UC Irvine Samueli
Department of Chemical and Biomolecular Engineering

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Designing Safer Energetics Under Multiple Property Constraints: Combining Chemistry-Informed Machine Learning with Multi-Scale Models

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Abstract: The design of new energetic materials that meet and exceed key safety and performance requirements is an important research area. Many relevant lab-scale experimental properties that correlate with safety and performance requirements are not conducive to physics-based modeling, while existing experimental datasets are too small for traditional machine learning (ML) approaches. In this talk, we highlight our development of transfer learning methodologies, including data-and physics-based approaches, that are uniquely suited to adapt ML models to small chemical property datasets. We employ these methods to predict experimentally measured impact sensitivity, vapor pressure, heat of vaporization, and transition temperatures via chemistry-informed directed-Message Passing Neural Networks (D-MPNNs). Our chemistry-informed D-MPNNs outperform direct-ML and physics-based models on diverse test sets. Using our chemical property models, we optimize a graph-to-graph translation model with multiple property constraints to generate new energetic molecules. We demonstrate this methodology to suggest molecules for melt-cast explosives that minimize volatility while also improving performance as estimated by oxygen balance and constraining on synthesizability. Finally, since the systems that deploy energetic molecules involve processes that occur at multiple length and time scales, we discuss applications of our property models to improve multiscale propellant simulations. These include estimating condensed phase propellant volatilization rates and elucidating propellant reaction pathways via automated mechanism generation.

Bio: Dr. Joshua Lansford is a Research Scientist at the DEVCOM Army Research Laboratory (ARL). His research focuses on the intersection of machine learning, chemical kinetics, and materials engineering, specifically for the design and discovery of novel energetic materials. He holds a B.S. in Chemical Engineering from the University of Virginia and obtained his Ph.D. in Chemical Engineering from the University of Delaware under the advisement of Professor Dion Vlachos, where he was a Blue Waters Graduate Research Fellow. While there, he developed theories in heterogeneous catalysis to understand trends in surface chemistry, implementing them to improve computational methods for characterization and microkinetic modeling. Following his doctoral studies, Dr. Lansford completed a postdoctoral fellowship jointly at the Massachusetts Institute of Technology and DEVCOM ARL. Working with Professor Klavs Jensen and Dr. Brian Barnes, he developed transfer learning methodologies to adapt machine learning models to the small datasets typical of energetic materials. Dr. Lansford's work has been published in numerous high-impact journals, including

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Nature Chemistry, *Nature Communications*, *Science Advances*, *ACS Nano*, and the *Journal of Chemical Information and Modeling*. His current interests lie in understanding the role catalytic processes play in propellant systems and surface erosion, developing computational frameworks to couple changes in surface structure with adsorbate reactivity, and using chemistry-informed ML and generative AI to accelerate materials design.

Hosted by: *Prof. Erdem Sasmaz*