C.* 124, 41, 22610-22618
- Zhang W., Liu F., Hu Y., Yang W., Guan H., Hao L. & Lu G. (2021). Pivotal Role of Chirality in Photoelectrochemical (PEC) water splitting. *Curent Chinese Science*, 115-121.
- Mtangi W., Tassinari F., Vankayala K., Jentzsch A. V., Adelizzi B., Palmas A.R. A., Fontanesi C., Palmas E.W., & Naaman R. (2017). Control of Electrons' Spin Eliminates Hydrogen Peroxide Formation During Water Splitting. *J. Am. Chem. Soc.*, 2794-2798.
- Mtangi W., Vankayala K., Fontanesi C., & Naaman R. (2015). "Role of the Electron Spin Polarization in Water Splitting", *J. Phys. Chem. Lett.*, 6, 24