From Random Networks to AI-Driven Glass Design

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Artificial intelligence is transforming glass science from empirical trial-and-error approaches to predictive design tools, enabling unprecedented control over structure-property relationships. This talk presents how modern AI-driven methodologies revolutionize glass structure understanding, simulation, and discovery across experimental, computational, and theoretical domains. We demonstrate how computational modeling provides critical insights into glass structure and enables tailored design of novel materials. Through systematic examples spanning oxide, chalcogenide, and specialty glasses, we will discuss how physics-informed machine learning achieves remarkable accuracy in predicting mechanical, optical, and transport properties while enabling rational design of glasses with targeted functionalities. Our framework integrates several cutting-edge approaches: reinforcement learning coupled with differentiable simulations to optimize glass structures and directly predict properties from atomic configurations, comprehensive benchmarking of universal interatomic potentials revealing critical limitations and improvement pathways, and materials-domain language models that extract decades of accumulated glass science knowledge from literature. The integration of topological descriptors, network connectivity analysis, and deep learning provides unprecedented insights into glass structure, capturing both short-range order and medium-range correlations that govern macroscopic behavior. This comprehensive approach accelerates glass discovery from decades to years or even months, enabling rational design of materials with tailored properties for applications ranging from nuclear waste immobilization to biomedical packaging, fundamentally transforming how we understand and design glassy materials.