Topical Symposium on Sustainable Surface Engineering
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Coatings and Surfaces for Thermoelectrical Energy Conversion and (Photo)electrocatalysis - TS4 Poster Session

TS4-ThP-1 Dopant-defect Engineering in SnS_2 Thin Films for Improved Gas-phase Photocatalytic CO_2 Reduction, ***Tadios Tesfaye Mamo (tadios.tesfaye@aau.edu.et)***, Department of Chemistry, National Taiwan University, Taiwan; *M. Qorbani,* Center for Condensed Matter Sciences, National Taiwan University, Taiwan; *A. Hailemariam,* Department of Applied Chemistry, National Yang-Ming Chiao Tung University, Taiwan; *A. Sabbah,* Center for Condensed Matter Sciences, National Taiwan University, Taiwan; *S. Kholimatussadiah,* Department of Physics, National Taiwan University, Taiwan; *C. Huang,* Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan; *L. Chen,* Center for Condensed Matter Sciences, National Taiwan University, Taiwan; *K. Chen,* Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan

To address the issue of CO_2 amount increment in the Earth's atmosphere, various semiconductor photocatalysts have been employed to convert CO_2 into valuable products. Designing an efficient photocatalyst that can activate the CO_2 molecule with the least amount of activation energy is one of the challenging problem. In this regard, we report a combined experimental and computational analysis on a thin film of SnS_2 doped with phosphorous ions at various ion doses. Thermal evaporation followed by sulfurization and ion implantation processes were used to prepare the regulated amount of phosphorous ion-implanted 20-nm SnS_2 thick thin films. Our findings reveal that phosphorous doping synergistically enhances light harvesting by lowering the band gap and energetically stable CO_2 binding sites with the lowest activation energy. The optimized P-SnS_2 photocatalyst has a three times higher CO_2 conversion rate than the pristine one, with a high selectivity of about 92% towards CH_4 formation. Because Phosporous play a vital role in the activation of CO_2 by serving as an active site and due to its low electronegativity, it increases the charge density of the Sn atom adjacent to it. Also, P-doping affects the charge density of the neighboring S atom by serving as a bridge to improve the charge distribution between Sn and S. This degree of electron density alteration would facilitate the electron transfer in the photocatalytic reaction.NAP- In-situ XPS and XAS results with formation energy, Bader charge, and Gibbs free energy calculations are used to carefully assess the overall impact of phosphorus in the SnS_2 sample. DFT calculations accord well with the experimental findings and help us to know the reaction pathway. We anticipate that our result will motivate additional ion implantation research to modify the material's active site for CO_2 reduction and examine its CO_2 conversion capability and related optical and charge transfer behavior.

TS4-ThP-2 e-Poster Presentation: Copper-Based Coatings on Polylactic Acid for Electrocatalytic CO_2 Reduction, *M. Lima,* University of Minho, Portugal; *J. Castro,* ***Sandra Carvalho (sandra.carvalho@dem.uc.pt)***, University of Coimbra, Portugal

The climate crisis caused by global warming is recognized by the United Nations (UN) as a trigger for catastrophic effects such as weather extremes and natural disasters. Carbon dioxide (CO_2) emissions constitute about three-quarters of the total greenhouse gases (GHG) released and have gathered global attention due to their significant contribution to global warming.

Developing new catalytic processes can accelerate the transition to a more sustainable Earth. Electrocatalytic methods are the most promising of all the catalytic processes because they are energy efficient, selective, easy to control, and flexible. They are also known as the most viable solution for the CO_2 reduction reaction (CO_2RR).

Metallic copper has notable electrical conductivity, making it suitable for many electrode-based applications. Additionally, copper-based materials were reported to be active and selective electrocatalysts capable of producing hydrocarbons from the CO_2RR. However, the updated version of the Element Scarcity—EuChemS Periodic Table by the European Chemical Society brings attention to the limited abundance of copper. Ensuring a sustained supply of this element is a significant challenge. Utilizing thin film coatings to produce electrodes is a potentially practical approach to mitigating element shortages. Furthermore, Cu-based electrodes using a polymeric skeleton can provide several benefits concerning cost, material accessibility, and weight.

This work used polylactic acid (PLA) as the substrate for Cu-based electrodes. PLA is widely used in additive manufacturing, a low-cost technique that enables the fabrication of 3D-structured electrodes. Magnetron sputtering (PVD technique) was applied to develop copper metallic surfaces on PLA. Different coatings with Cu/CuO_x/Cu layers were produced. Anodization was a secondary technique applied to enhance the electrochemical active surface area. The CuO_x in the middle of the coating might act as a barrier material to stop the oxidation reaction during the anodization process while maintaining film adhesion. The chemical and morphological characterization of the resulting films will be discussed, as well as the electrochemical properties for CO_2RR applications.

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