Title: Programmable Design of Plasmonic Nanoparticles: Machine Learning-Assisted Synthesis and Post-Synthetic Modification

Abstract: Plasmonic nanoparticles have attracted significant interest because their optical properties can be precisely tuned by controlling their composition, size, shape, and surface chemistry. These properties make them promising materials for applications in chemical and biological sensing, catalysis, and photonics. This seminar will present my doctoral research on the programmable design of plasmonic nanoparticles through two complementary strategies: autonomous machine learning-assisted synthesis and post-synthetic modification.

A major focus of my PhD work is the development of self-driving laboratories (SDLs) for the accelerated discovery and optimization of targeted nanomaterials. We first developed our group's first closed-loop oscillatory microfluidic platform, integrating real-time spectroscopic characterization with Bayesian optimization to autonomously navigate the synthesis parameter space and optimize the green synthesis of spherical gold nanoparticles. Building on this foundation, we developed the Autonomous Fluidic Identification and Optimization Nanochemistry (AFION) platform to expand the versatility of autonomous experimentation to a broader range of metal nanoparticle systems and photochemical synthesis pathways. The platform was demonstrated for the synthesis and optimization of diverse nanostructures, including gold nanorods, alloy nanospheres, core–shell nanospheres, and gold tetrapods, with minimal human intervention.

Complementary to direct synthesis, we investigated post-synthetic oxidative etching as a strategy to further tune nanoparticle morphology and optical response. Using polymer-capped penta-twinned gold nanorods as a model system, we demonstrated how end-grafted polymer brushes act as active interfacial regulators rather than passive barriers. The interplay between these polymer molecules, etchant concentration, and intrinsic crystallographic defects drives defect-selective etching pathways, yielding unique surface corrugations and precise plasmonic tuning.

Together, this research establishes an integrated framework for designing plasmonic nanoparticles, bridging artificial intelligence-guided chemical space exploration with nanoscale interfacial control.

Relevant publications:

1. **Wu, T.**, Kheiri, S., Hickman, R.J. et al. Self-driving lab for the photochemical synthesis of plasmonic nanoparticles with targeted structural and optical properties. *Nat Commun* 16, 1473 (2025).
2. H. Tao, **T. Wu**, S. Kheiri, M. Aldeghi, A. Aspuru-Guzik, E. Kumacheva, Self-Driving Platform for Metal Nanoparticle Synthesis: Combining Microfluidics and Machine Learning. *Adv. Funct. Mater*., 31, 2106725 (2021).
3. **T. Wu**, I. Koriakina, and F. Li, et al., Polymer Brushes Govern Defect-Selective Oxidative Etching of Penta-Twinned Gold Nanorods. *Angew. Chem. Int. Ed*. e8508304 (2026).

Short bio:

Dr. Tianyi (Taylor) Wu is a Postdoctoral Fellow at the National Research Council Canada's Quantum and Nano Technologies Research Centre, where she joined in June 2026 under the supervision of Dr. Chantal Paquete. She received her PhD in Chemistry from the University of Toronto, where she worked in Prof. Eugenia Kumacheva's group. Her doctoral research focused on self-driving laboratories, integrating machine learning, microfluidics, and closed-loop optimization to autonomously program plasmonic nanoparticles. She is currently exploring new research directions in volumetric additive manufacturing through functional photoresin design, nanomaterial integration, automated experimentation, and AI-assisted materials discovery.