Two-dimensional van der Waals heterostructures with asymmetric heat transport

Within this project, we intend to **exploit atomic-scale material engineering to revolutionize how heat is managed.** Imagine controlling heat as precisely as we control electricity. The purpose of this project is to create a new generation of thermal dissipation nanoscale devices that work more like "one-way valves" for heat flow, using innovative advances in **two-dimensional materials –** that is, sheets just one or a few atoms thick. These atomically thin layers, stacked like ultra-precise LEGO blocks, could transform how we manage heat in electronics, energy systems, and beyond.

Why does this matter? Heat is the invisible enemy of modern technology. From overheating smartphones to energy loss in power grids, inefficient thermal management limits performance and sustainability. While electrical diodes revolutionized electronics decades ago, controlling heat directionally remains a major scientific hurdle. Current solutions operate poorly at room temperature or rely on bulky materials. This project tackles these limitations by leveraging the unique properties of two-dimensional (2D) materials to design a vertical thermal nanodevice that outperforms existing technologies.

Why 2D Materials? Contrary to conventional bulk materials, two-dimensional structures offer outstanding control of physical properties: *(i)* Their extreme thinness minimizes unwanted heat leakage. *(ii)* Interfaces can be engineered without defects that minimize heat flow. *(iii)* Properties such as thermal expansion and vibrational spectra can be tuned at the atomic level.

The core of this research involves **van der Waals heterostructures**: artificially engineered stacks of 2D materials such as graphene, hexagonal boron nitride (hBN), and transition metal dichalcogenides (*e.g.*, MoS_2 and WSe_2). The choice of these structures originates from their mismatched vibrational properties – namely, imagine two grids of atoms vibrating at completely different frequencies. When stacked, the heat can flow more easily in one direction (top-to-bottom) than in reverse, which is known as a thermal diode effect (an asymmetric heat flow).

Key innovations of the project include: *(i)* Combination of heavy-element materials (e.g., tungsten-based layers) with lightweight counterparts (*e.g.*, graphene) to maximize vibrational mismatch. *(ii)* The use of advanced techniques like deterministic transfer and electron-beam lithography to assemble defect-free interfaces. *(iii)* Rotation of monolayers at specific angles to fine-tune heat flow, akin to adjusting gears in a machine. *(iv)* Application of microscopic stress to layers to alter their heat-conducting properties.

How do we go from the lab to real-world impact? The project team will prototype innovative thermal nanodevices using a three-step approach:

- **Predictive Modeling**: Quantum-level simulations identify optimal material pairs and stacking configurations.
- **Nanoscale Fabrication**: Cutting-edge cleanroom techniques create devices with integrated heaters and sensors smaller than a human hair.
- **Ultra-Precise Testing**: Combined Raman spectroscopy and electrical thermometry measure heat flow with atomic-scale resolution.

The expected breakthroughs are: *(i)* A prototype nanodevice showing vertical thermal rectification **-** far beyond the state of the art. *(ii)* Experimental identification and design rules for "dialing in" the desired thermal properties through material choice, thickness, and twist angles. *(iii)* Understanding of how atomic-scale vibrations (phonons) govern heat transfer at interfaces.

Big Picture Breakthroughs. This project could open the way to:

- **Cooler, faster electronics**: Prevent overheating in next-generation chips.
- **Smart energy harvesting**: Convert waste heat more efficiently into electricity.
- **Advanced thermal circuits**: Pioneering computing systems powered by heat instead of electrons.

In the end, the main goal of this project is to shed some light on a problem that has puzzled scientists for years, potentially opening doors to a whole new world of heat management technologies.