NDnano
Notre Dame Nanoscience and Technology

NDnano Summer Undergraduate Research
2026 Project Summary

1. Student name & home university:
Michael Schlesier, University of Notre Dame

2. ND faculty name & department: Rev. Bryan D. Paulsen, S.J., Ph.D.
Assistant Professor, Department of Chemical and Biomolecular Engineering, University of Notre Dame

3. Summer project title:
Optimizing Molecular Alignment of Mixed-conducting Thin Films with an Integrated Coating and Characterization Robot

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

I learned how to work with an automated spin-coating robot to rapidly fabricate and characterize polymer thin films. I also learned how to employ the Sobol-sequence method to design experiments. Finally, I became familiar with standard lab safety procedures and appropriate PPE.

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

This work lays the foundation for future work in solvent shearing post treatment processes for inducing molecular alignment in PEDOT:PSS thin films. In particular, the insights gained during this research stint will inform future researchers of which solvents and shearing steps are useful or not useful for inducing molecular alignment.

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

Poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) properties depend heavily on secondary doping and thermal annealing.. Using an automated meniscus-guided blade coating platform, we applied 40 solvent-shearing treatments (varying concentrations of Ethylene Glycol and DMSO in water, IPA, methanol) to induce molecular alignment. However, four-point probe analyses revealed high film instability and degradation rather than true molecular reorganization. Future work must identify optimal solvent concentrations that enable structural alignment without destroying the polymer film.

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

(1). Fenoy, G. E.; Azzaroni, O.; Knoll, W.; Marmisollé, W. A. Functionalization Strategies of PEDOT and PEDOT:PSS Films for Organic Bioelectronics Applications. *Chemosensors* **2021**, *9* (8), 212. https://doi.org/10.3390/chemosensors9080212.

(2.) *Bladecoating Robot*, www.sciprios.de/lab-automation/bladebot/. Accessed 24 July 2026.

(3.) *Four-Point Probe | Sheet Resistance Measurements | Ossila*, www.ossila.com/products/four-point-probe-system. Accessed 24 July 2026.

(4.) *V-780 Series UV-Visible/NIR Spectrophotometer | Jasco*, jascoinc.com/products/spectroscopy/uv-visible-nir-spectrophotometers/models/v-780-uv-visible-nir-spectrophotometer/. Accessed 24 July 2026.

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

As a foundational material in the field of organic electronics, poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) has drawn significant research interest due to its mixed ionic-electronic conduction, mechanical flexibility, optical transparency, and tunable conductivity. The optoelectronic and structural properties of PEDOT:PSS are sensitive to secondary doping—often achieved via solvent treatment—and thermal annealing. Consequently, our research focuses on engineering the microstructural characteristics of these thin films. We aim to precisely control molecular alignment, crystallinity, and the phase separation between the conductive PEDOT domains and the insulating PSS matrix through targeted pre- and post-deposition processing strategies. Achieving fine control over the microstructure of PEDOT:PSS thin films via processing is essential for tuning its material properties (e.g. electrical conductivity) for broader applications.Achieving record-level conductivities will allow this biocompatible polymer to serve as a viable alternative to conventional, rigid transparent conductors like indium tin oxide (ITO), while simultaneously opening doors for its use in emerging fields such as bioelectronics, thermoelectric power conversion, and high-performance electromagnetic interference (EMI) shielding.

To achieve the precise processing conditions required, our methodology utilizes the Sciprios automated experiment platform. This automated approach allows us to systematically explore a vast parameter space of post-deposition treatments, offering superior throughput, precision, and reproducibility compared to traditional manual methods. Specifically, we have investigated meniscus-guided blade coating techniques encompassing both dry and solvent-assisted shearing. In this process, the PEDOT:PSS thin film is already deposited and prepared on the substrate prior to the application of the shearing solvent. The mechanical shear forces applied during this secondary solvent pass have a significant impact on the film's sheet resistance. Enhancements in electrical performance are attributed to shear-induced conformational transitions within the PEDOT backbone; under the right conditions, disordered and coiled polymer segments reorganize into highly ordered, interconnected nanofibrillar networks that drastically reduce energy barriers and facilitate efficient, anisotropic charge transport.

To validate this hypothesized molecular alignment, Grazing-Incidence Wide-Angle X-ray Scattering (GIWAXS) is employed. This advanced characterization technique reveals the microstructural evolution of the film, tracking the transition from largely isotropic polymer grains to highly oriented crystalline domains. Analyzing GIWAXS data provides critical evidence of structural refinement, allowing us to

quantify increases in π-π stacking coherency and identify preferential edge-on or face-on molecular orientations relative to the substrate.

However, translating this theory into empirical success requires meticulous control over the solvent environment. To isolate the ideal processing conditions, a comprehensive matrix of 40 tests was conducted. Secondary dopants known for enhancing PEDOT:PSS conductivity—specifically Ethylene Glycol (EG) and Dimethyl Sulfoxide (DMSO)—were mixed at varying concentrations with a range of host solvents, including water, Isopropyl Alcohol (IPA), and Methanol. These complex solvent mixtures were then utilized during the automated shearing process, aiming to induce localized alignment in the pre-deposited PEDOT:PSS films.

The resulting data, gathered via four-point probe measurements, underscored the extreme sensitivity of the polymer matrix to chemical and mechanical disruption. The treated films exhibited high variability in conductivity and marked physical instability. Across the 40 test samples, structural integrity ranged from completely unaffected (no degradation) to moderate degradation, and in several cases, severe film degradation. When probing the conductivity in regions of the film that appeared visually undisturbed by the solvent shear, the electrical data revealed no statistically significant differences in anisotropic conductivity, indicating that alignment had not been achieved.

Interestingly, four-point probe measurements in the visibly degraded regions did reveal anisotropic conductivity profiles. However, structural analysis suggests this directionality was not the result of the desired molecular alignment or π-π stacking. Instead, the anisotropy was a false positive driven by the physical degradation and macro-scale tearing of the PEDOT:PSS film, which created artificial bottlenecks for charge carriers. Ultimately, these results demonstrate that our current solvent mixtures are either too aggressive, stripping the film from the substrate, or too passive to induce the necessary chain reorganization. Future research must identify an optimum of solvent concentration—a specific formulation that can successfully swell and disturb the pre-deposited film enough to allow shear-induced molecular realignment, without destroying the macro-structure of the film itself.