



## **SPEAKER SPOTLIGHT:**

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**Pacific Northwest**  
NATIONAL LABORATORY

### **EXPLAIN YOUR SESSION IN MORE DETAIL:**

- My session will focus on scientific drivers for AI-Accelerators, especially coming from the field of chemistry. Breakthroughs in chemistry, whether through discovery of novel catalysts for affordable biofuels, or developing next-generation electric vehicle batteries is essential for accelerating the transition to a sustainable future. Experimental validation of a new catalyst and its performance is expensive. AI-driven computing approaches aims to accelerate such discovery by down-selecting candidates that are most promising and merit extensive evaluation in a laboratory. The past few years have seen a lot of developments for applying AI to chemistry that range from predicting properties of atomistic structures or outcomes of reactions using graph neural networks (GNN). On the other hand, despite breakthroughs in large language models (LLMs) for scientific literature still have a long way to go for complex scientific reasoning. My talk will present a set of scientific challenge problems and datasets for LLMs and GNNs that represent unique workloads for these models in both standalone and combined forms.

### **WHY YOU CHOSE TO PARTICIPATE IN THE SUMMIT:**

- The national laboratories tackle large-scale, complex research and development challenges for hard multi-disciplinary problems. It is important for us to embrace breakthroughs in computing, especially in AI and evaluate their impact towards scientific discovery. The AI Hardware Summit seems like a perfect venue to reach out a broad audience with our challenges and form collaborations.

### **WHAT YOU ARE MOST LOOKING FORWARD TO:**

- Developing partnerships to drive breakthroughs in scientific discovery.

**VIEW THE AGENDA TO LEARN MORE ABOUT SUTANAY'S SESSION**



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