NDnano
Notre Dame Nanoscience and Technology

NDnano Summer Undergraduate Research
2026 Project Summary

1. Student name & home university:
Keiton Klein, Trine University

2. ND faculty name & department:
Rev. Bryan D. Paulsen, S.J., Department of Chemical and Biomolecular Engineering
Prof. Nosang V. Myung, Department of Chemical and Biomolecular Engineering

3. Summer project title:
Rational Design of Ionic Liquid–Conjugated Polymer Chemiresistive Gas Sensors for Volatile Organic Compound Detection

4. Briefly describe new skills you acquired during your summer research:

- Analyzing grazing-incidence wide-angle X-ray scattering (GIWAXS) and ultraviolet-visible (UV-Vis) spectroscopy data to determine thin-film morphology.
- Operating an iFOUR microdispensing robot for precise, automated sample fabrication and material deposition.
- Handling sensitive materials and fabricating sensor devices within an inert glove box environment.
- Employing Sobol sampling methods for efficient, comprehensive experimental design and parameter space exploration.
- Utilizing Python to process raw data sets and track scattering trends
- Synthesizing complex structural data into accessible science communication formats, including poster design and PowerPoint.

5. Briefly share a practical application/end use of your research:

This research enables the development of low-cost, room-temperature volatile organic compound sensors for real-time environmental monitoring, industrial safety, and wearable health diagnostics, where rapid detection of hazardous gases is critical.

6. 50- to 75-word abstract of your project:

Volatile organic compounds (VOCs) require sensitive, low-power detection for environmental and industrial safety. This work investigates poly(3-hexylthiophene) (P3HT)/ionic liquid chemiresistive sensors by examining how ionic liquid loading affects film structure and VOC sensing. Structural characterization (GIWAXS, UV-Vis) and chemiresistive testing with acetone and toluene demonstrated detection down to 10 ppm-v. These findings establish structure–property relationships that guide the rational design of selective, room-temperature VOC gas sensors.

7. References for papers, posters, or presentations of your research:

[1] K. Stewart, S. Limbu, J. Nightingale, et al., “Molecular understanding of a π-conjugated polymer/solid-state ionic liquid complex as a highly sensitive and selective gas sensor,” Journal of Materials Chemistry C, vol. 8, pp. 15268–15276, 2020.

[2] T. J. Quill, G. LeCroy, D. M. Halat, et al., “An ordered, self-assembled nanocomposite with efficient electronic and ionic transport,” Nature Materials, vol. 22, pp. 362–368, 2023.

One-page project summary that describes problems, project goal, and your research activities / results:

Volatile organic compounds (VOCs) are harmful gases that can be found in both industrial settings and everyday indoor environments. Being able to detect these gases quickly and accurately is important for protecting human health, monitoring air quality, and improving workplace safety. While many current gas sensors work well, they often require high operating temperatures and complex instrumentations, making them energy-intensive and difficult to integrate into portable, scalable, and low-cost devices.

This research focused on developing room-temperature chemiresistive gas sensors using blends of poly(3-hexylthiophene) (P3HT) and ionic liquids. A primary objective was to understand how changing the composition of these materials affects both their structure and their sensing performance. The long-term goal of this research is to aid in the design of gas sensors that are more sensitive, selective, and energy efficient.

The project encompassed comprehensive involvement in all stages of the research and development process. Experimental planning utilized a SOBOL sampling method to efficiently explore different material compositions. To prevent contamination, P3HT and ionic liquid mixtures were prepared inside a glovebox. Significant effort was also dedicated to building and improving the testing equipment. This included assembling a custom test station equipped with a vapor generator, humidifier, and data acquisition system to carefully control testing conditions and accurately measure sensor responses to different gases.

Following device fabrication, the materials were characterized using UV-Vis spectroscopy and grazing-incidence wide-angle X-ray scattering (GIWAXS). These techniques enabled the study of how the ionic liquids altered the polymer's molecular organization, crystallinity, and overall film structure. The resulting datasets were analyzed using custom Python scripts written to automate data processing and generate figures, which facilitated the comparison of structural changes across different samples.

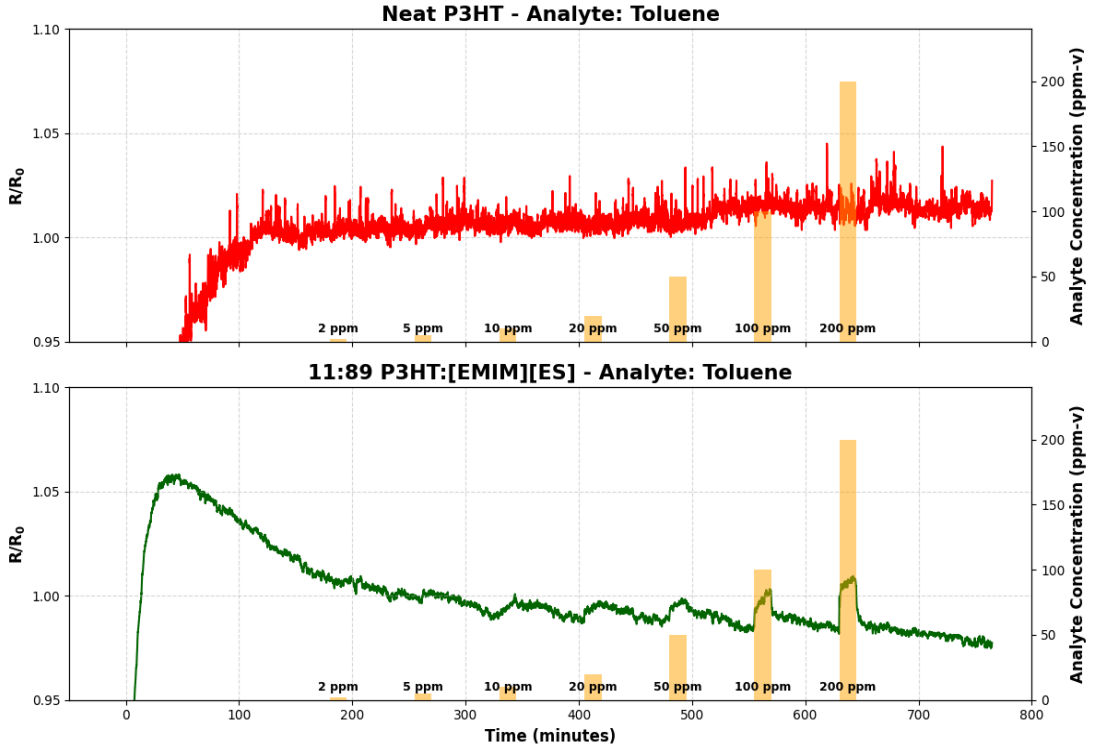


Figure 1: Dynamic normalized resistance R/R_0 of a Neat P3HT film (top panel, red trace) and an 11:89 P3HT:[EMIM][ES] composite film (bottom panel, green trace) exposed to sequential pulses of toluene vapor ranging from 2 to 200 ppm-v (orange bars). The composite material demonstrates significantly enhanced sensitivity and responsiveness to toluene compared to the neat P3HT, which fails to yield a measurable signal above the baseline noise.

Finally, the sensors were tested via exposure to acetone and toluene vapors at varying concentrations. The composite P3HT/ionic liquid films successfully detected both VOCs at room temperature, achieving detection limits as low as 10 ppm. A comparison of the structural characterization results with the sensing data revealed that changes in the film structure had a strong impact on sensor performance, indicating that increased structural disorder within the film correlates with enhanced sensing capabilities. Overall, this project provided valuable experience connecting materials processing, characterization, and device performance while actively contributing to the development of more efficient room-temperature gas sensors.