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Designing Complex Semiconductors: Tunable Mixed-Halide Chalcohalides and Transition Metal Dichalcogenides for Optoelectronic Applications

ABSTRACT:

Part 1. Chalcohalides are desirable semiconducting materials due to their enhanced light-absorbing efficiency and stability compared to lead halide perovskites. However, unlike perovskites, tuning the optical properties of chalcohalides by mixing different halide ions into their structure remains to be explored. We present an effective strategy for halide-alloying $Pb_3SBr_xI_{4-x}$ ($1 \leq x \leq 3$) using a solution-phase approach and study the effect of halide-mixing on structural and optical properties. We employ a combination of X-ray diffracraction, electron microscopy, and solid-state NMR spectroscopy to probe the chemical structure of the chalcohalides and determine mixed-halide incorporation. The absorption onsets of the chalcohalides blue-shift to higher energies as bromide replaces iodide within the structure. The photoluminescence maxima of these materials mimic this trend at both the ensemble and single particle fluorescence levels, as observed by solution-phase and single particle fluorescence microscopy, respectively. These materials exhibit superior stability against moisture compared to traditional lead halide perovskites, and IR spectroscopy reveals that the chalcohalide surfaces are terminated by both amine and carboxylate ligands. Electronic structure calculations support the experimental band gap widening and volume reduction with increased bromide incorporation, and provide useful insight into the likely atomic coloring patterns of the different mixed-halide compositions.

Part 2. Layered, transition metal dichalcogenides (TMDCs) such as MoS_2 and WSe_2 are under intense investigation due to their structural flexibility and optoelectronic tunability. The extent of mixing and alloying between two or more TMDCs is critical to their properties,yet elucidating these chemical transformations at the atomic scale remains difficult. To address this challenge, we probe TMDC mixing and alloying by using a combination of powder X-ray diffraction (XRD) and ^{77}Se solid-state nuclear magnetic resonance (SSNMR) spectroscopy. We find that the specific material and atmosphere used for ball milling and annealing strongly impact the formation of oxides during the mixing of TMDCs. Static wideband, uniform rate, smooth truncation (WURST)-quadrupolar Carr-Purcell-Meiboom-Gill (QCPMG), magic angle spinning (MAS), and dynamic nuclear polarization (DNP) SSNMR techniques allow us to detect and resolve ^{77}Se resonances in mixed bulk, exfoliated, and nanoscale TMDCs. Together, powder XRD and static WURST-QCPMG ^{77}Se SSNMR provide conclusive evidence for the formation of new alloyed multinary TMDCs, where all elements are intimately mixed at the atomic level, upon ball milling and subsequent annealing.

BIO:

Javier Vela is a University Professor of Chemistry at Iowa State University. He is a Fellow of the American Chemical Society (ACS) and the American Association for the Advancement of Science (AAAS). He serves on the editorial advisory boards of *ACS Energy Letters*, *Chemistry of Materials*, *Chemistry–An Asian Journal*, and *ChemNanoMat*. Along with former and current coworkers, Dr. Vela is the author of over ninety-five peer-reviewed scientific publications and patents on nanostructured materials, inorganic compounds, and their application to energy conversion, chemical catalysis, and fluorescence imaging. He has directed eighteen doctoral and four master's theses and successfully mentored numerous undergraduate researchers, among them three NSF graduate research fellowship awardees.

Dr. Vela has been a faculty scientist with the Ames National Laboratory since 2010. An active member of the American Chemical Society, he has served as Councilor for the Ames local section, Program Chair for the Midwest Regional Meeting in Ames in 2018, Treasurer of the Division of Inorganic Chemistry, and member of the Committee on Committees (ConC). He also worked as Equity Advisor for the ISU College of Liberal Arts and Sciences from 2015 to 2021. Dr. Vela holds a BS (Lic.) in Chemistry from UNAM and a PhD degree in Chemistry from the University of Rochester. After postdoctoral stints at the University of Chicago and Los Alamos National Laboratory, he joined Iowa State University in 2009. He was granted tenure in 2015 and became a full professor in 2019. He was named University Professor in 2020, and held the rotating John D. Corbett Endowed Professorship in Chemistry from 2020 to 2023. Dr. Vela grew up in Xalapa, Veracruz (Mexico) and is a proud US Citizen by naturalization.