

Semiconducting single-walled carbon nanotubes (SWCNTs) can glow in colours ranging from visible to near-infrared, depending on their exact structure. This makes them exciting candidates for optical sensors, but their glow—called photoluminescence—is naturally very weak. Scientists have recently found ways to boost this glow by adding special “defects” ( $sp^3$  defects) to their surface, helping light-emitting reactions happen more efficiently. These modified SWCNTs have already been used to detect important molecules like cholesterol or dopamine. Still, the chemical reactions used to add these defects don’t always work as expected, and the reasons behind this are not fully understood.

To use SWCNTs effectively, we also need to separate them by type, since they’re made as mixtures of different structures. A method called conjugated polymer extraction (CPE) is now one of the best ways to sort them, using special polymers that wrap around specific nanotube types—some of which I’ve helped study and improve. After sorting, SWCNTs are ready for chemical modification, but early results show that leftover polymers from the sorting process can interfere with later reactions. Surprisingly, no one has studied this effect in detail. Understanding how these polymers influence nanotube chemistry could help us design better materials for bioimaging, sensing, and future nanotechnologies.

This project aims to understand how conjugated polymers (CPs), stick to SWCNTs and influence their modification. SWCNTs are tiny, tube-shaped materials that can glow when exposed to light, but only if their surface is carefully modified. The polymers help separate and wrap around specific types of these SWCNTs, but we still don’t fully understand how this affects later chemical changes. By designing new polymers and studying how they work—both in the lab and using computer simulations—we hope to discover the rules that govern these interactions. This knowledge could help create more efficient materials for sensors and bioimaging tools in the future.

The project begins with the synthesis of new CPs based on fluorene and carbazole units using Suzuki coupling reactions, allowing precise control over polymer composition and structure. These polymers are characterized using techniques such as size exclusion chromatography (SEC), UV-VIS spectroscopy, and NMR to determine molecular weight, optical properties, and chemical structure. Next, the polymers are tested for their ability to disperse SWCNTs in toluene, where parameters like polymer-to-nanotube ratio, sonication time, and centrifugation speed are optimized to achieve high-quality, selective dispersions. Once optimal dispersion conditions are found, the original polymers are removed by filtration and washing, and the SWCNTs are re-dispersed using alternative polymer systems to allow for further surface modification. This polymer exchange process enables systematic investigation of how different polymer environments affect subsequent chemical reactivity of the SWCNTs. To chemically modify the SWCNTs, phenylhydrazine derivatives are introduced, which react with the nanotube surface to create luminescent  $sp^3$  defects. These functionalizations are monitored using UV-VIS-NIR, photoluminescence, and Raman spectroscopy to evaluate reaction efficiency and defect density. Finally, molecular dynamics (MD), Monte Carlo (MC), and DFT calculations are employed to model polymer–nanotube interactions, helping to rationalize experimental results and deepen the understanding of how polymer wrapping influences nanotube reactivity and functionalization potential.

This research will deliver unprecedented insight into how CPs interact with SWCNTs, both in terms of dispersion efficiency and their impact on chemical reactivity. By systematically studying polymer exchange and subsequent functionalization, it will unveil critical design principles for tailoring SWCNTs surfaces with atomic precision. The outcomes will not only fill a major knowledge gap in the field of polymer–nanotube chemistry but will also establish a transformative platform for creating highly tuneable, luminescent nanomaterials. These findings will significantly advance the development of next-generation optoelectronic and biosensing technologies. Ultimately, this project will shape the future of nanoscience and chemistry by setting new standards for the controlled, scalable modification of low-dimensional carbon materials.