

AI Agents: Unleashing the Power of Large Language Models in Chemistry and Computational Science

Dr. Neeraj Kumar

Pacific Northwest National Laboratory (PNNL)



The rapid advancements in artificial intelligence (AI), particularly in Large Language Models (LLMs), are advancing chemical research and computational methods. The emergence of AI agents powered by LLMs has ushered in a paradigm shift, enabling machines to autonomously learn, reason, and make decisions in complex chemical environments. In this talk, I will discuss the future of AI agents in chemistry and their transformative potential in various domains of molecular science. I will focus on the work initiated through CACTUS (Chemistry Agent Connecting Tool-Usage to Science), which integrates chemistry-specific tools with open-source LLMs. CACTUS represents a proof of concept for LLM-powered agents in molecular discovery, demonstrating the agents ability to

accelerate molecular and drug discovery processes, and streamline the development of autonomous experimentation in chemistry labs. However, the path to fully realizing the potential of AI agents in chemistry is not without challenges. Developing AI agents that can effectively integrate domain-specific knowledge, reason abstractly about complex molecular systems, and make reliable predictions requires significant advancements in machine learning algorithms and computational infrastructure. I will discuss the importance of bridging the gap between AI research and chemistry expertise, highlighting the need for close collaboration between computer scientists, chemists, and other subject matter experts. As we forge ahead in our quest to harness the power of LLMs and AI agents in science, we envision a future where these superintelligent systems serve as invaluable partners in molecular discovery, computational chemistry, and technological progress in the chemical sciences.

Bio: Dr. Neeraj Kumar is a Chief Data Scientist at Pacific Northwest National Laboratory (PNNL), where he manages a team of scientists and engineers to address important challenges in AI, energy, health, and biothreat sectors. As one of the co-founders of trillion parameter consortium TPC, he contributes to the consortium's efforts and collaborates with the national leadership team to drive progress in this field. With experience in quantitative research and data science, he focuses on developing innovative solutions and leading programs at the intersection of fundamental discovery and AI-driven tools development.