Hawai‘i Natural Energy Institute Research Highlights

Advanced Materials

Two-Dimensional Materials for Thin Film Manipulation

OBJECTIVE AND SIGNIFICANCE: Through this project, our objective is to develop methodologies to facilitate the manipulation of thin films utilizing two-dimensional (2D) interfacial layers. This approach has the potential to facilitate the physical transfer of high-efficiency devices, such as photovoltaics, from their original substrates to novel platforms, including clothing, vehicles, and buildings.

BACKGROUND: Monolithic integration – the process by which solid-state devices are made by sequentially depositing layers of materials on top of each other – is used in all commercial thin film-based technology. This process is so foundational that it is difficult to imagine any other way to create solid-state devices. Despite its wide acceptance, however, monolithic integration presents two major limitations. First, process compatibility is a challenge since the deposition of each layer must not damage the previously deposited underlying layers in any way. As such, the thermal, mechanical, and chemical compatibility between layers and their deposition processes is of prime importance, restricting materials selection to a subset of compatible systems, limiting the adoption of emerging promising candidates. Second, monolithic integration almost always leads to the formation of additional phases at the interface of two materials. The electronic and chemical properties of interfaces also generally differ significantly from those of a simple combination of the two constituting layers, which impacts device performance.

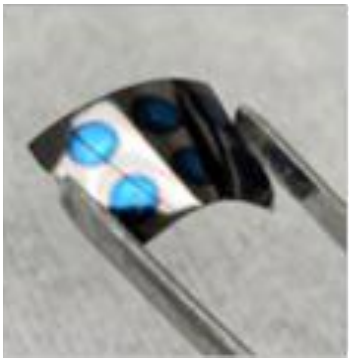
An integration scheme that combines materials regardless of their nature, while preserving or even enhancing their intrinsic performance, could revolutionize the manufacturing of renewable technologies that rely on material stacking, including photovoltaic (PV) devices. Such an integration approach, using 2D materials for thin film manipulation, is proposed in this program.

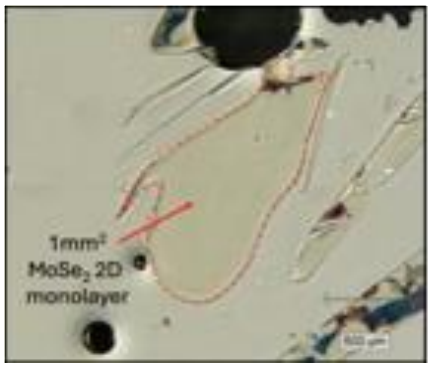
PROJECT STATUS/RESULTS: In this project, the University of Hawai‘i (UH) and the University of Nevada, Las Vegas (UNLV) partners with the Lawrence Livermore National Laboratory (LLNL) and National Renewable Energy Laboratory (NREL) to develop the concept of 2D material-assisted thin film exfoliation, focusing on the chalcopyrite class (e.g., $Cu(In,Ga)Se_2$, CIGSe) and transition metal dichalcogenides (e.g., MoS_2 and $MoSe_2$) 2D interfacial layers that can naturally form when sulfur- or selenium-containing semiconductors are deposited onto transition metal substrates.

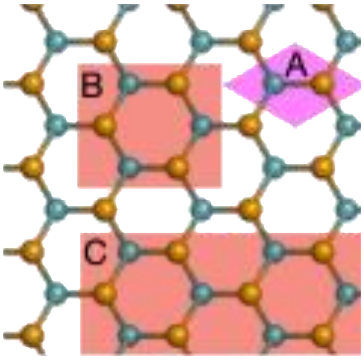
Current efforts are focused on: 1) the exfoliation of commercially available 2D materials; 2) the characterization of their chemical properties using advanced spectroscopic techniques; and 3) the theoretical modeling of their energetics when interfaces with CIGSe.

Graphene and $MoSe_2$ 2D layers were isolated through the mechanical exfoliation method. Flakes of both materials were delaminated from bulk seed crystals by pressing a transfer strip onto them. The process involved folding the tape on itself a predetermined number of times to further separate the remaining crystals. Subsequently, these separated layers were transferred onto silicon wafers. X-ray photoelectron spectroscopy and Raman spectroscopy carried out at UNLV and HNEI, respectively, evidenced the 2D nature of the layers isolated with HNEI’s method.

Lastly, theoretical modeling efforts conducted at both UH and LLNL focused on understanding the impact of mechanical strain on the energetic properties of 2D materials. This crucial information will be







instrumental in analyzing how mechanical deformation, such as stretching or bending, affects the performance of flexible PV devices.

To date, this research has produced the following work:

- 2024, M. McLean, A.T. Nguyen, W. Lee, and N. Gaillard, **Periodically Strained 2D Materials for Tunable Optoelectronic Applications**, Presented at the Electrochemical Society PRiME Meeting, October 6-11, Symposium H03, Abstract 2468.

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