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2D/2D MXene-based Van der Waals heterostructures for next-generation optoelectronic applications

Optoelectronics is considered a technology of the future. It has already contributed to the massive development of technology not only in the development of the information industry but also in other various aspects, such as medical, aerospace, defense, and solving environmental problems. Based on Market Insight Report, the optoelectronics market is expected to grow by around 10% in 2024. Nowadays, almost every aspect of daily life is exposed to the rapid development of optoelectronics. For examples, the development of thin and foldable electronic devices, the utilization of photocatalysts for degrading harmful substances, the usage of various smart sensors to make people’s lives easier, and the use of solar cells as green energy to reduce carbon emission. Basically, optoelectronic devices are based on light-matter interaction in the materials. Therefore, to push forward the development of optoelectronic devices, one needs to discover more suitable materials with excellent properties, easy processing, and low-cost.

Combining two different materials into a single block is considered a promising way to obtain materials with hybrid physicochemical properties. Nowadays, 2D nanomaterials are viewed as an ideal building block for fabricating 2D/2D Van der Waals (VdW) heterostructure. In 2011, Naguib *et al.* introduced Ti_3C_2 MXene to the world by etching it from the parental Ti_3AlC_2 MAX phase. In particular, MXene offers several advantages compared to other 2D nanomaterials, such as good dispersibility in aqueous solution and excellent conductivity. Recent studies have shown the possibility of MXene-based heterostructure to improve the optoelectronic performance of semiconductors, for example, prolonged charge transfer, light absorption, and electrical conductivity. Furthermore, Ti_3C_2 is the most popular MXene, with 70% of MXene studies devoted to this material. It is believed that the synergistic mechanism in Ti_3C_2/2D leading to improvement in photogenerated carrier lifetime. However, as MXene is a complex optical material that may behave as a semiconductor or metallic, the mechanism behind the improvement of optoelectronic properties of MXene-based heterostructure is still unclear.

As MXene family member comes with distinct physicochemical properties, it is important to discover the complex light-matter interaction in other MXenes. In this study, three different MXenes with distinct stability and electronic structure are selected, i.e., Ti_2C (semiconductor), Nb_2C (conductor), and V_2C (very unstable). It is expected that different MXene heterostructures will give different electron transport mechanisms. For the construction of heterostructure, MXene will be coupled with graphene as graphene has a high theoretical specific surface area, superior carrier mobility, high stability, and high thermal conductivity.

The coupling between graphene and MXene is also expected to give heterostructure with robust adhesion, prevention towards self-restacking problems, and interestingly this structure can be easily fabricated by self-assembly methods. The project's final objective is to implement the proposed VdW heterostructure in optoelectronics applications. Thus, two different optoelectronic application models will be demonstrated i.e., wearable photodetector and photocatalysis for pollutant degradation. This project will give an insight into understanding the mechanism of MXene charge carrier behavior and open the pathway for MXene-based heterostructure to be implemented in next-generation optoelectronic applications.