ZABs may soon emerge as a viable solution for large-scale energy storage and transportation. Combining high energy density, eco-friendly materials, and reduced costs, ZABs hold promise as a cornerstone of sustainable energy solutions. (Reported by Chi-Liang Chen)

This report features the work of Shih-Yuan Lu and his collaborators published in Energy Storage Mater. ***67****, 103286 (2024), and the work of Yuan-Yao Li and his collaborators published in Nano Energy* ***121****, 109236 (2024).*

TLS 17C1 EXAFS

- XAS, WT
- Materials Science, Chemistry, Condensed-matter Physics

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Novel $ZnIn_2S_4$ Combines Piezopotential and Dipole Field for Hydrogen Technique

This study offers an in-depth examination of vacancy engineering in ZIS nanosheets, utilizing piezopotential and dipole fields to optimize photocatalytic performance.

Visible-light-driven photocatalysts often suffer from significant charge recombination due to their limited carrier diffusion lengths, which constrain their practical applications. A common strategy for mitigating this challenge is the development of heterostructure photocatalysts with built-in junction fields to promote charge separation. Alternatively, leveraging the dipole field within the internal bulk phase of photocatalysts has demonstrated considerable effectiveness in enhancing charge separation and transport. This dipole field arises naturally in photocatalysts with non-centrosymmetric crystal structures and can be introduced through the structural modifications. Piezoelectric polarization, a macroscopic built-in potential, is generated in piezoelectric crystals with non-centrosymmetric structures in response to applied mechanical stress. Piezo-photocatalysis synergistically integrates the piezoelectric effect with the light-harvesting capabilities of piezoelectric semiconductors, facilitating the separation and movement of photogenerated charge carriers through the macroscopic built-in potential field.

Jih-Jen Wu (National Cheng Kung University) and his coworkers recently investigated the influence of In- and S-vacancy concentrations on the photocatalytic activity of zinc indium sulfide (ZIS) nanosheets for hydrogen evolution reactions (HERs). Using X-ray absorption spectroscopy (XAS) measurements, including X-ray absorption near edge structure (XANES) and extended X-ray absorption fine structure (EXAFS), conducted at **TPS 32A** and **TPS 44A**,[1] they gained deeper insights into the structural transformations of defective ZIS after hydrazine treatment. For clarity, the unmodified ZIS powder, as well as the modified ZIS powders that had been subjected to hydrazine treatment for 1 hour and 5 hours, are designated as ZIS-0, ZIS-1, and ZIS-5, respectively. **Figure 1(a)** presents the XANES spectra of the ZIS samples at the S K-edge, revealing a notable increase in sulfur vacancies and unoccupied states at sulfur sites following hydrazine treatment. **Figures 1(b) and 1(c)** illustrate the XANES and EXAFS spectra at the Zn K-edge for ZIS-0 and ZIS-5. The reduced coordination number and elevated electron density observed at Zn sites in ZIS-5 compared to ZIS-0 are attributed to the higher concentration of sulfur vacancies in ZIS-5. Similarly, **Figs. 1(d) and 1(e)** display the XANES and EXAFS spectra at the In K-edge for ZIS-0 and ZIS-5. Because of the contrasting trends in electron density changes driven by sulfur and indium vacancies, it was determined that sulfur vacancies have a more pronounced effect on the electron density at the indium sites in ZIS-5 than do indium vacancies, resulting in increased electron density at these sites compared to ZIS-0. Additionally, ZIS-5 exhibits a slightly diminished sulfur coordination environment relative to ZIS-0, which is attributed to a higher sulfur vacancy concentration post-treatment. The atomic arrangement of sulfur and indium vacancies within

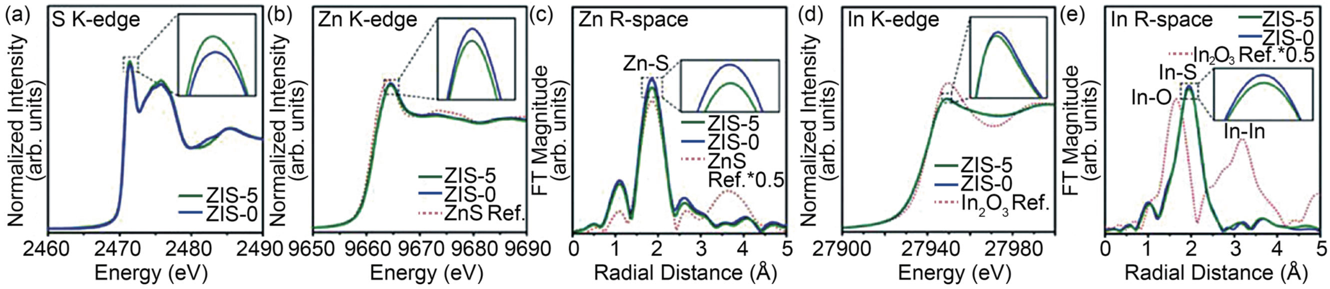

Fig. 1: (a) Normalized S K-edge XANES spectra for ZIS-0 and ZIS-5. (b) Normalized Zn K-edge XANES spectra and (c) Fourier transformed (FT) EXAFS spectra in R-space of ZIS-0, ZIS-5, and ZnS reference. (d) Normalized In K-edge XANES spectra and (e) FT EXAFS spectra in R-space of ZIS-0, ZIS-5, and In_2S_3 reference. [Reproduced from Ref. 1]

the ZIS structure plays a pivotal role in facilitating rapid charge transfer and effective charge separation, ultimately enhancing hydrogen production. This investigation meticulously explores how sulfur and indium vacancies improve charge dynamics and hydrogen evolution rates. By integrating the experimental data with multi-scale simulations, the study demonstrates how these vacancies optimize hydrogen production, offering valuable insights into the mechanisms by which structural vacancies in ZIS influence its electrochemical performance, particularly in hydrogen generation applications.

In summary, defect engineering of ZIS nanosheets with varying levels of indium and sulfur vacancies was successfully realized through hydrazine post-treatment of hydrothermally synthesized ZIS nanosheets. The photocatalytic HER rates show a positive correlation with the combined concentrations of indium and sulfur vacancies in the ZIS nanosheets. This study provides a detailed exploration of vacancy engineering in ZIS nanosheets, leveraging piezoelectric polarization in conjunction with the dipole field to enhance photocatalytic efficiency. (Reported by Yan-Gu Lin)

This report features the work of Jih-Jen Wu and his coworkers published in Adv. Mater. ***36****, 2403228 (2024).*

TPS 32A Tender X-ray Absorption Spectroscopy
TPS 44A Quick-scanning X-ray Absorption Spectroscopy

- XAS
- Materials Science, Chemistry, Condensed-matter Physics, Environmental and Earth Science

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Defect-Engineering for Selective Methanol Decomposition

Undercoordinated Pt sites in $PtTe_2$ are crucial in facilitating methanol decomposition and promoting formaldehyde production.

Two-dimensional transition metal dichalcogenides (TMDs) have garnered significant attentions in catalysis due to their unique electronic properties, high surface area, and tunable surface chemistry. Unlike conventional noble metal catalysts, which exhibit disadvantages such as high costs and susceptibility to poisoning, TMDs are promising alternatives owing to their structural versatility and defect engineering capabilities.[1,2] However, the basal planes of pristine TMDs are often inert, limiting their catalytic utility. Surface defects, particularly chalcogen vacancies, introduce the undercoordinated metal sites that can serve as highly active catalytic centers, significantly altering their chemical reactivity. Among TMDs, platinum telluride ($PtTe_2$) is of particular interest due to its intrinsic metallic nature, which provides superior conductivity compared to semiconducting TMDs such as MoS_2 or WS_2. A research team led by Meng-Fan Luo (National Central University), Jyh-Pin Chou (National Changhua University of Education), and Chun-Liang Lin (National Yang Ming Chiao Tung University) is investigating the catalytic properties of $PtTe_2$ with engineered Te vacancies. Their study focuses on $PtTe_2$, a metallic group-10 TMD, emphasizing the role of undercoordinated Pt (Pt_{uc}) sites at Te vacancies in methanol decomposition, which is a crucial reaction for hydrogen production and direct methanol fuel cells. To explore the catalytic behavior of $PtTe_2$, controlled Ar^+