## <u>Defect Engineering of 2D Transition Metal Dichalcogenides for Nitrogen</u> Reduction Reaction

The current process for producing ammonia, a crucial substance in fertilizers and various industrial products such as textiles and pesticides is creating environmental problems leading the world population into an energy crisis. Ammonia can also be a potential green energy carrier and transportation fuel. Unfortunately, the traditional production methods heavily rely on fossil fuels, making them unsustainable. In particular, the widely used Haber-Bosch process consumes a significant amount of energy, accounting for about 1-2% of the total energy consumption resulting in a large amount of CO<sub>2</sub> emissions. This not only harms the environment but also establishes ammonia as an expensive and inefficient product.

To overcome these challenges, researchers are pursuing an environmentally friendly alternative known as nitrogen reduction reaction (NRR). By exploiting nitrogen, an abundant element in the Earth's atmosphere, we aim to revolutionize ammonia production and address the environmental concerns associated with current practices. However, this procedure has been proven to be quite challenging. This project aims to seek a new class of materials called transition metal dichalcogenides (TMDs) to improve the NRR process. These materials are cost-effective and show promise in making ammonia production more sustainable.

Our specific research objectives include:

- 1. Developing and preparing various TMDs suitable for efficient ammonia production.
- 2. Modifying the structure of TMDs to enhance their ability to interact with nitrogen, making the production process more effective.
- 3. Exploring engineering approaches, namely creating vacancies and adding certain elements (doping), to enhance the performance of TMDs in ammonia production.
- 4. Thoroughly examining the engineered materials to understand how they work and their potential contribution to cleaner ammonia production.
- 5. Assessing the efficiency, stability, and environmental impact of the new materials in the ammonia production process.

Our research will focus on finding better ways to produce ammonia, a vital component in our modern lives. By exploring novel materials and methods, we hope to create a cleaner, more sustainable future for ammonia production, greatly reducing its impact on the environment.