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Introduction to emerging materials for solar energy harvesting

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In this themed edition of *Journal Materials Chemistry A*, organized in collaboration with the ICMAT 2023 Symposium O, we present innovative work at the forefront of materials research aimed at addressing the carbon crisis. This includes experimental works, reviews, and perspectives on carbon dioxide reduction, photovoltaics, hydrogen evolution photocatalysis and water oxidation electrocatalysis. The studies span a large spectrum of materials, ranging from metals to oxides, sulfides, selenides, halides, Kesterites, nitrides, oxynitrides, and perovskite-inspired materials.

In overall water splitting as a pathway to green hydrogen fuel, several advances are highlighted. In one contribution, Ji-Hyun Jang and coworkers review developments on heteroatom-doped hematite for photoelectrochemical water oxidation (**https://doi.org/10.1039/D3TA04520J**). This is followed by a perspective by Kazunari Domen and coworkers on cost-effective solar hydrogen production with photocatalyst sheets (**https://doi.org/10.1039/D3TA04353C**). Separately, Qian Wang and coworkers review methods to improve the photocatalytic hydrogen evolution efficiency of covalent triazine frameworks (**https://doi.org/10.1039/D3TA04472F**). Oxynitride materials are attractive photocatalysts for water splitting, and accordingly, Kazuhiko

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Joel M. R. Tan

Joel M. R. Tan, a Senior Research Fellow at the School of Materials Science and Engineering, Nanyang Technological University, Singapore, has an interdisciplinary research career. His work, deeply rooted in chemistry, spans a wide array of fields: from the intricacies of DNA origami and synthetic food chemistry to the synthesis of inorganic nanoparticles. Joel has made contributions to the development of materials for renewable energy harvesting, the formulation of inks for printed electronics, and the advancement of 3D printing technology and 3D design for soft robotics applications. Joel actively collaborates with industry partners to innovate in the field of printed electronics, aiming to bridge the gap between academic research and practical applications. As of December 2023, Joel's contributions to the field are reflected in his H-index of 16.

Frank E. Osterloh

Frank E. Osterloh is a Professor in the Chemistry Department at the University of California, Davis, United States. His research interests are centered on the chemical and photophysical properties of inorganic materials and their use for solar energy conversion. This includes the development of photocatalysts for overall water splitting (artificial photosynthesis), the sustainable fabrication of inorganic photovoltaics, and the study of photochemical charge-transfer reactions with surface photovoltage spectroscopy. Frank has authored 135 peer-reviewed scientific publications, including three book chapters and several review articles. As of November 2023, his works have received over 10 000 citations, based on the Web of Science, and his H index is 45.

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Maeda and coworkers demonstrate that the transformation of $K_2LaTa_2O_6N$ into nanosheets enhances catalytic hydrogen evolution (https://doi.org/10.1039/D3TA01387A). While most photoanode studies focus on solar irradiation conditions, Sophia Haussener and coworkers study the function and stability of Sn-doped Fe_2O_3 and $BiVO_4$ photoelectrochemical cells under high-irradiance (https://doi.org/10.1039/D3TA05257E). Water electrolysis in combination with photovoltaics offers higher efficiencies, but stable and inexpensive electrocatalysts are lacking. In their paper, Chuan Zhao and coworkers explore the factors that limit the stability of FeNiCr and FeNi oxygen evolution electrocatalysts under industrial conditions (https://doi.org/10.1039/D3TA03905F). Along similar lines, Roland Marschall and coworkers demonstrate Ni_2FeS_4 as a non-precious-metal hydrogen evolution co-catalyst in combination with TiO_2 (https://doi.org/10.1039/D3TA02439C). Lastly, report from Ong Wee-Jun's group identifies the morphology–activity relationship in $ZnIn_2S_4$ photocatalysts for hydrogen evolution coupled to benzyl alcohol oxidation (https://doi.org/10.1039/D3TA04204A).

Key to improved photovoltaics is the expansion of the material library and the development of new materials as superior solar absorbers. Reports include a comprehensive study on combinatorial sputtering and theoretical calculations in the Ba–Sn–S ternary phase system, identifying promising candidates for optoelectronic applications (https://doi.org/10.1039/D3TA04431A). The exploration of intrinsic defects and hydrogen impurities in Zn_3P_2 through hybrid functional calculations reveals subtle yet beneficial impacts on its electrical properties (https://doi.org/10.1039/D3TA03697A). In the quaternary I_2–II–IV–X_4 system, efforts to mitigate anti-site defects are discussed, with a focus on alkali element doping in $Cu_2BaGe_{1-x}Sn_xSe_4$ films (https://doi.org/10.1039/D3TA01494K). Ding-Jiang Xue and coworkers show that copper can replace gold as the electrode material in selenium photovoltaics to yield efficiencies of up to 10.4% under indoor illumination (https://doi.org/10.1039/D3TA04530G). Additionally, Robert Hoye and coworkers highlight the promising applications of bismuth sulfobromide (BiSBr) in indoor photovoltaics and optoelectronics (https://doi.org/10.1039/D3TA04491B). Innovative syntheses of antimony chalcohalides to produce photovoltaics with high open-circuit potential are provided by Edgardo Saucedo and coworkers (https://doi.org/10.1039/D3TA03179A). It is also shown that prebaking of a SnS source with sulfur can achieve higher performance in SnS solar cells (https://doi.org/10.1039/D3TA05204D) and that doping of silver into Cu_2CdSnS_4 leads to doping-type inversion (https://doi.org/10.1039/D3TA04529C). Finally, a review article by Marit Kauk-Kuusik and others focuses on flexible PV solar cells from Cu_2ZnSnS_4 (CZTS) monograin layers (https://doi.org/10.1039/D3TA04541B).

Improved photovoltaic performance is achieved by improving overall device design. For example, in antimony-based solar cells, $InCl_3$-modified SnO_2 improves both electron transport and the quality of the heterojunction (https://doi.org/10.1039/D3TA03358A). It is also shown that incorporation of InOCl layers between the In_2S_3 buffer layer and the $Sb_2(S,Se)_3$ absorber reduces defects and allows higher conversion efficiency (https://doi.org/10.1039/D3TA01736B). An improved photovoltaic efficiency of 8% is achieved by combining hydrothermal deposition with vapor transport to grow $Sb_2(S,Se)_3$ films with graded bandgaps (https://doi.org/10.1039/D3TA05489F).

The potential of photovoltaic semiconductors in photoelectrochemical water splitting is further explored. CZTS's performance and stability in PEC applications have been examined by one of us, particularly the role of ITO interface modifications between buffer layers and catalysts (https://doi.org/10.1039/D3TA05227C). With antimony selenide, solution treatments boost photocathode performance for hydrogen generation, as reported by David Tilley and coworkers (https://doi.org/10.1039/D3TA00554B).

Finally, we address direct carbon conversion and CO_2 removal for fuel production. In one contribution, Lydia Wong and coworkers show that electrochemical CO_2 reduction to CO is improved by replacing Sb sites with sulfur in Cu–Sb–S photocathodes (https://doi.org/10.1039/D3TA04777F). In another paper by Lianzhou Wang and coworkers, they emphasized the influence of carbon contamination on product analysis for catalytic CO_2 reduction (https://doi.org/10.1039/D3TA00834G). Finally, using Sn as a growth surfactant to mitigate oxygen and carbon impurities, Ann Greenaway and coworkers showed single-crystal-like Sn:$ZnTiN_2$ films with improvements to optoelectronics properties, aiming to advance photoelectrochemical CO_2R performance (https://doi.org/10.1039/D3TA06200G).

We hope that this themed issue on emerging materials for solar energy harvesting in the *Journal of Materials Chemistry A* will not only provide readers with new insights, but also stimulate new ideas. We thank all the contributing authors, reviewers, and editorial and production staff for making this themed issue possible.

Lydia Wong

Lydia Wong is an Associate Professor at the School of Materials Science and Director of the Global Alliance of Industries at Nanyang Technological University, Singapore. A Fellow of the Royal Society of Chemistry, she serves on editorial boards for leading journals in energy and materials chemistry. She specializes in the synthesis and development of emerging materials for next-generation solar harvesting, including photovoltaics, solar water splitting and CO_2 conversion. Lydia has authored more than 160 reviewed scientific publications, including several review articles. As of January 2024, based on the Web of Science, her work has been cited more than 9000 times and her h-index is 55.

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