FACETS

Shattering the Boundaries of Conventional Thinking

By harnessing information and data science tools to advance knowledge discovery, MDI is establishing a new paradigm for materials science research and education.

Chair's Welcome

Dear Friends,

Welcome to the Department of Materials Design and Innovation (MDI) at the University at Buffalo! Established in 2015, our department is the first to dedicate its entire educational and research program to train material scientists and engineers in the methods of data driven discovery, design and innovation. We are committed to accelerating science-based solutions to solve pressing societal problems such as climate change, environmental sustainability and public health.

Never has this goal been more pressing as now, as we are witnessing a surge of problems in all aspects of our lives – climate change, emerging diseases, challenges in food, water, and energy supplies – and these problems are becoming more frequent and complex. Their seriousness and urgency demand solutions that are effective, robust, and rapidly deployable, and can address interdependent problems in a holistic way. This, in turn, requires a new paradigm: one that can accelerate scientific discovery and problem-solving abilities so that we can work faster and smarter.

The concept of nucleating and building a new department in the field of materials science and engineering entirely from the ground up was a bold and audacious goal. Spurred by the endowment by UB alumnus Erich Bloch, former director of the National Science Foundation, vice president of IBM and Medal of Technology and Innovation holder, MDI launched with the goal of establishing a new paradigm for research and education. Inspired by Bloch's perspective that "science is changing, the tools of science are changing,

and that requires different approaches," MDI was built from scratch in five years, hiring an entirely new entourage of faculty, establishing a unique graduate and undergraduate curriculum that aims to rewrite how materials science research is done, and educating a new genre of students.

Our distinguished faculty are pioneering a unique learning and discovery framework involving the convergence of materials science and information science – Materials Informatics. Through the lens of data, we explore and discover connections between experiments and modeling for a deeper understanding of existing relationships to uncover information that cannot be easily detected by experiments or computational methods alone, and to detect new trajectories of materials exploration that have not been recognized in the past.

In this, the inaugural issue of FACETS, we introduce you to MDI, to share how we have grown and where we are heading in exciting and inspiring ways. We hope FACETS serves to build connections and conversations with the readership, and we look forward to hearing from you and welcoming you to the MDI family!

Erich Bloch Chair, SUNY Distinguished Professor and Empire Innovation Professor
Department of Materials Design and Innovation

"...science is changing, the tools of science are changing and that requires different approaches."

– Erich Bloch

Our History

6 STUDENTS FIRST ENROLLED IN 2016

ENROLLMENT: 2020–2021

26 MASTERS STUDENTS
19 PHD STUDENTS

51 MASTERS STUDENTS **+** **2** PHD STUDENTS
HAVE GRADUATED SINCE 2016

3:1 GRADUATE STUDENT TO FACULTY RATIO

15 FULL TIME FACULTY

MDI IS HOST TO NSF SCIENCE & TECHNOLOGY CENTER **BioXFEL**

$250,000 – $300,000 AVERAGE RESEARCH EXPENDITURES PER FACULTY

OVER $6 MILLION
FROM INDUSTRY AND PRIVATE FOUNDATION INVESTMENTS

2014 — The Beginning

The Department of Materials Design and Innovation (MDI) was approved in Spring 2014, and is jointly managed by the School of Engineering and Applied Sciences and the College of Arts and Sciences.

2015 — Leading Light

Krishna Rajan joined the University at Buffalo to lead MDI as its inaugural Erich Bloch Chair.

2016 — A Year of Firsts

The first MDI faculty members were hired, the first class of grad students were enrolled, the first Erich Bloch Symposium took place, and the MDI industry–resident scholar program was initiated.

2017 — Making the Grade

The MS and PhD curriculum was approved, the inaugural class of MS students graduated, and the CoRE Center was established.

2018 — Gaining Momentum

The NSF Science and Technology Center BioXFEL Phase 2 was awarded, and MDI teaching and lab space was established in Bonner Hall.

2019 — Leaps to Success

Quanxi Jia was elected to the National Academy of Inventors, MDI joined the SUNY-Applied Materials Research Institute board, and NSF-REU program in Data Driven Materials Design was awarded.

2020 — Establishing Alliances

The first PhD students graduated, the BS degree was approved, the Center for Materials Processing Data industry – academia consortia was established, CoRE was renewed, the nations first accelerated BS-Chemistry/MS-Materials Science degree program was established and Ed Lattman was elected Fellow of AAAS.

16 World-Class Faculty and Staff

Since our inception, 11 of our 15 faculty members joined the University at Buffalo, while four others moved into MDI from other units. Collectively, our faculty have lived, worked or studied in 19 states and 12 countries, and offer 75 years of industry experience and over 130 years of teaching experience.

Baishakhi Mazumder

Assistant Professor

PhD, physics and material science, University of Rouen

E. Bruce Pitman

Professor

PhD, mathematics, Duke University

Edward Snell

Professor and Director of BioXFEL NSF Science and Technology Center

PhD, chemistry, University of Manchester

Erik Einarsson

Associate Professor, joint appointment with electrical engineering

PhD, mechanical engineering, University of Tokyo

Kristofer Reyes

Assistant Professor

PhD, applied and interdisciplinary mathematics, University of Michigan

Olga Wodo

Assistant Professor

PhD, mechanical engineering, Czestochowa University of Technology

Prathima Nalam

Assistant Professor

PhD, surface science and technology, materials science, ETH Zurich

Quanxi Jia

National Grid Professor of Materials Research and Empire Innovation Professor; Scientific Director, New York State Center of Excellence in Materials Informatics

PhD, electrical and computer engineering, University at Buffalo

Fei Yao

Assistant Professor

PhD, energy science and physics, Sungkyunkwan University

Grace Wang

Professor

PhD, materials science and engineering, Northwestern University

Jung-Hun Seo

Assistant Professor

PhD, electrical and computer engineering, University of Wisconsin-Madison

Krishna Rajan

Erich Bloch Chair, SUNY Distinguished Professor and Empire Innovation Professor

ScD, materials science, Massachusetts Institute of Technology

Scott Broderick

Assistant Professor of Research

PhD, materials science and eginering, Iowa State University

William J. Bauer

Assistant Professor of Research

PhD, structural biology, University at Buffalo

Ed Lattman

Emeritus Professor

PhD, biophysics, The Johns Hopkins University

Margaret Poniatowski

Director of Administration

MBA, University at Buffalo

A New Paradigm in Materials Science Education

Finding solutions to society's major problems, both local and global, through interdisciplinary partnerships is at the core of MDI's research and teaching missions. MDI faculty have pioneered new genres of experimental and computational techniques, and new paradigms for materials development that facilitates an **"atom-to-applications"** framework for materials science.

We have developed a unique educational **paradigm** that uses new concepts, cross-disciplinary methodologies, and novel pedagogical approaches to promote the convergence of advances taking place, often separately, in different fields such as physics, computer science, mathematics, chemistry, engineering disciplines and materials science. At the graduate and undergraduate levels, we have introduced a completely novel curriculum by bringing a data perspective to all core subjects for the study of materials theory, characterization, synthesis, processing, and computational and simulation techniques.

Our curriculum uses the mathematical rigor of data science to explore and navigate the core concepts that define structure–property–processing relationships in all classes of materials, and informatics serves as the 'connective tissue' between experiments and computation to help students uncover patterns and relationships in an accelerated manner. MDI's pedagogical approach heightens **awareness** of data in all facets of materials science and engineering, develops statistics, machine learning and mathematics skills, and shows how to judiciously use the tools of data analytics with the theory of materials behavior.

The department has succeeded in attracting students from diverse backgrounds who, through their formal coursework and research projects, are learning to communicate and collaborate across disciplines. Some of the students come with physical / life sciences and engineering backgrounds, interested in adding informatics training to their repertoire; while students with computer science and mathematics backgrounds find opportunities to explore domain application areas.

Diversity and Inclusion in MDI

Critical to our students' success and the department's excellence is our commitment to promoting and nurturing an inclusive culture that welcomes, supports and enables all those who are interested in and capable of contributing to the field. A third of our faculty are women and all of our faculty are intellectually diverse, have brought with them stellar resumes, and diverse educational and work experiences from around the globe. These international experiences that forced them to live and work in cultures and places outside their comfort zone, provides them with a unique and empathetic view of the world, and the ability to understand and relate with others – faculty, staff, and students – who find themselves in a new and unfamiliar place.

MDI Achieves Landmark of Graduating First Two PhD Students

In May of 2020, Aparajita Dasgupta and Edward Swinnich (left) became the first two PhD students to graduate from the Department of Materials Design and Innovation.

Dasgupta joined the Department of Chemical Engineering at Massachusetts Institute of Technology (MIT) as a post-doctoral researcher, where she is researching the development of machine learning models that will have an impact on human health and the drug development and manufacturing process. For her PhD, she worked with Krishna Rajan to use data science and statistical analysis techniques to uncover fundamental relationships in materials science and find new materials of interest. She earned her BS in chemical engineering at BITS Pilani Dubai, and an MS in chemical engineering from the University at Buffalo.

Swinnich is a senior process engineer at GlobalFoundries, where he is in charge of electroplating at the company's Fab10 facility. For his PhD, he worked with Jung-Hun Seo to combine dissimilar semiconductors that have never been researched together before – gallium oxide and diamond – for the creation of new electronic devices for high power applications. He completed his BS in electrical engineering from the University at Buffalo.

Our Outstanding Students

Aparajita Dasgupta, PhD student

[Advisor: Krishna Rajan]
Best Poster Award, "Data Driven Analysis of Volcano Plots and Prediction of New Binary Catalysts," Materials Research Society Meeting, 2019.

Olivia Licata, PhD student

[Advisor: Baishakhi Mazumder]
Summer Internship Position, Idaho National Lab, July 2020; Winner of the CAMECA Calendar Image Competition, January 2020; Second Place, SEAS Student Poster Competition, April 2019; International Field Emission Society Travel Award, August 2019; Oral Presentation, Microscopy and Microanalysis, August 2019.

Jith Sarker, PhD student

[Advisor: Baishakhi Mazumder]
Oral presentation, 62nd Electronic Materials Conference, June 2020; Advanced Short-Term Research Opportunity Program, February 2020.

Yingjie Gao, PhD student

[Advisor: Bruce Pitman]
Best Poster Award, "Data Driven Analysis of Volcano Plots and Prediction of New Binary Catalysts," Materials Research Society Meeting, 2019.

Eric Oliverio, MS student

[Advisor: Prathima Nalam]
Career Experience Program Fellowship, NYS Center of Excellence in Materials Informatics, February 2019; MidAtlantic Rubber and Plastic Group, MARPG scholarship, October 2019.

Behnoosh Sattari, PhD student

[Advisor: Prathima Nalam]
Mark Diamond Research Fund, MDRF Fellowship, July 2020; First Place, MRS Science is Art Competition, December 2019; Best Poster Award, MRS Student Poster Competition, December 2019; First Place, STLE Student Poster Competition, May 2019; Second Place, SEAS Student Poster Competition, April 2019; George Norton SEAS Scholarship, June 2019.

Weimin Jiao, PhD student

[Advisor: Fei Yao]
AVS 66th International Symposium & Exhibition Travel Award, October 2019.

Mruganka Parasnis, PhD student

[Advisor: Prathima Nalam]
Mindsumo Fellowship, July 2020; Career Experience Program Fellowship, NYS Center of Excellence in Materials Informatics, February 2020.

Thaicia Stona de Almeiada, PhD student

[Advisor: Scott Broderick]
Best Poster Award, "Data Driven Analysis of Volcano Plots and Prediction of New Binary Catalysts," Materials Research Society Meeting, 2019.

### Robert Waelder, PhD student

[Advisors: Erik Einarsson and Kristofer Reyes]
Graduate Student Participant, Air Force Research Lab Summer Faculty Fellowship Program, June 2020.

Research Areas: Making Possibilities Realities

MDI's research portfolio is highly interdisciplinary and pushes the boundaries of traditional classifications in materials science research to establish a new paradigm for materials design and innovation. The department is organized into two broad overlapping research themes: **Methodology Science** and **Discovery Science.**

Methodology Science Cluster

The Methodology Science research cluster focuses on advancing and/or developing new techniques in experimental and computational materials science.
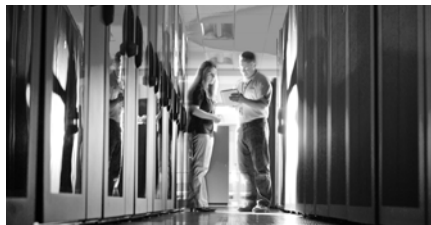
Materials Informatics

Advancing the tools of applied mathematics, statistics, machine learning, machine vision and information science, into experimental and computational materials science.

### Computational Materials Science

Research in the field of computing, multiscale modeling, and simulation of structure-property relationships in hard and soft materials.

Imaging, Spectroscopy and Metrology

Specialized research in high resolution imaging, time-resolved spectroscopy and property measurements for molecular scale materials characterization, and research directed towards instrumentation development and sensor design.

Discovery Science Cluster

The Discovery Science research cluster emphasizes innovations in the development of new materials, processes and expanding the design envelope for building devices and systems for a broad range of technological applications.
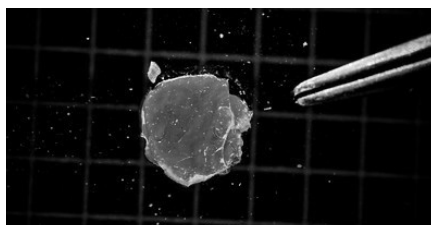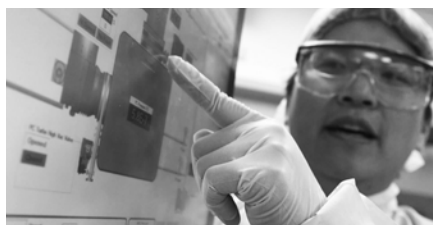
Synthesis and Materials Discovery

Exploring all aspects of materials synthesis and processing methods that promote the accelerated discovery of new materials and emergent phenomena, including high throughput protein crystal growth, low dimensional materials, nanostructured multifunctional materials and alloy design.

Renewable Energy and Sustainability

Advancing accelerated discovery, modeling, characterization and nanofabrication of materials for energy storage and conversion for renewable energy and carbon neutral technologies.

Artificial Intelligence for Materials Innovation

Research at the nexus of materials informatics, human-machine interactions and robotics leading to accelerated innovation in environmentally conscious materials manufacturing and sustainable materials design.

Major Projects

BioXFEL: An NSF Science and Technology Center, represents a new paradigm for materials science research. For the first time, data sciences, physics, materials and chemistry of soft matter are converging to enable scientists to view the shape of a molecule as well as how it changes in real-time. The research aims to transform a broad range of scientific fields focused on fundamental aspects of structural biology that has impact on a wide range of problems in medicine and biomedical sciences and extending into fields of soft matter.

The research in BioXFEL, which stands for Biology with X-ray Free Electron Lasers, captures the duality of the confluence of the "Methodology Science" and "Discovery Science" research thrusts of MDI. The activities in BioXFEL also serve as an excellent example of the merging of research interests in the life sciences and materials sciences in the fields of high throughput crystallography, crystal growth, X-ray scattering and data science. This type of intellectual convergence typifies the MDI research paradigm.
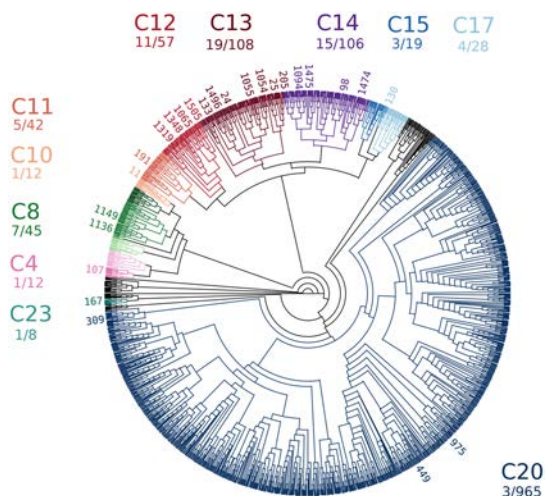

Comparing Chemistry to Outcome: The Development of a Chemical Distance Metric, Coupled with Clustering and Hierarchal Visualization Applied to Macromolecular Crystallography, by A.E. Bruno, A.M. Ruby, J.R. Luft, T.D. Grant, J. Seetharaman, G.T. Montelione, J.F. Hunt, E.H. Snell. PLOS ONE 9(6): e100782.

The Collaboratory for a Regenerative Economy (CoRE) is a unique research, education and civic entrepreneurship initiative that links materials design with manufacturing technologies in coordination with the needs of industry and front-line communities. CoRE explores, at the onset of technology design, strategies that reduce the footprint of materials and chemicals, guide industry practices, and build the infrastructure for a safe and sustainable environment in industrial communities. This approach has the potential to develop and deploy technologies that are capable of delivering better processes, products, and outcomes.

A key objective of our materials informatics work is to establish a platform for artificial intelligence (AI) driven materials chemistry discovery that meets the dual objectives of chemical performance, and human and environmental health and safety. The research focuses on the simultaneous and integrated consideration of technical and sustainability factors in chemical design, while factoring the needs of industry and health and well-being of industrial communities and workers. By applying our AI methods to health and environmental data (available through this network), we explore and identify pathways for reducing and eliminating the use of known chemicals and materials of high concern and replacing them with inherently safer and healthier alternatives.
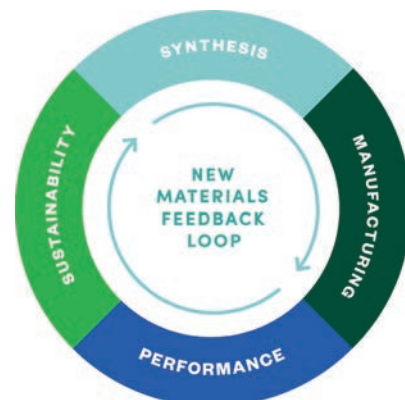
Building Communities: Here is How We Make the Greatest Impact

The MDI Hub is the focal point for a broad range of engagement and outreach activities for the department. We forge critical partnerships with community groups and non-governmental organizations to ensure our research and educational activities have the greatest impact on a broad range of areas such as health, climate change, and energy sustainability.

MDI-Industry Resident Scholar Program: Enabling Co-design for Materials Discovery with Engineering Innovation

MDI has established a unique genre of university-industry partnerships aimed at creating a research environment which significantly accelerates the implementation of basic science research into direct technological use. The philosophy of the MDI-Industry Resident Scholar program is to make MDI a home for industry-based scientists to work directly with MDI faculty and students. In this manner, both academia and industry can develop a meaningful understanding of the scientific and technological issues that each community of scientists face. Each perspective informs the other in adapting and guiding research goals to solve challenging engineering design problems driven by advances in materials science.

MDI has hosted companies such as Toyota Engineering Manufacturing of North America (TEMA) and Murata Corp., who have sent their scientists from Japan for one to three years in the MDI Resident-Scholar program. As an example, the TEMA-MDI partnership is a long-standing alliance that has allowed Toyota scientists and MDI faculty and students to work in a collaborative space to advance the harnessing of materials informatics to close the gap between materials discovery and engineering design. This research partnership has permitted the latest advances in our respective labs to be rapidly linked to solve difficult engineering problems.

Collaboratory for a Regenerative Economy: Innovative Materials Design for Health and Sustainability

Expanding beyond an initial focus on solar production and advanced manufacturing in industrial communities like Buffalo, New York, CoRE is developing scientifically-based, solution-oriented strategies to mitigate environmental health and safety risks by examining solar and other renewable energy technologies throughout their entire lifecycle, including manufacturing, use, decommissioning, and recycling. This includes identifying critical stages in the production of solar cells and other technologies, and how choices in materials and chemicals at different stages of production influence each other.

This information guides the development of scientific information and data-driven tools for the renewable energy economy to help change how industries approach materials innovation, and create pathways to accelerate the transition toward safer materials and clean production. CoRE actively engages and partners with industry, nonprofit, government, and academic leaders in the assessment, analysis, diagnosis, development, and implementation of new solutions and strategies for materials innovation. [corebuffalo.org]

Center for Materials Processing Data (CMPD)

CMPD is a consortium involving University of Connecticut, Worcester Polytechnic Institute and MDI in collaboration with ASM International to support partnerships with industry organizations. It is dedicated to the stewardship of materials data for modeling of material and process design for targeted industrial needs via computational materials engineering. Its aim is to serve as a data hub for accelerating the transfer of knowledge discovery in materials science to implementation in manufacturing. [cmpd.asminternational.org]

SUNY Applied Materials Research Institute (SAMRI)

SAMRI is a strategic alliance between the different campuses of the State University of New York (SUNY) system and Applied Materials, Inc. that serves as a research hub for academic-industry partnerships in the development of advanced materials, devices, manufacturing, and emerging areas of science and technology. It provides a unique platform to showcase MDI students and faculty and bridges the research activities of the department to industrial platforms.

Erich Bloch Symposium: A Convivium for Innovation

From right to left, distinguished leaders of American science including former NSF colleagues of Erich Bloch, **Robert W. Corell**, Principal, Global Environment Technology Foundation, **Rita R. Colwell**, Distinguished Professor, University of Maryland at College Park and Johns Hopkins University Bloomberg School of Public Health, President and Chairman of CosmosID, Inc., and former director of NSF, **William C. Harris**, President and CEO, Science Foundation Arizona, and **C. Daniel Mote, Jr.**, President, National Academy of Engineering, join Krishna Rajan, SUNY Distinguished Professor and Erich Bloch Chair of the Department of Materials Design and Innovation, to launch the inaugural Erich Bloch Symposium for MDI.

Linda Sapochak, Division Director of the Division of Materials Research, National Science Foundation, talks with Mugdha Kasarekar, a PhD student in the UB Department of Materials Design and Innovation, about her research poster during the 2018 Erich Bloch Symposium.

Attendees of the 2019 Erich Bloch Symposium pose for a group photograph in Grace Plaza, in front of Barbara and Jack Davis Hall, at the University at Buffalo.

The Erich Bloch Symposium is the flagship event of the Department of Materials Design and Innovation (MDI). Dedicated to the late Erich Bloch, the former director of the National Science Foundation whose endowment helped to create MDI, the annual event has developed into an "idea laboratory" for the future of materials science.

World leaders and thinkers from a wide variety of fields, including policy makers, business leaders, social scientists, educators, social activists and community leaders, along with numerous scientific disciplines covering all aspects of physical, life and mathematical sciences, come together to explore innovative strategies for research and education in materials sciences. Their overarching goal is to identify accelerated solutions to address a broad range of societal needs and catalyze new ways of thinking that help to define the future strategic trajectories of where and how materials science can help accelerate the development of solutions.

Data Takes the Center Stage in Unique Approach to Teaching Materials Science

A fundamental challenge in teaching a subject like materials science is that students need to absorb and rapidly connect concepts that link materials behavior at the engineering scale with molecular scale phenomena. The pedagogical framework of materials science and engineering requires that the perspectives of chemistry, physics and engineering all converge.

To better build the interconnections between diverse but foundational concepts, faculty in the department analyzed the curriculum using network representations and relevant concepts from graph theory.

Over a two-year period, they analyzed the entire core courses of the MDI master's curriculum. Two of the courses focused on data science and informatics concepts, and the other presented a blend of traditional materials science and data science. They created a comprehensive database that evaluated syllabi, homework assignments, and numerous exam questions.

From the over 200 specific topics addressed in the courses, they condensed the topic list to 10–15 topics for analysis. Finally, they identified how each of these topics connected to other topics across the curriculum, a process that involved active discussions among teaching faculty and peer-auditing each other's lectures.

This type of data driven network-based approach, enabled by MDI's unique collaborative teaching approach, facilitates a personalized education environment by showing students exactly what topics will be covered in a curriculum.

Detailed findings and analysis of the network-based approach to curriculum development are provided in "Data-driven visualization schema of a materials informatics curriculum: Convergence of materials science and information science," published earlier this year in **MRS Advances**. Authors, all from the Department of Materials Design and Innovation, are Erik Einarsson, Krishna Rajan, Olga Wodo, Prathima Nalam, Scott Broderick, Kristofer Reyes and E. Bruce Pitman.
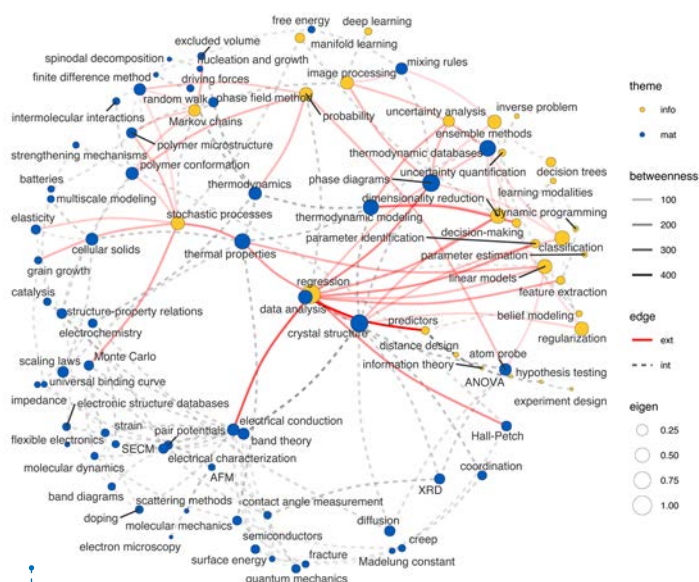
The highly interconnected MDI curriculum is represented in this graph, where blue and yellow vertices are used to denote materials science and informatics concepts, respectively.

Connect with MDI

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