

# NATIONAL SCIENCE FOUNDATION

## Proposal Abstract

Proposal:1937017

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**Proposal Title:** Convergence Accelerator Phase I (RAISE): MPrint-OKN  
**Institution:** Virginia Commonwealth University  
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The NSF Convergence Accelerator supports team-based, multidisciplinary efforts that address challenges of national importance and show potential for deliverables in the near future.

The broader impact and potential societal benefit of this Convergence Accelerator Phase I project is to create a knowledge network and design platform (the MPrint-OKN) for the accelerated, highly targeted creation of advanced products ranging from medicines to smart materials. The MPrint-OKN plans to create predictive tools that will attract a user-base eager to contribute their data to the collective whole in order to gain access to powerful tools that help them maximize the value of their data. This mutually beneficial exchange will result in an ever-growing collection of critically important scientific data, revolutionizing the design and manufacture of more efficient, less costly, and environmentally friendly end-products. By converging academic, government, and industrial researchers in computer, data, and formulation science with chemical, materials, and product engineers, the MPrint-OKN platform will act as a hub with two main goals: 1) create tools enabling partners to discover molecular systems that provide improved performance, lower environmental impact, and/or better economics relative to state of the art and 2) accelerate the speed of research transition from laboratory to marketplace by decreasing the discovery cycle time. The team already has partnerships in place with national laboratories and government agencies (such as Argonne, Idaho, Los Alamos, and NIST) as well as corporations (including Dow, Merck, Schlumberger, and Suez). This project will foster a vibrant, collaborative, multi-disciplinary community, and create innovative approaches to machine learning and data science in important economic sectors which will help the U.S. maintain its global leadership in data sciences and material sciences.

The research objective of MPrint-OKN is to create a valuable collaborative system that develops and distributes the most advanced molecular models, machine learning, data science, and data visualization tools available to the many disciplines requiring molecular systems for product development. We seek to reduce both the cost and time of discovering and developing next-generation molecular-based applications by placing advanced tools in the hands of more researchers. One aspect of the intellectual merit of the MPrint-OKN is derived by intersecting quantum-mechanical molecular representations with experimental data through machine learning. This creation of these new machine learning tools will enable partners to predict how molecules interact in complex systems and enable new insight into the relationships between molecular structure and product performance. Complementing the development of scientific tools, the MPrint-OKN project will help foster the ecosystem of thought leaders from all sectors of our economy that rely on molecules to drive their innovation.

This award reflects NSF's statutory mission and has been deemed worthy of support through evaluation using the Foundation's intellectual merit and broader impacts review criteria.