



# Swiss Science Concentrates

## A CHIMIA Column

Short Abstracts of Interesting Recent Publications of Swiss Origin

### Interfacial Stabilization by Prelithiated Trithiocyanuric Acid as an Organic Additive in Sulfide-Based All-Solid-State Lithium Metal Batteries

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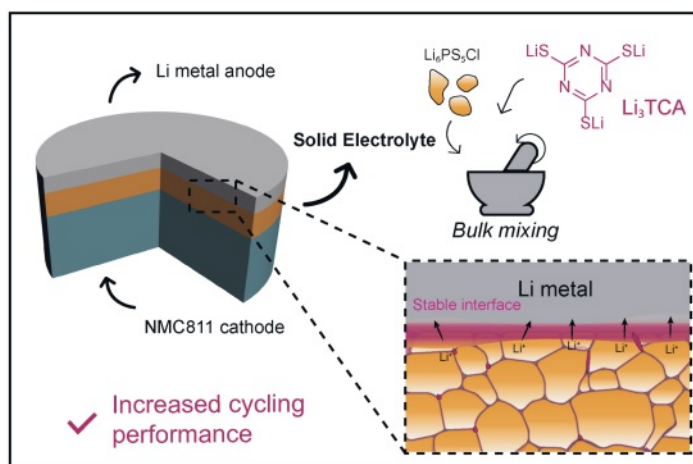
<https://doi.org/10.1002/anie.202408238>

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Sulfide-based all-solid-state batteries (ASSBs) with lithium metal anodes (LMAs) are promising due to their safety and potential for higher energy density compared to conventional Li-ion batteries. However, the narrow electrochemical stability window and chemical reactivity of sulfide solid electrolytes with LMAs lead to interfacial degradation and reduced performance. To mitigate this, the authors propose adding prelithiated trithiocyanuric acid ( $\text{Li}_3\text{TCA}$ ) to  $\text{Li}_6\text{PS}_5\text{Cl}$ , which stabilizes the interface and maintains high ionic conductivity. Incorporating 2.5 wt %  $\text{Li}_3\text{TCA}$  decreases  $\text{Li}_2\text{S}$  formation in the solid-electrolyte interface (SEI), enhancing stability. This approach increases the critical current density in LiLi symmetric cells from 1.0 to 1.9  $\text{mA cm}^{-2}$  and allows stable cycling for over 750 hours. It also extends the lifespan of Li|NbO-NCM811 full cells to over 500 cycles at 0.3 C.

#### Authors' comments:

“The pioneering use of a simple molecular additive in solid-state batteries for interfacial stabilization opens up new avenues for harnessing organic molecules to fine-tune the properties of solid-state electrolytes.”



### NSPs: Chromogenic Linkers for Fast, Selective, and Irreversible Cysteine Modification

Yong Hua, Zhi Zhou, Alessandro Prescimone, Thomas R. Ward, Marcel Mayor, and Valentin Köhler\*

*Chem. Sci.* **2024**, *15*, 10997.

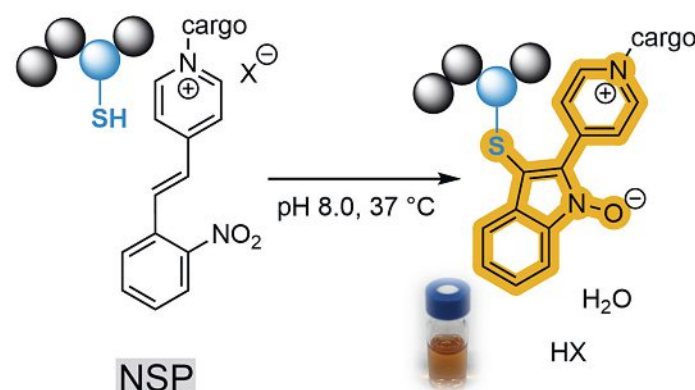
<https://doi.org/10.1039/d4sc01710b>

University of Basel

A Click & Lock reaction sequence involves the addition of a sulfhydryl group to water-soluble *N*-alkyl(*o*-nitrostyryl)pyridinium ions (NSPs), resulting in a stable S–C  $\text{sp}^2$  bond through rapid, irreversible cyclization and aromatization. This process selectively targets cysteine residues, forming *N*-hydroxy indole pyridinium ions. The reaction causes a red shift of over 70 nm, allowing easy monitoring by UV-vis spectroscopy with extinction coefficients of  $\geq 2 \times 10^4 \text{ M}^{-1} \text{ cm}^{-1}$ . Its versatility is demonstrated in peptide stapling and protein derivatization, such as modifying trastuzumab with Val-Cit-PAB-MMAE. The method offers high stability, rapid reaction rates, and high selectivity, making it a promising alternative for cysteine conjugation.

#### Authors' comments:

“NSPs are easily prepared, tuned, and modified. Bioconjugation reactions of NSPs reach high conversion within short time frames and a developing coloration indicates reaction progress.”



## Excited-State Dynamics of MAPbBr<sub>3</sub>: Coexistence of Excitons and Free Charge Carriers at Ultrafast Times

Natalie Banerji, Demetra Tsokkou, Nikolaos Droseros, Parnian Ferdowski, Efrain Ochoa Martinez, and Michael Saliba.

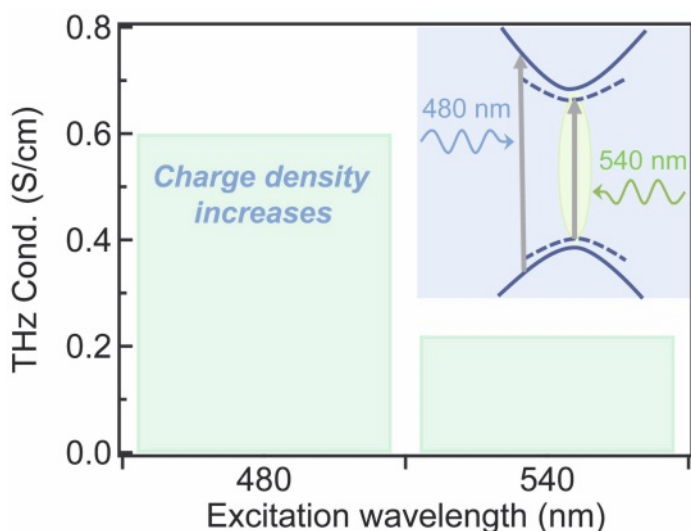
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<https://doi.org/10.1021/acs.jpcc.3c08509>

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This study explores the photophysical properties of methylammonium lead tribromide perovskite (MAPbBr<sub>3</sub>), an important material for light-emitting applications and tandem solar cells. Using transient spectroscopies, the researchers explore how excitons and free charge carriers behave under various excitation conditions. They found that both excitons and free charges are rapidly generated within 50–100 femtoseconds and coexist in the material. The ratio of excitons to free charges increases as the excitation photon energy approaches the band gap. At high excitation densities, complex interactions like band gap renormalization, excitonic repulsion and others occur. The study shows that excitons can localize in shallow traps before being released, highlighting the potential of MAPbBr<sub>3</sub> for light-emitting applications and tandem solar cells.

### Authors' comments:

“Our study highlights the value of collaborative work, combining outstanding materials synthesis with detailed photophysical characterization. We are confident that our findings pave the way for educated design of perovskite materials for optoelectronic devices.”



## Direct Anchoring of Molybdenum Sulfide Molecular Catalysts on Antimony Selenide Photocathodes for Solar Hydrogen Production

Pardis Adams, Jan Bühler, Iva Walz, Thomas Moehl, Helena Roithmeyer, Olivier Blacque, Nicolò Comini, J. Trey Diulus, Roger Alberto, Sebastian Siol, Mirjana Dimitrievska, Zbynek Novotny\*, and S. David Tilley\*

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<https://doi.org/10.1021/acsenergylett.4c01570>

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Molybdenum sulfide is a promising non-precious metal catalyst for hydrogen evolution, with activity concentrated at its edge sites. To enhance catalytic performance at low loading densities, two molybdenum sulfide clusters, [Mo<sub>3</sub>S<sub>4</sub>]<sup>4+</sup> and [Mo<sub>3</sub>S<sub>13</sub>]<sup>2-</sup>, were investigated. These molecular catalysts were deposited on Sb<sub>2</sub>Se<sub>3</sub> via a simple soaking process, forming a thin catalytic layer. Under illumination, the catalysts achieved up to 20 mA cm<sup>-2</sup> of current density. Both clusters demonstrated activity, with [Mo<sub>3</sub>S<sub>13</sub>]<sup>2-</sup> proving superior, delivering higher photovoltage and achieving a faradaic efficiency of 100% for hydrogen evolution. This enhanced performance is attributed to the more efficient loading and higher catalytic activity of [Mo<sub>3</sub>S<sub>13</sub>]<sup>2-</sup> on the Sb<sub>2</sub>Se<sub>3</sub> surface, validated through X-ray photoelectron and Raman spectroscopy.

### Authors' comments:

“Earth-abundant molecular catalysts play a crucial role in the future success and commercialization of photoelectrochemical water splitting, due to their high selectivity and widespread availability.”

