Artificial Intelligence for Accelerated Material Design

Participating Departments:

Department of Mechanical Engineering and Engineering Science, The William States Lee College of Engineering

Department of Chemistry, College of Liberal Art and Science

Department of Civil and Environmental Engineering, The William States Lee College of Engineering

Department of Physics and Optical Science, College of Liberal Art and Science

Department of Mathematics and Statistics, College of Liberal Art and Science

Department of Electrical and Computer Engineering, The William States Lee College of Engineering

School of Data Science

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Target Category: Future Opportunity and Investment

Key Words: Artificial Intelligence, Machine Learning, Material Design, Data Science, statistical analysis

Executive Summary: The main goal of the proposed thematic area is to establish an interdisciplinary research cluster across UNC Charlotte's multiple colleges and departments toward using *artificial intelligence for accelerated material design*. This emerging research area is directly linked to the nation's priorities, such as the NSF 10 Big Ideas "Harnessing the Data Revolution" and "Growing Convergence Research" foci. Moreover, artificial intelligence (AI) for materials design is directly linked to the research activities already occurring by individual faculties or small teams across the campus. For example, faculties of Departments of Mechanical Engineering, Chemistry, Civil Engineering and Physics have been utilizing experimental and computational techniques in material design and behavior prediction. Faculty of the Departments of Electrical and Computer Engineering, Computer Science, Mathematics and Statistics, and School of Data Science are involved in research on different aspects of AI and intelligent data analysis. *The emerging collaboration between these two groups of faculties will establish outstanding interdisciplinary strength toward utilizing artificial intelligence for accelerated material design.* Establishing such collaborations is timely, given the recent developments in AI algorithms and the initiatives launched recently by the U.S. government on accelerated material design. Due to its high impact on the future of material design, it is envisioned that such research collaborations have the potential of winning large federal and industrial awards.

Developing tools and methodologies for discovering and designing innovative new materials that can enhance the competitiveness of U.S. manufacturing are essential for the economic growth and national defense. The design and discovery of new materials is costly and time consuming. The current time frame for designing new materials is typically between 10 to 20 years from the initial research to the first use. The importance of accelerating design and deployment of new materials has led to the launch of Material Genome Initiative (MGI) in 2011 by the U.S. government aiming at accelerating material design, discovery and analysis. The problem of material design is mathematically formulated as an optimization problem where a vast number of design parameters are available and the goal is to find the best set of parameters which meet the target material property. By increasing the complexity of materials, the number of design parameters affecting material properties become intractable by the conventional experimental and computational simulation methods. This makes it difficult to use only experimental and simulation methods for the purpose of accelerating material design and behavior prediction.

Artificial intelligence (AI) is becoming a powerful tool in the field of materials engineering due to its power in predicting material properties with high accuracy and at a lower cost. Recent breakthroughs in AI methodologies have created new horizons for overcoming long lasting issues in material design strategies. Materials and manufacturing communities are seeking to complement the conventional experimental and computational techniques by leveraging the capabilities of AI toward accelerated design of materials, prediction of structure-property relations and deploying the new materials to the existing and emerging manufacturing sectors. Significant efforts are devoted to seamlessly integrate conventional experimental and computational modeling with AI and intelligent data analysis to improve the efficiency of the conventional methods and reduce the error rate of AI models. In this new paradigm, AI acts to unify the experimental and simulation efforts by using the large datasets properly prepared and processed using the domain knowledge of materials science. Advanced AI models trained by large datasets can accurately and rapidly predict the behavior of materials and significantly accelerate the design and deployment of new materials. To achieve this goal, close collaboration among material scientists and AI experts is required as is proposed in this proposal.

Evidence of Strength and Excellence: The proposed emerging thematic area encompasses three subfields consisting of materials, artificial intelligence (AI) and data science. The faculties participating in this thematic have a long history of conducting high impact research in each of the subfields (see **Table 1**). As shown in Table 1, a large group of faculties have research interest and expertise in materials. This group of faculties use advanced experimental and computational methods to understand structure-property relationships of materials to tailor various aspect of material properties including mechanical, photonic, electronic and energy storage properties. The other faculties in the team use and develop data science and artificial intelligence methods for various purposes including functional dynamics of polymers, visual analytics, dimension reduction of complex data, experimental design, model parameter estimation, computer vision systems, advanced manufacturing and predicting fracture and strength of materials.

The faculties participating in this proposal have a long history of collaboration in various aspects of research and education including co-supervising Ph.D. students, joint publications and proposals. Such collaborations are exemplified by their participation in the UNC Charlotte's nanoscale science program [1] and are elaborated further in this section. These established collaborations can serve as a springboard for the creation of new and large multi-disciplinary collaborations **specially between the materials faculties with those with expertise in artificial intelligence and data science to take advantage of AI for accelerated material design and behavior prediction**. Such emerging collaborations provide a unique and excellent opportunity toward the development of new research programs and research centers such as the Center of Excellence of Material Informatic focusing on using AI in material design.

The faculties participating in this thematic area have received several awards from multiple federal agencies including NSF, DOD, ARL, ARO, ONR, NASA and DOE. This includes not only single PI awards [2-8] such as the prestigious NSF CAREER awards of Drs. Xu [2] and Li [3] and the NSF IUCRC award on the Center for Visual Decision and Informatics of Dr. Dou [4], but also includes several proposals prepared by collaboration among the participating faculties [10-24]. For example, Drs. Fang and Weggel have received three joint grant awards with a total amount exceeding $650,000 [14-16]. Dr. Cherukuri is the PI on an NC ROI grant on Self-Aware Machining [5]. This is a multiyear and multiuniversity grant with faculties from UNC Charlotte, NCSU, and Fayetteville State University. The high number of joint proposals is a clear indication that the team of participants have complementary expertise which will allow them to solve complicated multi-facet research problems collaboratively.

Table 1. List of participants conducting research in each subfield.

Field of Expertise		Faculties names
Materials	Mechanical Properties	Y.Chen, Cherukuri, Fang, Jacobs, Li, Tabarraei, Weggel, Wei, J. Xu
	Photonic Properties	Astratov, Fiddy, Falaggis, Her, Hoffman, H. Zhang, Y. Zhang, Poler,
	Electronic Properties	Haitao Zhang, Yong Zhang
	Energy Application	T. Xu, Poler, J. Xu
Artificial intelligence		C. Chen, Cherukuri, Jacobs, Khan, Tabarraei
Data Science		Dou, Jiang, Pan, Song, Khan

The research results of the participant faculties are published in several hundred journal papers. Many of the published papers are a result of the collaborative work among the team members. A select number of them are presented in references [25-32]. The high number of publications and their high citations provides a strong support of the prominence of the research team in materials, artificial intelligence and data science fields. For example, due to their high impact research, Dr. Wei (studying mechanical properties of materials), Dr. Astratov (working on photonic materials) and Dr. C. Chen (an assistant professor in the Department of Electrical and Computer Engineering working on developing efficient AI methods) have been listed as top 2% highly cited world scholars according to the Stanford University ranking.

The high impact research of the team has also received media attention. For example, Dr. Jun Xu's work on lithium-ion batteries was reported by NPR news [6]. Dr. Astratov's work on superresolution microscopy was highlighted in SPIE News [7]; his work on resonant optical forces was highlighted by Optics and Photonics News [8]; and his research on optical scalpels was highlighted by SPIE Newsroom [9]. The collaborative work of Drs. Her and H. Zhang on self-assembly of tungsten nanograting was also highlighted by Optics.org [10].

In addition to collaborating with the UNC Charlotte's faculties, the team is engaged with external entities as well. For example, Dr. Fiddy has served as a DARPA program manager in the past. Dr. Jun Xu has been collaborating with NASA, Argonne National Laboratory and National Renewable Energy Laboratory on several research projects since 2019. Dr. Tabarraei has worked and engaged with Energy Power Research Institute (EPRI), Oak Ridge National Lab and other regional industry on developing computational tools for modeling behavior of materials. Dr. Astratov has a 10-year long collaboration with the Air Force Research Laboratory (AFRL) along with collaborations in Europe including Center for Nanoscience and Nanotechnology (C2N) in Paris and Center for Physics of Materials in San Sebastian, Spain. Dr. Wei has been involved in the Johns Hopkins University MEDE Program supported by US ARL for the past 5 years and has established collaborations with US ARL. He was a visiting Senior Fellow of US ARL, Aberdeen Proving Ground, MD from Feb. 2020--August 2020, working in WMRD (Weapons and Materials Research Directorate). Dr. Dou from the School of Data Science has multiple year of collaborations with the Pacific Northwest National Laboratory and was selected as a summer faculty fellow by PNNL. Dr. Khan has collaboration with the Air Force Research Lab in San Antonio, with the Center for Industrial Mathematics at U of Bremen, Germany and LIMOS at University Clermont Auvergne for machine learning research. Dr. Jiang has been collaborating with worldwide leading econometricians and data scientists at Princeton University in the past 20 years. Dr. Cherukuri has an ongoing collaboration with NIST and LLNL on additive manufacturing and machining.

Cross-Discipline Education: Applying AI and statistical modeling and quality control techniques to material design is a multidisciplinary effort requiring experts from various fields including material science, chemistry, mechanics, mathematics, computer science and data science. Some public and private sectors now hold boot camps on artificial intelligence for material design and manufacturing. However, to answer the high demand in this field a larger and more organized effort is required. The collaboration among the UNC Charlotte's faculties on the proposed thematic area will lead to better knowledge sharing among them and will facilitate the development of new multi-disciplinary programs such as Material Informatic with focus on training Ph.D. students at the intersection of material science, engineering and data science.

Alignment with Regional and National Priorities: The critical need for accelerated design of materials for the national economy and security and has led to the launch of Material Genome initiative (MGI) by the U.S. government in 2011. MGI is a federal multi-agency program which "*creates policy, resources and infrastructure to support U.S. institutions in the adoption of methods for accelerating materials development*". Due to the importance of accelerated material design, 18 federal agencies including NSF, NIST, NASA, DOD, DOE, DARPA and U.S. Army are contributing toward this goal by partnering with MGI. For example, in 2017 NSF sponsored the workshop "Advancing and Accelerating Materials Innovation Through the Synergistic Interaction among Computation, Experiment, and Theory: Opening New Frontiers" to present accomplishments and opportunities that has emerged under the MGI. The Advanced Manufacturing Office of DOE also held a workshop on "Artificial Intelligence Applied to Materials Discovery and Design" to identify opportunities and challenges for applied research in advancing the artificial intelligence applied to material design and discovery in energy and other related materials.

The launch of MGI and the coming of the big data era has led to the creation of several large dataset of material properties including Harvard Clean Energy Project, Cambridge Structural Database, and Crystal Structure Database. The availability of such large databases along with efficient data mining techniques and artificial intelligence models have provided a powerful impetus for accelerated material design. The team of this proposal participates in completing these databases and will harness these databases in their material research using AI. Such activities are directly aligned with the NSF's 10 Big Idea on "Harnessing the Data Revolution" and paves the way toward receiving large funding from federal agencies. Furthermore, the interdisciplinary nature of the proposed activities which converges various scientific fields to establish an emerging discipline are well aligned with the NSF 10 big ideas on Growing Convergence Research.

In addition to its alignment with the national priorities, the activities of this proposal are well aligned with the priorities of the state of North Carolina and Charlotte's region in both North and South Carolina. North Carolina manufactures produce 17% of the gross state product and Charlotte manufacturing accounts for 14% of local gross product, second only to finance and insurance which produce 15% of Charlotte gross product. Due to the importance of manufacturing for the region, North Carolina has recently launched its manufacturing sector of research initiative and workforce development program. Additive manufacturing (AM) which is a new manufacturing paradigm has enabled the fabrication of an object with accurate deposition of different types of materials. The full realization of AM requires advanced and novel materials which are suitable for unique characteristics of AM (rapid solidification and thermal cycles). The development of new materials which are suitable for additive manufacturing is of high importance for the industries of the state of North Carolina and Charlotte. Therefore, the proposed collaborations for accelerated material design will provide an excellent opportunity to receive funding from various industries and programs such as the "Research Opportunities Initiative" (ROI) program of UNC System. This program which is funded by the North Carolina General Assembly represents a significant investment in UNC system's strategic goals with priority research areas such as Advanced Manufacturing and Data Science.

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Supporting Documents

Name	Title	Expertise and Contribution
Alireza Tabarraei	Associate Professor of Mechanical Engineering and Engineering Science	Dr. Tabarraei's research is on computational material and mechanics. He uses various computational tools to study the property of materials at different scales from atomistic to continuum. Recently, he is using machine learning in combination with other computational tools such as molecular dynamics (LAMMPS) and finite elements (ABAQUS) to study the mechanical, fracture and thermal properties of materials. He has published more than 50 papers and currently is supervising 5 Ph.D. students working on federally funded projects.
Jordan Poler	Professor of Chemistry	Dr. Poler's research entails fundamental studies of molecular and nanoscale systems to understand directed and self-assembly processes. We aim to design new particles and materials with higher functionality and effectiveness. Our long-term interests are toward: novel mechanisms for mechanical transducers and sensors in NEMS, energy storage in supercapacitors, catalytic solar fuel production, water purification, and optical metamaterials. We use an array of computational methods to model the new nanomaterials. Using tools such as Gaussian, LAMMPS, GROMACS, and Materials Studio we use multiscale modeling from atomist to the mesoscale. He has published 47 peer reviewed journal articles with 500 citations. He has been PI or co-PI/SP on external funding exceeding $3M.
Taufiquar Khan	Professor and Chair, Mathematics and Statistics	Dr. Khan's research is in mathematical modeling, simulation, and computational aspects of inverse problems involving PDEs or distributed parameter systems particularly for model parameter estimation. His recent interest is in deep learning using neural networks with applications to AI for model parameter estimation.

Name	Title	Expertise and Contribution
Harish Cherukuri	Professor and Chair, Mechanical Engineering and Engineering Science	The current research interests of Harish Cherukuri are in the areas of modeling additive manufacturing (AM) processes and machining processes, thermomechanical properties of AM parts, heat-transfer characteristics of AM surfaces, application of machine learning to manufacturing processes, particle-based computational methods, thermal modeling in biomaterials, and effective properties of porous materials.
Qiuming Wei	Professor of Mechanical Eng. and Engineering Science	Qiuming Wei's research and teaching at UNC-Charlotte focus on mechanics, materials science, esp. the relationship between microstructure and mechanical properties of structural materials. He has published more than 100 journal articles, many of which have received significant citations by his peers. According to Google Scholar, his current H-index is 41, with a total citation of ~7000. He has been recently listed by a Stanford University ranking system into the 2% highly cited world scholars. He has produced 9 PhD at UNCC, and more than 10 PhD's with joint efforts at John Hopkins University, NC A&T State University, Northwestern Polytechnical University and Beihang University. He has received more than 1.0 million external funding as PI and CO-PI.
Mike Fiddy	Professor of Dept. of Physics and Optical Science	Dr. Fiddy started his career as a physicist, and he realized early on that curiosity driven research is less likely to have societal impact and attract funding if it is not directed towards a tangible goal that will make a difference. Since the mid-1990s he has fostered collaborations between researchers both as a Dept. Head and director of various Centers. His preference is to engage in inter- or multidisciplinary research since he believes interaction between individuals with different approaches and coming from different backgrounds leads to new ideas, new knowledge, and a deeper understanding of problems. His past collaborations have led to Fellow status recognition by professional societies and almost all his publications include co-authors. The opportunity he had recently to create and manage research programs while at DARPA has provided a unique insight into what makes a fundable proposal and has reinforced the fact that well-coordinated teams constantly build momentum behind their work, deliver to agencies and their success creates further opportunities.

Name	Title	Expertise and Contribution
Xingjie Li	Associate Professor of Mathematics and Statistics	Dr. Li's main research area lies in the area of applied and computational mathematics with a focus on mathematical modeling and analysis for materials science and development of computational tools to enhance the design and manufacturing and has a solid record of successes regarding publications and external funding supports.
Youxing Chen	Research Assistant Professor at Mechanical Engineering and Engineering Science	Youxing's research focuses on the microstructure - mechanical behavior correlation at the nanoscale, emphasizing materials behavior in extreme environments, such as large strain, high strain rate, elevated temperature, and radiation. He is also interested in developing high-throughput nanomechanical techniques for fast mechanical property measurement. He has published 60 peer-reviewed articles with a total citation of 1800, according to google scholar.
Chen Chen	Assistant Professor of Electrical and Computer Engineering	Dr. Chen's research focuses on developing machine learning techniques that can achieve computation and memory efficiency, label/sample efficiency, and energy efficiency for real-world intelligent computer vision systems. He has published over 70 peer reviewed journal and conference papers with 6452 citations. He has been PI or co-PI/SP on external funding exceeding $1M.
Terry Xu	Professor of Mechanical Engineering and Engineering Science	Dr. Xu's research areas include synthesis and characterization of boron-based 1D nanostructures, measurement of mechanical properties of individual nanostructures and exploration of their applications in thermoelectric energy conversion. Her research has been funded by National Science Foundation (NSF) including the CAREER award, Department of Defense (DoD), American Chemical Society – Petroleum Research Fund (ACS-PRF), Lockheed Martin Corporation and others. Her work has been published in high impact journals, such as *Nature Nanotechnology*, *Physical Review Letters* and *Nano Letters*.

Name	Title	Expertise and Contribution
Haitao Zhang	Associate Professor of Mechanical Engineering and Engineering Science	Dr. Zhang's general research interests are focused on the study of functional materials in forms of thin films and nanostructures for electronic and optoelectronic applications. His research areas range from materials synthesis and growth mechanism study, materials characterization, and property measurement & testing. He has been funded by National Science Foundation (NSF) and Department of Defense (DoD). As an experimental materials scientist, Dr. Zhang could provide experimental data in materials design, synthesis, structure characterization, and property measurement for the artificial intelligence (AI) training. He can also perform experimental verification of the AI predicted material designs.
Jun Xu	Assistant Professor of Mechanical Engineering and Engineering Science	Dr. Xu's research area includes the characterization, modeling and analysis of lithium-ion battery safety and mechanics design materials/structures upon dynamic loading. Dr. Xu has published more 100 peer-reviewed papers with total citation over 2600 times. He serves as the Chair of Electrochemical Energy Conversion and Storage Committee, and Multifunctional Materials Committee, ASME. Dr. Xu has been PIs on external funding exceeding $1.5M in the past three years.
David Weggel	Professor of Civil and Environmental Engineering	Dr. Weggel's general interests involve experimental and analytical research of structures. Specific areas include full-scale testing of structural, mechanical,and vehicular systems under extreme loading such as blast and impact; engineering mechanics (including FEA, AEM modeling); and forensic investigations. He has been funded by the NSF, DOE, NIJ, FEMA, USDOT, NCDOT, and the private sector. As an experimentalist, he could provide datasets that investigate the performance of systems composed of new AI-designed materials. Collaborating with mechanical and materials engineers, he could contribute to constitutive models at various stages of material design and integrate experimental results/models with AI..

Name	Title	Expertise and Contribution
Tino Hofmann	Assistant Professor of Applied Optics	Dr. Hofmann's research work covers a broad range of experimental condensed matter physics and photonics with a strong emphasis on characterizing the anisotropic optical response of spatially coherent nanostructured materials in the visible and THz spectral range. Dr. Hofmann has published over 120 peer-reviewed, technical articles and 14 books and book chapters. Google Scholar is listing over 2800 citations to his publications resulting in an H-index of 31. He is the recipient of a 2014 EU Marie Curie Fellowship and a VINNMER Fellowship. Dr. Hofmann is co-directing the UNCC Center for Metamaterials with a focus on marketing, member recruitment, and communications.
Jun Song	Assistant Professor of Statistics	Dr. Song's research is centered around developing statistical methodologies of dimension reduction for complex data, including high-dimensional data, functional data, manifolds, and tensors. This research field gets tremendous attention with increasing demand to adapt to new types of data with drastically increased dimension, volume, and complexity. Consequently, it has great potential in collaborative research within statistics as well as inter-disciplinary research. The potential research areas include pattern recognition, economics, finance, fMRI research, and a combination of these complex data. In recent years, Dr. Song wrote papers regrading the dimension reduction for functional data in top-tier statistics journals in statistics, including the premier journal, The Annals of Statistics (one published, one under major revision) and other journals of statistics and interdisciplinary fields. Currently, Dr. Song is working on dimension reduction of general tensor products and feature screening of multivariate functional data.
Yong Zhang	Bissell Distinguished Professor of Electrical and Computer Engineering	Yong Zhang's research interests include electronic and optical properties of semiconductors and related nanostructures, organic-inorganic hybrid materials, impurity and defects in semiconductors, and novel materials and device architectures for energy and related applications (e.g., photovoltaics, solid-state-lighting, electronic-photonic integrated circuits). His expertise areas include microscopic scale material and device characterization, optical spectroscopy, material and device simulation.

Name	Title	Expertise and Contribution
Tsing-Hua Her	Associate Professor of Physics and Optical Science	Tsing-Hua Her's research interests encompass many aspects of light-matter interaction, including laser material synthesis and modification, laser resonators and quantum electronics, guided-wave physics, optical sensing, optical metrology, ultrafast and nonlinear optics, nanomaterials and metamaterials. Almost all his publications include co-authors and many of whom are colleagues at UNCC.
Wenwen Dou	Assistant Professor of Computer Science	**Dr. Wenwen Dou** is a core faculty member of the Ribarsky Center for Visual Analytics. Her research interests include Visual Analytics, Text Mining, and Human Computer Interaction. She works in the cutting-edge research area of Visual Text Analytics, which integrates statistical and machine learning methods with powerful interactive visualization for analyzing large amounts of textual data. Dou has worked with various analytics domains in reducing information overload and providing interactive visual means to analyzing unstructured information. She has experience in turning cutting-edge research into technologies that have broad societal impacts, partially demonstrated by support from both academic and industry partners, including the Pacific Northwest National Laboratory, US Army Research Office, US Special Operations Command, National Science Foundation, US Army Engineering Research and Development Center, and Lowe's company Inc. Dou has served on the organizing and program committee of the IEEE VIS conference, the premier conference for visualization research for the past 5 years.

Name	Title	Expertise and Contribution
Donald Jacobs	Professor of Physics	**Dr. Donald Jacobs** research activities include simulation of biopolymers, development of models for rapid free energy calculations using importance sampling, and algorithms that aid advanced simulation methods. Applications include optimizing metastable liquids that are fragile glass formers as formulations, and the identification and prediction of allostery and long-range cooperative effects in proteins. Most recently, Dr. Jacobs has developed novel supervised projection pursuit neural network machine learning to identify functional dynamics in biomolecular systems. Different from classification, a discovery likelihood is used within a molecular design pipeline that combines simulation, experiment and machine learning. The simulation data represents digital twins of experimental systems, which is analyzed in the context as a comparative analysis. Through iterative learning, a multivariate hypothesis is refined as the functional dynamics is resolved, making it possible to optimize material properties.
Hongbing "Howie" Fang	Professor of Mechanical Engineering and Engineering Science	Dr. Fang's research area is computational mechanics with specific interests in numerical modeling and simulation of impact problems such as vehicular crashes and ballistic impacts, design optimization algorithms and solution methods, and surrogate modeling for complex systems. He published over 40 journal articles and organized over 10 minisymposia for the U.S. National Congress on Computational Mechanics and World Congress on Computational Mechanics. Dr. Fang received more than $3M external research funding in which he served as the PI of projects over $2.5M.

Name	Title	Expertise and Contribution
Yinghao Pan	Assistant Professor of Statistics	Dr. Pan's research is centered around developing novel statistical and machine learning methods to analyze data from medicine and public health, with particular focus on precision medicine. Specific applications of his work include improving health outcomes for patients with depression and monitoring of complex diabetic patients. Dr. Pan has published articles in top-tier statistics journals, including Journal of the American Statistical Association, the premier journal of statistical science.
Jiancheng Jian	Professor of Statistics, Department of Mathematics and Statistics	Dr Jiang's focus is on statistical analysis of big data. His current research directions are Bayesian statistics, quality control, statistical learning with big data. He is currently the associate editor of two journals and serving at the editorial board of two other journals. He has supervised 12 Ph.D. students and has published more than 60 journal papers.