Artificial Intelligence

Thursday Oct. 16, 2025 307/309 Lake St. Claire/Huron – University Center		
1:25 to 2:00	**Matthew J. DiTucci** PPG	Enterprise Applications of Large Language Models (LLMs) in Materials Science
2:00 to 2:35		
	Break	
2:45 to 3:25	**Mikola Lysenko** Socket	Fighting cybercrime with generative AI: A case study
3:25 to 4:00	**Wenyan Xu** eurofins	Beyond the Bench: Navigating the Future of Chemistry in the Age of AI and Automation

Enterprise Applications of Large Language Models (LLMs) in Materials Science
Matthew J. DiTucci, PhD
Data Science Research Associate, Digital Science & Technology
PPG

Transformer-based models are shaping a new paradigm in how researchers and technical professionals interact with data, enabling the conversion of unstructured content into structured formats that support downstream analysis and decision-making. By leveraging Large Language Models (LLMs), new capabilities emerge across summarization, information extraction, and classification tasks, each of which can be applied in scientific workflows to streamline routine processes and accelerate insight generation. In this presentation, we explore the application of LLMs for industrial research and development, with emphasis on materials and chemical research. Case studies include automated extraction of chemical variables from literature and product data sheets, summarization across large corpora of technical reports, and classification of patent literature to assess strategic relevance and innovation gap analysis. These examples illustrate how LLMs can be incorporated within programmatic frameworks to support scalable processing of diverse and complex data sources. Additional topics include retrieval-augmented generation (RAG) for internal knowledge search, and the use of transformer-derived embeddings for molecular data representations. Collectively, these methods demonstrate how LLMs can be systematically integrated into scientific methodologies to enhance efficiency, scalability, and data-driven insight.

Fighting cybercrime with generative AI: A case study

Mikola Lysenko
Principal Software Engineer
Socket

Abstract: This two-part talk for a general technical audience shows how we use LLMs at Socket to catch malware and fix software supply chain issues before they hurt anyone. Part I demystifies autoregressive language models, how they work, how they're built, and what that means for how you should use them. We'll cover pragmatic patterns for shipping real products with LLMs: when batch APIs are enough, when to use retrieval or agents, and how to think about evaluation, latency, and reliability. Part II dives into Socket's production pipelines: the patterns that worked, the ones that didn't, and why, covering schema design, chunking, guardrails, caching, and monitoring. I'll close with opinions on today's AI tooling, trade offs between local/open and closed models, cost and scale considerations, and fast prototyping tricks for small tasks.

Beyond the Bench: Navigating the Future of Chemistry in the Age of AI and Automation

Wenyan Xu, PhD
Group Leader, Analytical Chemist
Eurofins Lancaster Laboratories, Professional Scientific Services

Artificial intelligence (AI) and laboratory automation are rapidly transforming the practice of chemistry, reshaping not only how experiments are designed and executed but also how scientists define their professional identities. My talk will reflect on the evolving role of the bench scientist in this changing landscape. After framing the discussion with a personal anecdote from the laboratory, I will trace the trajectory of automation in bioanalytical chemistry—from early instruments such as auto-titrators to today's high-throughput robotic platforms and AI-powered tools like IBM's RXN for Chemistry and DeepMind's AlphaFold. While these technologies accelerate discovery, they also raise pressing challenges: skills displacement, diminished ownership of experimental work, and a sense of disconnection among scientists whose expertise risks being reduced to system operation. I will explore how the profession can adapt by embracing hybrid scientific identities that combine hands-on experimentation with data literacy, while highlighting what remains uniquely human—intuition, creativity, troubleshooting, and ethical judgment. Case

studies of effective human–machine collaboration will illustrate opportunities for synergy. Finally, I will discuss how academic training can evolve to prepare the next generation, emphasizing critical thinking, experimental design, and interdisciplinary fluency. The session concludes with a call for dialogue among educators, students, and professionals to ensure that chemistry's future remains both technologically advanced and deeply human.

References

1. Schwaller, P.; Laino, T.; Gaudin, T.; Bolgar, P.; Hunter, C. A.; Bekas, C.; Lee, A. A. *ACS Cent. Sci.* **2019**, *5*, 1572–1583.
2. Jumper, J.; Evans, R.; Pritzel, A.; et al. *Nature* **2021**, *596*, 583–589.
3. McKinsey & Company. *Artificial Intelligence in Life Sciences: Transforming R&D Productivity*. Report, 2022.