Novel 2D materials (2D pnictogen and palladium chalcogenides): a new Self-powered platform for optoelectronics and sensors.

Project goal

Photodetectors and sensors are an irreplaceable part of our daily life thanks to their wide range of applications from health, security, electronic devices to smart systems. Several investigations in this direction have already been carried out with different materials. Nevertheless, we need to improve their response time and responsivity for practical applications. For this reason, researchers are always striving to find new materials for better applicability. In this direction, we have extended our search to various emerging 2D materials. The emerging 2D materials (pnictogens, palladium thiophosphate ($Pd_3(PS_4)_2$), and palladium phosphochalcogenides (PdPS)) have tremendous attraction due to their intriguing structures and extraordinary electronic properties. In the group of pnictogens, only the famous member BP has been better studied by researchers, but the other members such as arsenene, antimonene and bismuthene are largely unexplored. Also, the optical properties of $Pd_3(PS_4)_2$ and PdPS have hardly been explored experimentally, although theoretical calculations predict a preferred band gap (2.60 eV) with an unprecedented absorption coefficient on the order of 106 cm-1 in the UV-vis region, which have emerged as future candidates for sensors and photodetector applications. The above reason has led us to investigate the optoelectronic and sensing properties of these 2D materials. Our main goal in this project is to develop new self-powered photodetectors and sensors using a photoelectrochemical based system that can be efficiently used for broadband or targeted IR photo sensing by the above single materials or the combination of 2D materials and upconverting nanoparticles. We will also extend our research to the development of photodetectors and sensors using 2D pnictogens and new 2D materials ($Pd_3(PS_4)_2$ and PdPS) to achieve better device performance.

Description of the research

The main motivation of this project is to fill this gap and provide a platform for future optoelectronic applications. The success of this project is based on an interdisciplinary approach combining materials chemistry, electronics, and optical physics. The path can be summarized:

1. Realization of high-quality ultrathin film 2D materials by mechanical/chemical exfoliation.
2. Fabrication of novel device architectures to demonstrate superior device performance and explore the underlying science.
3. Explore optoelectronic and sensing properties of novel pnictogens, $Pd_3(PS_4)_2$ and PdPS.
4. Attempt to develop a novel self-powered (PEC), ultrasensitive and ultrafast sensing platform.

Justification for tackling a specific scientific problem

Two-dimensional (2D) materials have attracted much attention and have been extensively studied in recent decades due to their intriguing physical, electronic, and chemical properties resulting from their 2D quantum confinement. It is immensely important to find new 2D materials that offer the right bandgap, environmental stability, and high carrier mobility to meet the requirements of high-efficiency future devices. One of the example is member of pnictogen group, black phosphorus (BP), which is promising to address the bottlenecks created by graphene (high carrier mobility but zero band gap) and TMDs (low carrier mobility, with a relatively large band gap of 1.5−2.5 eV) with tunable band gap (0.3 to 1.5 eV) and a high carrier mobility (1000 $cm^2 V^{-1} s^{-1}$). Along this way the emerging layered semiconductors such as metal phosphochalcogenides (i.e., palladium thiophosphate ($Pd_3(PS_4)_2$) and palladium phosphochalcogenides (PdPS)) also possess tremendous potential as their theoretical calculations predict an ideal band gap (2.45 eV) with a measured carrier density and Hall mobility of 2.36×10^{16} cm^3 and 87 $cm^2 V^{-1} S^{-1}$, respectively. To fulfil the goal of prepare novel devices for sensors and photodetector applications, we explore the emerging photoelectrochemical (PEC) photodetectors, which are inherently self-powered photodetectors and have a low-cost, environmentally friendly, and simpler fabrication process compared to other types of self-powered photodetectors. We believe that our attempt to develop a new self-powered, ultrasensitive, and ultrafast sensing platform will be effective toxic gas detection and photodetection for practical use of warfare agents.

The impact of the project results on the development of the research field and scientific discipline

The PEC-based, self-powered photodetector with novel 2D materials enables the design and construction of highly effective photodetectors for a wide spectral range, from the ultraviolet to the far infrared. They achieve sensitivity that exceeds the current state of the art of commercially produced photodetectors by several orders of magnitude. Volatile organic molecules are of particular interest in biochemistry and public health. Detection of explosives, which are also typically based on organic compounds with nitro or nitric ester groups, is critical. Detection of underwater hazards (e.g., sea mines, torpedoes) is another important but difficult task. Our preliminary results showed superior responsivity and frequency-dependent selectivity for various organic vapors with an ultrafast response and recovery time of less than 1 s. This phenomenon made it a suitable candidate for practical sensing applications. This novel material with the fascinating phenomenon described above will pave the way for practical future applications in optoelectronics and sensing.