CORE COLLABORATORY FOR A REGENERATIVE ECONOMY

Elements of Change

NOVEMBER
2020

Moving forward together toward a cleaner, safer future

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Executive Summary

The renewable energy industry has the potential to significantly improve human health, safety, and the environment around the globe. Unfortunately, the industry's products rely on toxic chemicals, from lead contained in solar cells to hydrofluoric acid used in manufacturing processes, which in turn pose challenges to the decommissioning and recycling of the products.

The Department of Materials Design and Innovation at the University of Buffalo, Clean Production Action, and Niagara Share created the Collaboratory for a Regenerative Environment (CoRE) in 2017 to address this growing problem, and accelerate progress toward cleaner, safer solutions.

CoRE brings together academic experts in materials science with entrepreneurial nonprofit organizations to accelerate clean production and sustainable materials in the renewable energy economy. Our innovative collaborations and data-driven tools enable business, government, and nonprofit leaders to identify and select inherently safer chemicals and sustainable materials for a healthier renewable energy economy.

In this report, you will learn more about the ongoing impact of our work—from using artificial intelligence to discover new materials, to helping some of the world's largest technology companies measure their "chemical footprint," and collaborating with leaders to create safer, healthier communities.

About CoRE

Who we are

In partnership with Clean Production Action and Niagara Share, the Department of Materials Design and Innovation at the University at Buffalo houses the Collaboratory for a Regenerative Economy (CoRE). The JPB Foundation funds the program.

Buffalo-Niagara: An ideal environment for developing effective solutions

CoRE's work in the Buffalo-Niagara region and Western New York (WNY) areas provides a unique opportunity to pilot and scale solutions with industrial suppliers and solar manufacturers in the region. Manufacturing is the largest contributor to the WNY regional economy, and clean, safe manufacturing is a priority for the protection of the Great Lakes watershed.

WHAT WE DO

Department of Materials Design and Innovation (MDI)

An interdisciplinary department at the University at Buffalo (UB)—a premier, public, research-intensive university in the top 1% of universities in the world.[1] MDI is a pioneering new department focused on establishing knowledge discovery in materials science by harnessing the tools of information and data science.[2]

Niagara Share

Creates lasting partnerships across thought leaders to formulate new ideas and policies designed to positively impact people, the environment, and the bottom line in industrial communities.

Clean Production Action (CPA)

Designs and delivers strategic solutions for green chemicals, sustainable materials, and environmentally preferable products.

University at Buffalo

Facilitates connectivity of platforms and oversees CoRE's operations and integration.

LEADERSHIP

Dr. Krishna Rajan, Erich Bloch Endowed Chair

- Leading proponent in the field of materials informatics
- SUNY Distinguished Professor
- Leader in the fields of computational studies, and advancing quantitative methods for the interpretation of nanoscale chemical imaging techniques

Alexandra McPherson, Principal

- Launched the startup Clean Production Action (CPA)
- Delivered tools and services to CPA partners such as Apple, HP, Kaiser Permanente, leading nonprofits, and the U.S. Environmental Protection Agency
- Served on the national advisory board of IEEE's EPEAT—the world's largest green electronic product registry

Dr. Mark Rossi, Executive Director

- Founder of BizNGO, a collaboration focused on advancing safer chemicals and sustainable materials
- Co-author of the GreenScreen®, the gold standard in hazard assessment used by industry leaders such as Hewlett Packard, Seagate, and DSM
- Co-founder of the Chemical Footprint Project, and author of a United Nations report on safer alternatives to toxic chemicals

Dr. Chitra Rajan, Associate Vice President for Research Advancement

- 25-year career as a senior administrator at universities
- Coordinated large scale, multi-institution teams to create research programs and consortia to advance technology-enabled solutions in health, manufacturing, renewable energy, and other sectors

What we do

OUR MISSION
Empower all stakeholders with science- and data-driven tools to reduce the chemical and material footprint of the renewable energy sector and its supply chains, thereby creating meaningful, measurable progress toward a regenerative materials economy.

OUR FOCUS
Developing strategies and solutions that improve chemicals management as well as accelerate sustainable material development for renewable energy technologies. Sustainable development of clean and safe technologies can be achieved only through simultaneous and integrated consideration of technical, environmental, and social factors in all aspects of the design, development, and adoption of renewable energy technologies.

Our approach

CoRE engages and partners with business, nonprofit, government, and academic leaders in the development and implementation of new solutions and strategies for data-driven, materials innovation frameworks. By doing so, we create pathways for the inclusion of environmental and human health considerations at the front end, especially in materials development and selection, and chemicals management.

At CoRE, we:

- **Identify pathways to accelerate solutions for safe and clean technologies to benefit all stakeholders**
- **Reduce the chemical footprint of manufacturing operations and the renewable energy sector and its supply chains**
- **Build on our knowledge infrastructure to support research platforms and the translation of that knowledge for stakeholder needs**
- **Use multiple modes and avenues to engage and share project results with various stakeholder communities**

Our values

HEALTHY PEOPLE, PLANET, AND ECONOMY
First and foremost, we seek to transform the chemicals and materials economy into one that sustains the lives of all, especially the most vulnerable populations

CONVERGENCE
Our cross-sector, multi-organization, deliberate approach to developing implementation strategies yields greater social, environmental, and economic value

SCIENCE-BASED SOLUTIONS
Scientific knowledge and tools enable us to analyze complex, multi-faceted societal problems and create innovative solutions

A SYSTEMS APPROACH
We address the entire life-cycle of products, while simultaneously exploring the use of alternate materials without compromising cost-effectiveness or engineering integrity

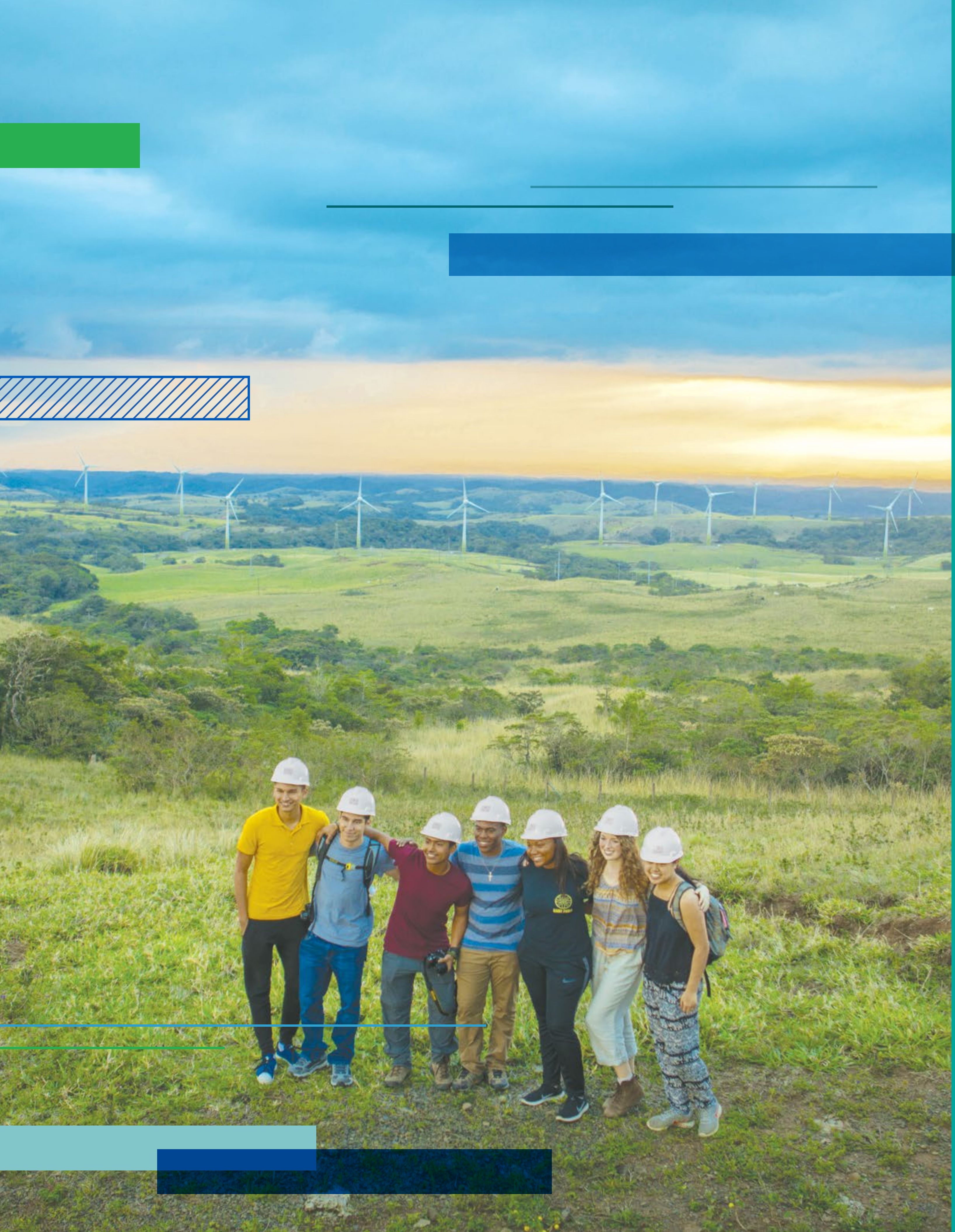
ACCELERATED DISCOVERY AND ITS TRANSLATION TO PRACTICE
Transferring research to practice typically takes years, even decades; our goal is to use an accelerated discovery paradigm to get results faster

ENGAGEMENT AND CAPACITY BUILDING
We make deliberate efforts to work together with key stakeholders, including workers and industrial communities, that can contribute to (and reap the benefits of) advancements in a regenerative economy

BROAD DISSEMINATION
A publicly accessible web portal and other initiatives to broaden and deepen the network of stakeholders engaged in the regenerative economy at the regional, national, and global levels

How we demonstrate our values:

- **Utilize the power of science and technology to understand and address complex, societal problems**
- **Recognize the importance of addressing root causes through preventive, rather than remedial, measures**
- **Value collaborations with industry, nonprofits, and government agencies, as we work together in stakeholder collaborations for systemic change**
- **Identify and disseminate proven and evidence-based practices for scalable, lasting impact**



The problem: How to safely meet demand for renewable energy

CoRE's Grand Challenge

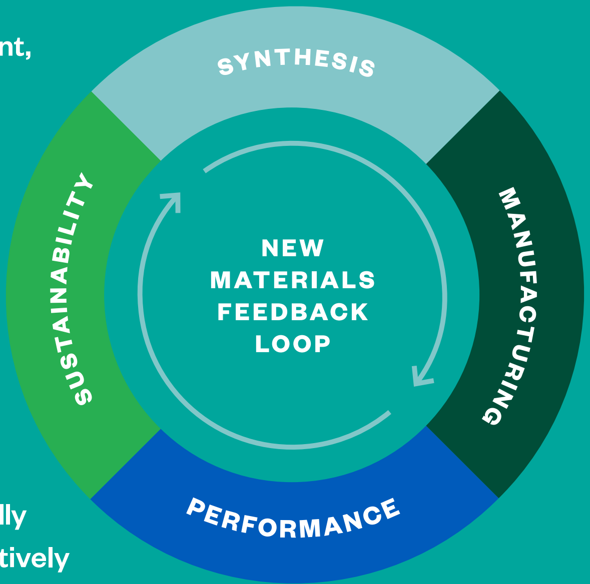
Build a collaboratory that supports wide-scale inclusion of environmental and human health considerations at the front end in the design of high-performance materials and clean manufacturing processes essential for a clean and safe renewable energy economy.

What is a collaboratory?

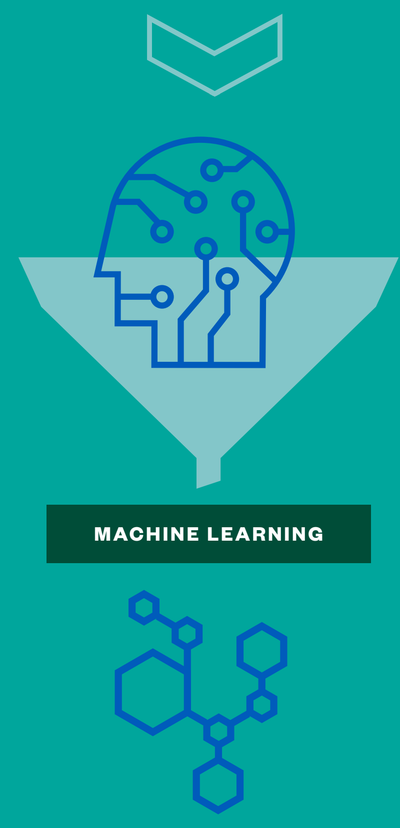
A collaboratory is a network that brings people together from multiple disciplines, and is intentionally designed to facilitate the sharing of ideas, expertise, and resources as stakeholders work together toward common goals.

Innovative materials design for health and sustainability

We take a holistic view of materials development, including determining the ability to synthesize a new material, as well as studying how it will perform, and its impact on the manufacturing process and sustainability. For example, a material may perform exceptionally well, but may be prohibitively time-consuming to manufacture.



When we identify potential chemistries that meet all four of these criteria, we use an artificial intelligence framework to discover the most promising new chemistries, as well as new tools for analyzing them.



More than a dozen states, including New York and California, have passed legislation mandating a net zero carbon economy. This demands a concerted effort in the rapid development of renewable energy technologies to address the climate crisis and avoid the ensuing catastrophic social and environmental impacts.

Many renewable energy industries, including solar energy, depend on novel materials to reduce costs and optimize efficiencies.

However, some of these materials are:

- Unsafe for the environment and human health
- Being rapidly depleted
- Scarce and can be difficult to access due to technological or political reasons

Workers, in particular, are exposed to hazardous chemicals throughout the supply chain, from extraction and manufacturing to recycling and disposal of renewable energy technologies. Industrial use of toxic chemicals has been largely ignored by businesses despite the risks these chemicals pose for workers, communities, and our economy.

Currently lacking: A proactive, systemic approach

Published data on current solar manufacturing lifecycle technologies are primarily retrospective and "forensic" in nature; they provide information on the impact of manufacturing and processing strategies *after the fact.* Important as it is, this approach can, at best, help with remediation, but not in preventing these problems. We need systemic changes in the design and development of renewable energy technologies to accelerate the development and discovery of safer materials without compromising performance.

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. Such an approach offers the potential to develop and deploy technologies that are capable of delivering better processes, products, and outcomes.

COVID-19 Impact

"We are an unhealthy nation—and many of our elevated disease rates are linked to environmental chemicals. COVID-19 is bringing into sharp focus the need to prevent this widespread exposure."[3]

Former director and program administrator of the National Institute of Environmental Health Sciences

At CoRE, we're concerned about megatrends, including:

2.7M+
deaths worldwide.

Nearly **20%**
of cancers attributable to environmental factors, including chemicals.

- More than 2,780,000 workers globally die from unsafe or unhealthy work conditions each year, according to the International Labour Organization (ILO). This is tantamount to a worker dying somewhere in the world every 30 seconds from exposure to hazardous chemicals in the workplace.[4]
- Chemical pollution has been identified as a significant "and almost certainly underestimated" contributor to the global burden of disease, highlighting the gaps in data and knowledge on many chemicals currently in use.[5]
- More than 78 million tons of waste related to solar panels will be produced by 2050.[6]
- Cancer is the second leading cause of death globally—responsible for 8.8 million deaths in 2015.[7] The World Health Organization (WHO) has estimated that approximately 19 percent of all cancers are attributable to environmental factors.[8]

Hazardous chemicals: A vast, fast-growing concern

In the 2019 Global Chemicals Outlook (GCO) II report, the United Nations concluded that the 2020 target of minimizing adverse impacts of chemicals and waste set in the Strategic Approach to International Chemicals Management (SAICM) will not be met, and will be further exacerbated as the chemical industry doubles in size from $5 trillion US in 2017 to $10 trillion in 2030.[9]

Further, the UN GCO II report highlights the need for filling global knowledge gaps by harmonizing research protocols, using health and environmental impact information to set priorities, and strengthening the collaboration of scientists and policy makers. These mega impacts exacerbate systemic racism, poverty, and chronic health problems that surround many of our industrial communities throughout the United States and the world.

COVID-19: Further impacting the most vulnerable communities

The COVID-19 pandemic has demonstrated the additional risks faced by industrial communities and workers due to compromised immune systems that arise from exposure to these contaminants. Cellular-level disruptions arising from exposure to such chemicals have been shown to be an important upstream determinant that influences individual functioning and health outcomes.

CoRE is working on identifying key molecular signatures that could be used to guide the selection of safer substitutes for some of the chemicals that are categorized as endocrine disrupting chemicals (EDCs). These chemicals interfere with the normal functioning of hormones and adversely impact inflammation and healthy immune responses that are linked to diseases like cancer, and increase our susceptibility to COVID-19.

The CoRE solution: Innovative materials design for health & sustainability

Our approach acknowledges the role that scientific knowledge and tools can play in analyzing complex, multi-faceted societal problems and in creating innovative solutions, but recognizes that the development and implementation of new technologies and practices will accelerate and scale when researchers collaborate with leaders and stakeholders.

Sustainable development of clean and safe technologies can be achieved only through **simultaneous** and **integrated** consideration of technical, environmental, and social factors in **all aspects** of the design, development, and adoption of renewable energy technologies.

The CoRE Theory of Change

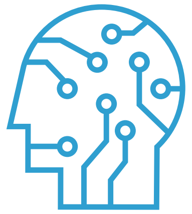
Empower stakeholders with science- and data-driven solutions to accelerate the discovery and market adoption of sustainable materials for renewable energy technologies.

Using data to accelerate discovery

While the development of new performance materials typically takes decades, CoRE seeks to accelerate this discovery with data-driven tools that can assess, process, integrate, and internalize the technical, environmental, and social considerations into the design and development of new high-performance materials.

Three key platforms

CoRE integrates three platforms to systematize common currencies of data needed for the development of sustainable renewable energy technologies. These platforms support and inform each other, enabling CoRE to develop more innovative solutions in a more timely manner.



- **Science Platform: shows what is possible**
  Accelerates the discovery and development of safer materials by advancing state-of-the-art materials informatics that leverages artificial intelligence (AI) and data-driven materials science

- **Tools Platform: enables what is possible**
  Organizes and simplifies complex data, thereby enabling decision-makers and change agents to assess and measure chemical footprints and make safer substitutions

- **Stakeholder Platform: advocates for what is possible**
  Convenes multi-stakeholder groups to co-create, disseminate, and implement practical solutions that accelerate business, nonprofit, and government decisions and policies for developing and using safer chemicals and materials innovation

Goal

Create a new framework for innovative materials design for health and sustainability by bringing together academic, industry, nonprofit, and government partners to accelerate the development of clean and safe renewable energy technologies.

Focused on the entire lifecycle of renewable energy

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 Science Platform in developing the 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.

Working toward the United Nations Sustainable Development Goals

The United Nations Sustainable Development Goals (SDGs) are “the blueprint to achieve a better and more sustainable future for all.”[10] CoRE’s strategy for achieving the SDGs is to transform how the renewable energy sector and its supply chains, including operations in Buffalo, manage chemicals—by moving them to eliminate the use of chemicals of high concern as defined by the GreenScreen® for Safer Chemicals, and building demand to replace them with safer and healthier alternatives.

CoRE Goal

Reduce the renewable energy economy’s chemical footprint by 50% by 2030 to make significant progress toward the United Nations Sustainable Development Goals for Good Health and Well-Being, Clean Water and Sanitation, and Sustainable Consumption and Production. Key performance indicators in each of these goals set 2030 targets for responsible management and reduction of hazardous chemicals.

CoRE strives to contribute to the University at Buffalo’s efforts to positively impact metrics and targets set in the United Nations Sustainable Development Goals (SDGs); the university was recently rated #1 among U.S. universities working on SDG #13, which addresses urgent action to address climate change.[11]

Identifying new pathways to accelerate solutions

Materials are central to every technology, and future technologies will place increasing demands on materials’ performance. Our goal is to identify pathways that will lead to accelerated solutions for developing clean, safe, and sustainable renewable energy technologies that benefit all stakeholders. Our approach to materials discovery and design is to help identify solutions that are effective, robust and address various problems associated with the lifecycle of solar technology.

Learning from peers

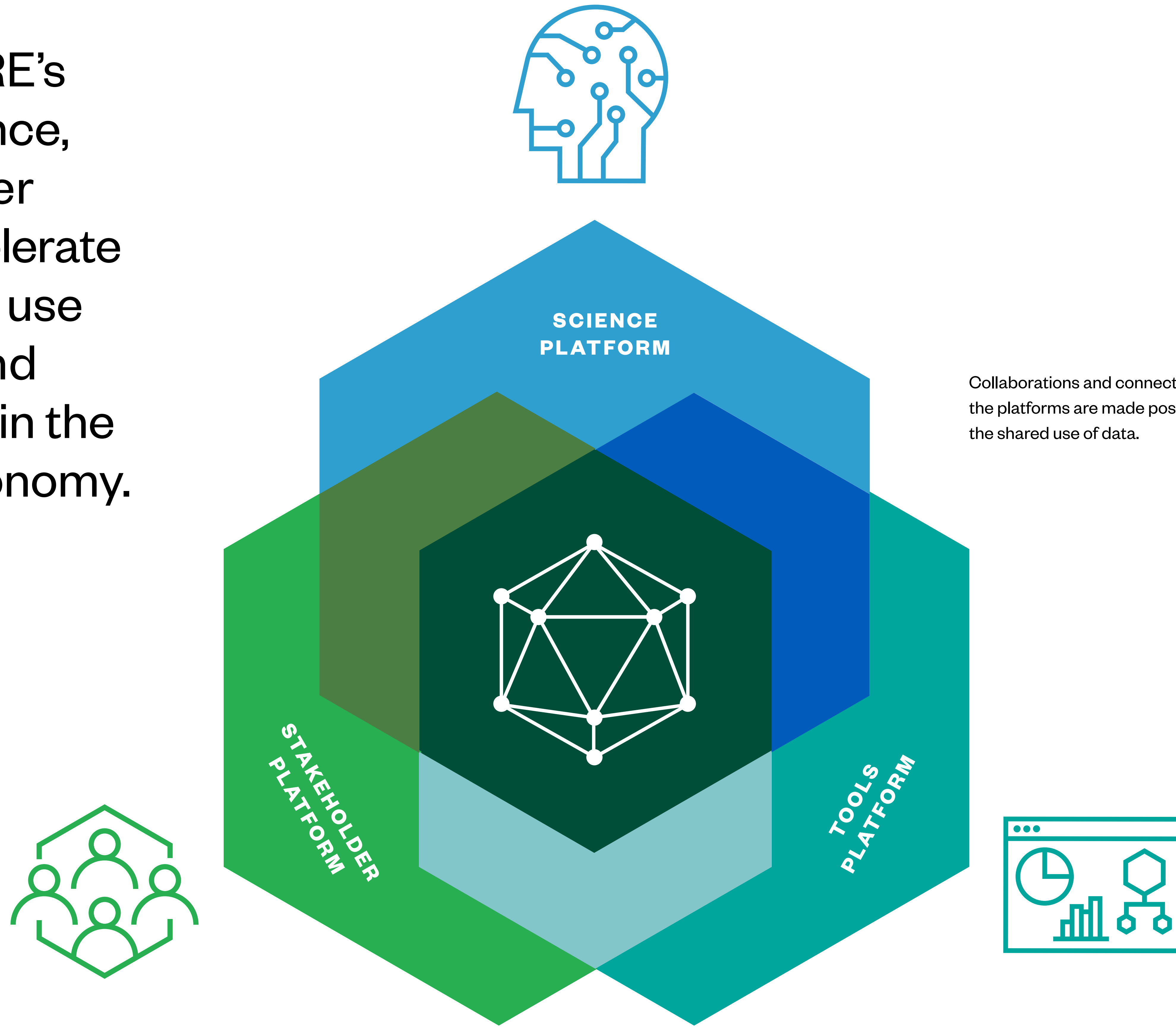
CoRE is continually assessing emerging research on the solar sector, including the analysis published in *Solar Power: Innovation, Sustainability, and Environmental Justice.*[12]

Key findings include:

- Safer substitution is needed for high-risk hazardous materials including exotic chemical combinations, metal compounds, and nanoparticles used commonly in solar technologies
- Industry leaders and environmental stakeholders need to identify positive social and environmental practices that can be supported at every stage of the commodity value chain of solar technologies
- Society needs to scale solar rapidly to address climate change but be intentional about just and sustainable design
- Worker health and safety standards need to be established to address human rights challenges that are elevated by the rise of “contract manufacturing” and “offshoring production”—labor processes similar to those in electronics and semiconductor industries

Integrated platforms for more effective results

The integration of CoRE's three platforms (Science, Tools, and Stakeholder Engagement) will accelerate the development and use of safer chemicals and sustainable materials in the renewable energy economy.



Collaborations and connections across the platforms are made possible through the shared use of data.

The Science Platform

Using artificial intelligence to address technical and human needs

Our arsenal of multifaceted data-analytical tools—which combines computational materials science and experimental data with machine learning methods—enables us to fuse information in a robust, but accelerated, manner.

This approach, known as materials informatics, allows CoRE to:

- Assess the overall impact of selected materials and their use
- Provide parameters for finding alternatives and target areas for making changes
- Simulate materials properties, structure, and performance
- Streamline time-consuming trial and error experiments
- Quickly discover correlations and connections that merit further exploration[13]

What is materials informatics?

Materials informatics is the science of harnessing the tools of information science coupled with experimental and computational data to provide new insights into the structure-property relationships of materials. The computational foundations of materials informatics permit researchers to significantly accelerate the discovery and design of new material founded on a concurrent understanding of the mechanisms governing such behavior.

Focused on rational design and data-driven tools

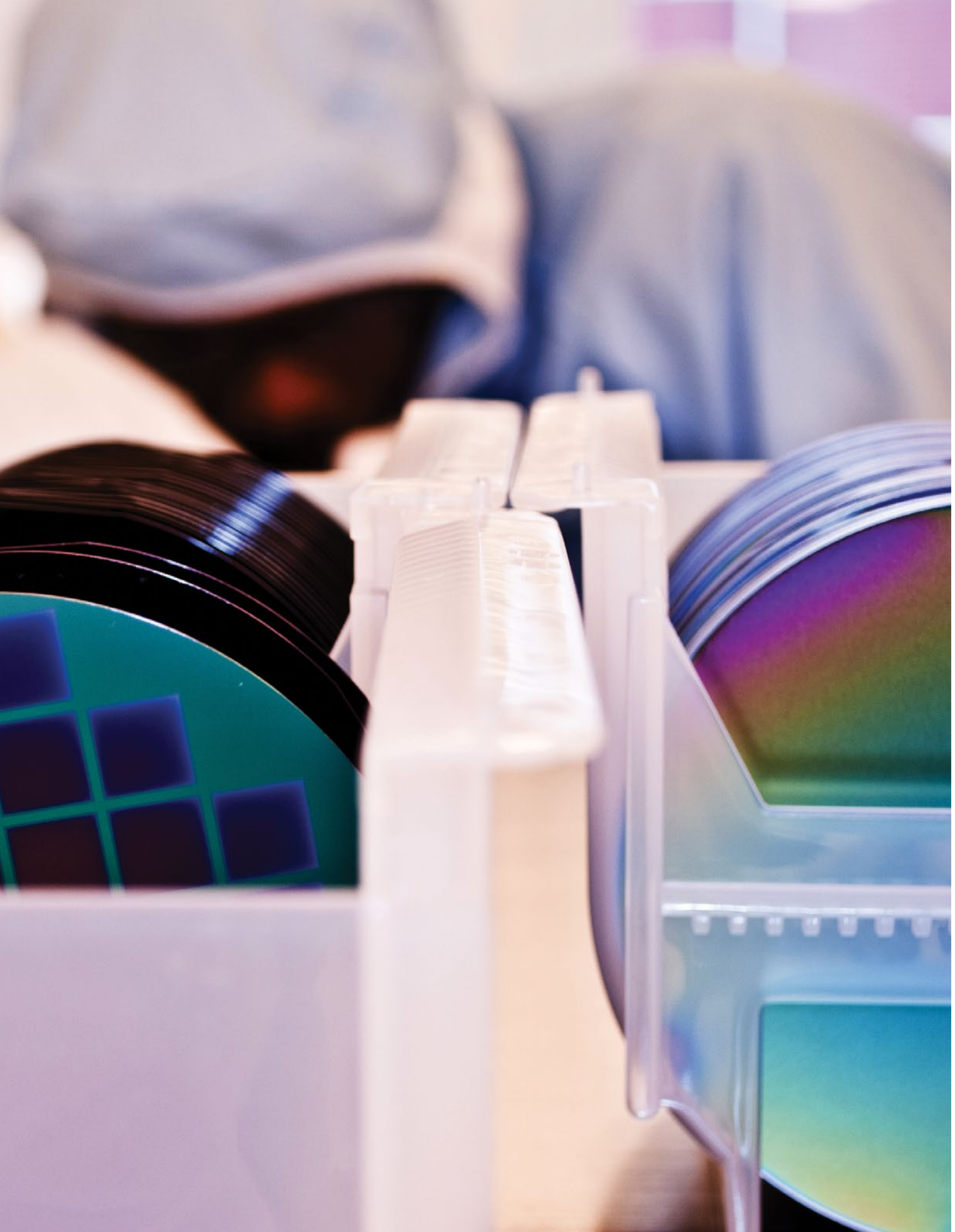
The Science Platform has two broad objectives:

1. Harness advanced materials modeling and informatics techniques to identify pathways for the rational design of new materials chemistries for renewable technologies (e.g., solar energy) that minimize adverse environmental and human health impacts without compromising functionality. Through the Science Platform, we are working on problems including identifying new lead-free material chemistries for state-of-the-art solar devices, such as the perovskite family of materials that is being used for enhanced performance of solar systems. Searching for the proper chemistry of materials that meet multiple functionality metrics of minimal hazard and enhanced engineering performance requires us to explore a chemical search space that is prohibitively too large to explore and make critical discoveries within a reasonable time frame using traditional methods. CoRE seeks to address this challenge by applying materials informatics and physics-based modeling to fill the gaps in scientific knowledge, which then guides accelerated materials discovery and design for solar technologies. At CoRE, our goal is to gain a greater understanding of how atomic scale changes in chemistry have multiscale influence on materials manufacturing, performance, and sustainability of solar cells.

2. Develop data-driven screening tools that can estimate potential toxicity and inform the design of safer alternatives. CoRE is harnessing advanced machine learning methods to help navigate the complexity of information associated with new and emerging chemicals used in the manufacture of solar devices. Our modeling tools can provide insight into the molecular-scale mechanisms that govern the toxicity of hazardous chemistries. For example, we have developed classification models for persistent and hazardous chemicals such as PFAS compounds and other organic chemistries used in the synthesis of new high-performance solar devices. Additionally, these tools provide guidelines for identifying potential candidates for safer materials chemistries.

What is rational design?

Rational design is a process in which we bypass trial-and-error approaches, and create new materials based on a predictive understanding of the fundamental science governing materials performance.



A key objective of our materials informatics work is to establish a science 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 will provide pathways for reducing and eliminating the use of known chemicals and materials of high concern and replacing them with inherently safer and healthier alternatives.

The Tools Platform

Shifting the market from toxic to safer chemicals

CoRE's Tools Platform plays a key role in enabling our strategy of reducing the use of toxic chemicals. On the demand side, we work with investors, retailers, governments, health care organizations, and nonprofits, and provide them with tools that simplify and clarify their demands for safer chemicals in products, manufacturing operations, and supply chains. On the supply side, our tools assist manufacturers and their suppliers to develop corporate-wide chemicals management policies and programs, identify toxic chemicals as well as safer alternatives, measure their chemical footprint, set chemical footprint reduction goals, and report to their stakeholders and customers regarding progress toward those goals.

Our tools include:

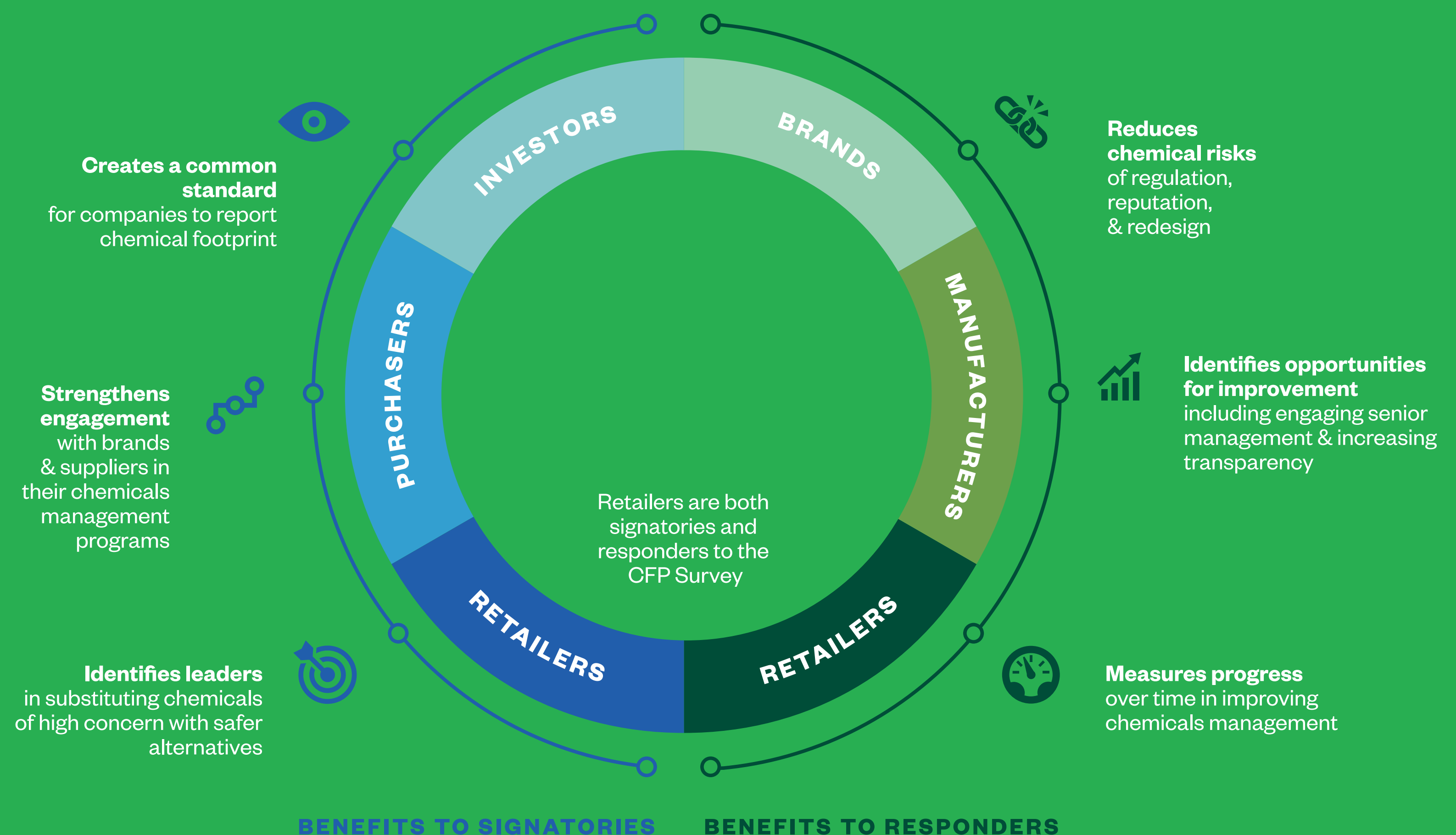
- GreenScreen for Safer Chemicals: Assesses and benchmarks chemicals based on their hazards. Companies can use GreenScreen benchmark scores to identify chemicals of high concern, safer chemicals, and safer products.
- The Solar Scorecard: Assesses overall corporate performance in the solar industry based on sustainability and social justice benchmarks, integrating questions from the Chemical Footprint Project Survey.
- Materials science research tools: Give us informatics and machine learning tools that are essential to mapping chemical footprints across the renewable energy sector as well as fast tracking safer material development and innovation.[14]
- The Chemical Footprint Project: A Clean Production Action program to develop and advance the concept and practice of chemical footprinting of products, packaging, manufacturing, supply chains, and facilities with the goal of reducing the use of chemicals of high concern. The Chemical Footprint Project Survey evaluates responders' chemicals management systems against best practice to measure and reduce chemical footprints.

Visualizing the impact of toxic materials

CoRE's research will be used to map material streams and their lifecycle impacts using machine learning and artificial intelligence (AI) tools to close the knowledge gaps on safer substitution of toxic chemicals, and accelerate the development of sustainable, high-performance materials chemistry for solar technologies. CoRE has also developed interactive visualization tools that would be valuable to a broad range of stakeholders. CoRE's application of new AI tools to incorporate diverse, complex, and often poorly organized information—including environmental and human health data sets—into user-friendly assessment tools will help decision-makers understand and apply complex environmental, socio-economic, and health data for safer material innovation and chemical footprinting. This includes increasing applicability and scalability of such leading hazard assessment tools as the GreenScreen for Safer Chemicals and quantitative metrics to measure and reduce chemical footprints. The intent is for these decision-making frameworks and tools to make chemicals management and materials innovation more feasible and affordable for industry leaders. These tools help stakeholders effectively use data (including information that may be critical to solving a specific problem) to meet their goals, discover new scientific knowledge, or advocate for a position.

Chemical Footprint Project Survey Value

The annual CFP Survey of brands, manufacturers, and retailers provides benefits both to CFP Signatories and Survey Responders.



Chemical footprint: A measure of chemicals of high concern, either by count or by mass, in a defined product, space, or process.

The Stakeholder Platform

Working closely with key organizations

CoRE is modeling a process for stakeholder engagement with people, organizations, and companies—a process that is iterative and capable of incorporating new knowledge arising from scientific discoveries, evolving social and environmental conditions, community impact, and the needs of the local and global economy.

Through the annual Erich Bloch MDI Symposium and CoRE Change Agent Summit, for example, CoRE disseminates, pilots, and tests its solutions with a large network of scientists, business leaders, influencers, investors, and representatives of non-governmental organizations. We work in partnership with change agents in the nonprofit advocacy community, the renewable energy industry, and industrial manufacturers to drive industry demand for new, cleaner, and safer high performance materials through a variety of benchmarking tools and hazard assessment metrics.

Key collaborations include:

- Western New York Small Business Roundtable and its Clean Production Leadership program
- Investor Environmental Health Network (IEHN), a community of investors working to reduce corporate financial risks of toxic chemicals in products, manufacturing, and supply chains
- BizNGO, a collaboration of businesses and advocacy organizations working together to advance safer chemicals and sustainable materials
- Chemical Footprint Project signatories—organizations that sign on and engage companies in reducing their chemical footprint, which include retailers, NGOs, health care organizations, and investors

Clean Production Leadership

CoRE co-created Western New York's first Clean Production Leadership program with the Western New York Sustainable Business Roundtable (WNY SBR) and New York State's Pollution Prevention Institute (NYSP2I), a five-year, $30 million New York State funded program at the Rochester Institute of Technology. Renewable energy manufacturers and solar installers—including Tesla, Solar Liberty, and Montante Solar—are leading members in the WNY SBR.

In addition, we integrate market-shifting visualization tools into existing and new stakeholder collaborations to expand and hasten companies' demands to reduce their chemical footprint.

Co-creating user-friendly tools

Moving forward, we will continue to pilot and scale our tools to make it easier for companies in the renewable energy sector and their supply chains to reduce their chemical footprint.

- With industry and nonprofit leaders, we will create GreenScreen assessments and certifications to replace high-concern chemicals used in solar manufacturing processes and products
- With investors and Chemical Footprint Project (CFP) Signatories, we will tailor the Chemical Survey for solar manufacturers to demonstrate for the solar industry and its supply chains how corporations can measure and reduce their chemical footprint
- With the Silicon Valley Toxics Coalition (SVTC) and their Solar Scorecard, we will evaluate, compare, and impel solar manufacturers to replace toxic chemicals in manufacturing with safer alternatives—including our partnership to support SVTC's development of the next generation of the Solar Scorecard
- With WNY SBR, we will take this work on the ground to demonstrate how clean production practices can be implemented in the middle of the supply chain as well as by major renewable energy manufacturers and suppliers with operations in Buffalo
- With leading scientists, nonprofits, and industries, we will leverage the resources in CoRE's Science Platform, and pilot tools in our data laboratory (including data-driven models on materials and chemistry related performance) that are relevant to minimizing the costs of reducing chemical footprints and investing in material innovation

Global Impact

CoRE worked with the investment firm and CFP Signatory Boston Common Asset Management to engage Panasonic in Tokyo on chemical footprinting.

Impact and lessons learned

Impact

Safer materials for solar cell device

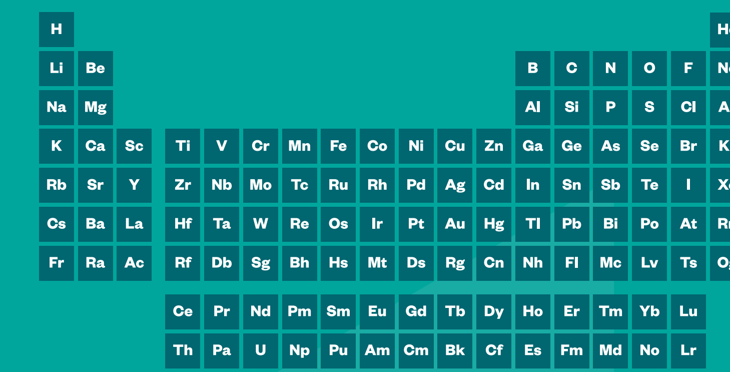
One of our objectives is to establish a comprehensive strategy for designing toxic-free materials for solar technology—specifically, in solar devices. While there are many efforts around the world, new materials that meet the multitude of properties required for high-performing solar cells and are free from toxic elements are so complex that the search is very slow. Using our materials informatics approach, we have discovered a new way to navigate the information landscape that achieves this. We need to understand how the many different characteristics of a material's chemistry interact to collectively influence both the functionality of the material (for example, solar energy conversion performance) *and* impact human and environmental health. CoRE's Science Platform has identified a cohesive design strategy for the next generation of solar materials chemistry that addresses this problem.

Our materials informatics (or in-silico) approach to designing materials with targeted properties involves choosing structural, chemical, and processing parameters based on experimental and theoretical evidence, while making sure that we do not miss critical descriptors that may hold clues for materials discovery and design. We have created a single machine-readable representation of molecular structure to rapidly explore and successfully predict properties of large numbers of material chemistries.

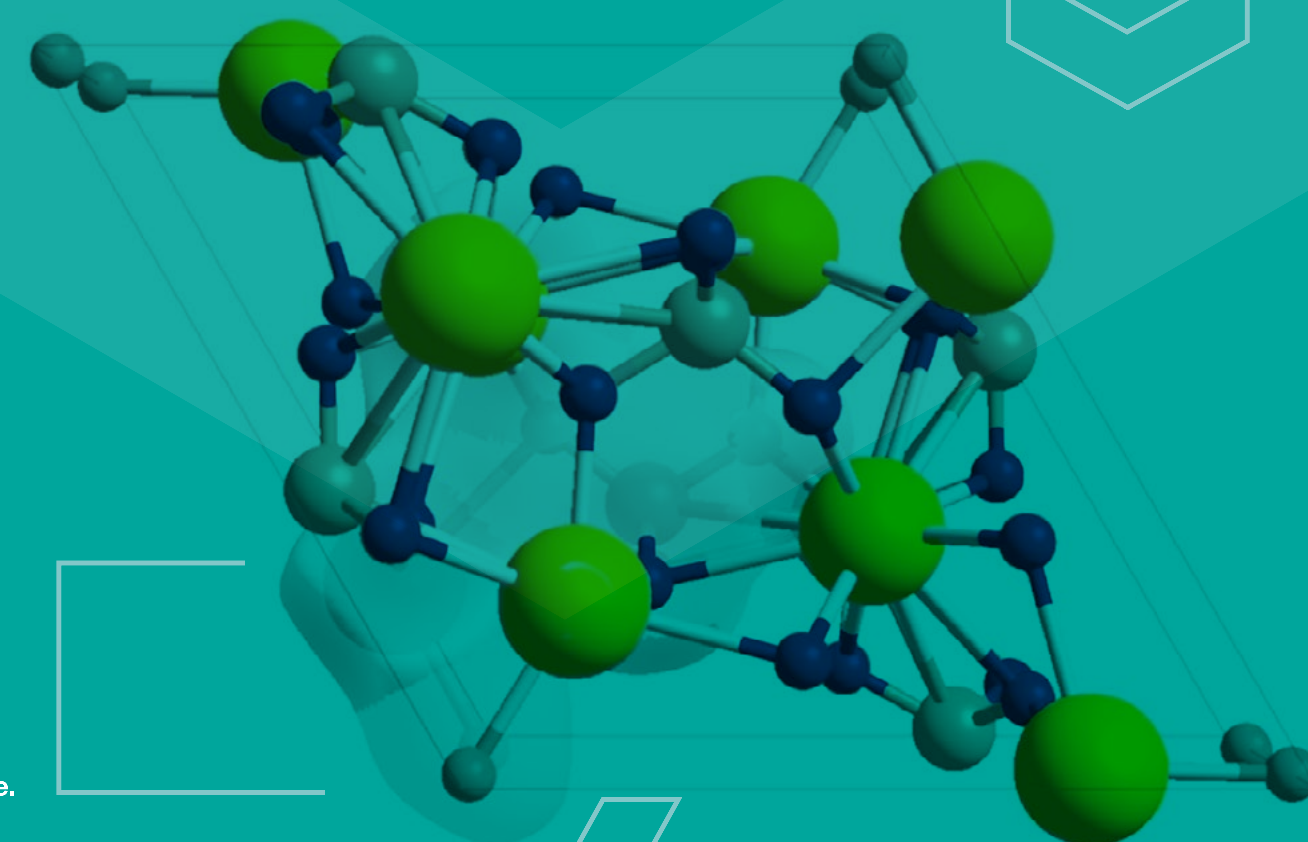
Using a new genre of data representation, we have captured the synergistic effects of chemical formulas, bonding intermolecular packing, crystallographic parameters, and building blocks characteristics to create a data motif that can be expanded to predict additional properties and generalized to an entire genre of complex inorganic solids. We have demonstrated that our data fingerprints provide a powerful representation of perovskite crystal chemistry, thus overcoming some fundamental theoretical and computational bottlenecks. We are now in a position to quickly guide the design of new chemistries that can be substitutes to toxic elements.[15]

Chemical fingerprinting

We have developed new accelerated computational methods linking computational chemistry with machine learning to establish chemical "fingerprints," which can serve as strategic markers to rapidly a) predict the properties of emerging candidates for solar technology, and b) provide guidelines for developing materials chemistry that meet the dual objectives of performance and safety.



Chemical fingerprint:
A representation of a material's properties

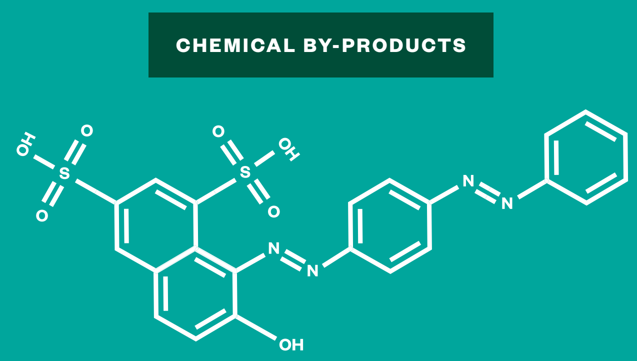


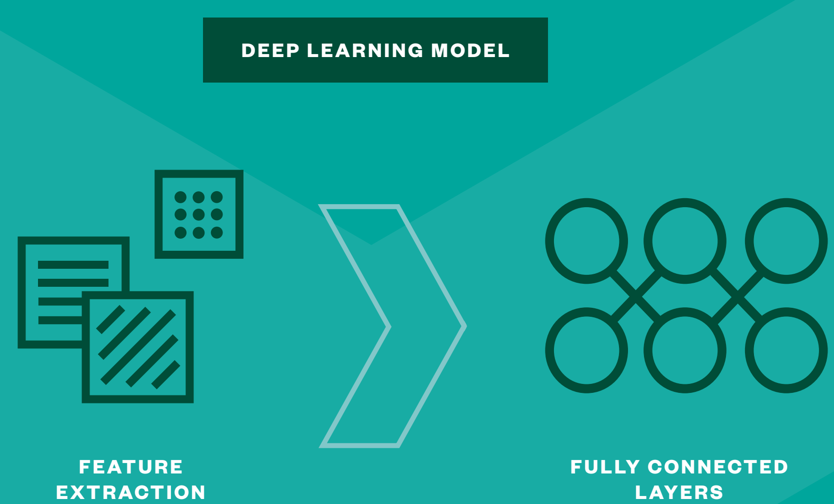
MATERIALS MODELING

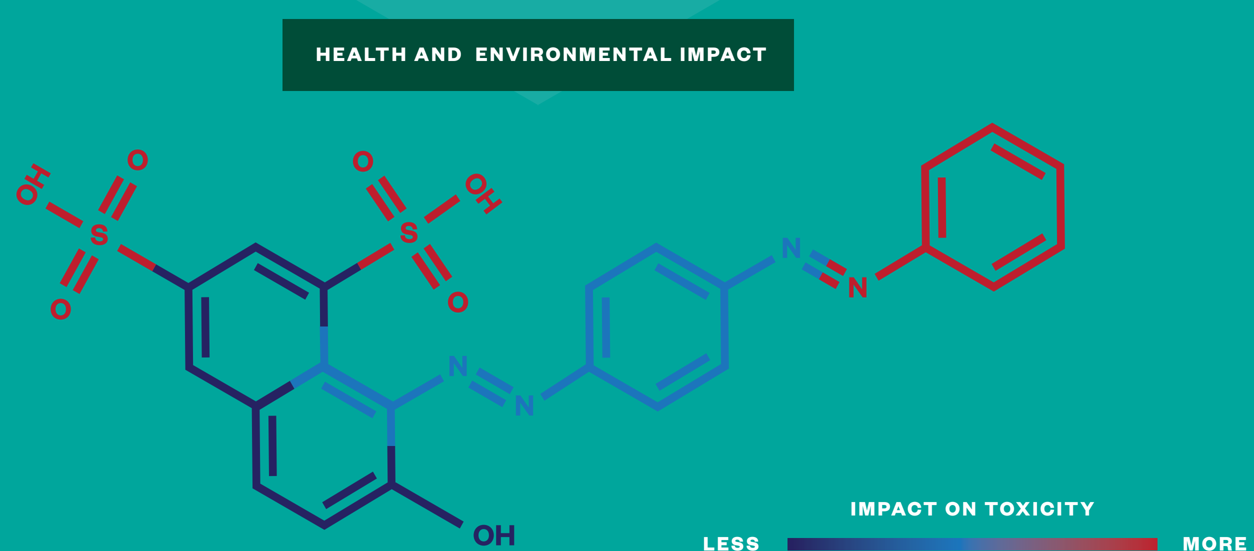
Machine learning coupled to computational materials science helps us to accelerate the design of new materials chemistries with enhanced performance.

Molecule toxicity assessment

We use artificial intelligence (AI) to identify and visualize the most critical parts of the molecule in terms of its toxicity.







Impact

Tracking molecular data fingerprints for hazardous chemicals

PFAS (per- and polyfluoroalkyl) compounds represent some of the most serious contaminants to human and environmental health due to their persistence, toxicity, and bioaccumulation. Although legacy PFASs (i.e., perfluorooctane sulfonates/PFOSs and perfluorooctanoic acids/PFOAs) have been banned worldwide, alternative PFASs with unknown structures and/or properties are being produced every day. Among the large family of PFAS chemistries, only a few have been experimentally studied, resulting in significant gaps in data linking chemistry to PFAS properties as well as hazard impact.

Due to the high cost and amount of time needed for measurements, it is impossible to fill the gaps solely based on traditional experiments.

To overcome this problem, CoRE has:

- Built research protocols to track hazardous chemicals commonly used in solar panels from public domain databases
- Combined this information with an informatics-based analysis of molecular characteristics of PFAS compounds
- Created an atlas that can readily uncover patterns of classifications and eliminate any ambiguity or vagueness of classifications due to chemical terminology and labeling; this atlas captures high-dimensional information, yet makes the classification of PFAS clearer and easier than the previously published descriptive classifications

With this technique, we are now able to uncover the molecular origins that govern the behavior of toxic chemicals and the degree of toxicity. Visualizing PFAS compound properties in this manner provides an accelerated approach for filling data gaps by allowing us to estimate the unmeasured properties, rapidly classify the potential toxicity of new compounds, and provide guidance on where research and safety concerns should focus. It can also capture high-dimensional information that can be used to develop guidelines for classifying new and emerging PFAS compounds. This approach will help us develop similarity metrics to guide the selection of alternative safer chemicals.

Impact

Creating metrics for chemicals management in the solar industry

Foundational to CoRE's work to transform the solar industry is defining, developing, implementing, and disseminating the process of how to measure and reduce chemical footprints. But very few companies measure their chemical footprint in the way they track their carbon footprint. Most companies externalize the societal risks and costs of using toxic chemicals and rely heavily on exposure controls that do not provide adequate protection to vulnerable populations working in, and living near, industrial production and disposal facilities.

CoRE is advancing the concept of chemical footprinting in the renewable energy sector through Clean Production Action (CPA) and their Chemical Footprint Project (CFP) Survey, which provides a robust framework for evaluating overall corporate chemicals management practices, including the measurement of a company's overall chemical footprint.

Solutions for multiple sectors

CoRE provides tools and resources like the Chemical Footprint Project, the GreenScreen for Safer Chemicals, and MDI's Safe Manufacturing data analytics to support clean production. This magnifies CoRE's impact and allows us to scale solutions across multiple industrial sectors, including solar.

In *Hewlett-Packard's Use of the GreenScreen® for Safer Chemicals*, researchers wrote that:

"Formal, traditional risk assessment provides valuable information and analysis for regulators and industrial hygienists, but it may not be the right tool for comparing the relative impacts of replacement and restricted substances. Nevertheless, there is a concern among some practitioners that shifting away from risk-based screening overemphasizes the inherent hazard of substances and does not account for exposure controls that are available to protect human health. While exposure controls are important, especially in industrial settings, a key reason to pursue hazard reduction is that perfect exposure control is not possible."[16]

GreenScreen's 18 Endpoints

GreenScreen is a scientifically robust and peer-reviewed method for assessing chemical hazards across 18 human health and environmental endpoints, aggregated and organized across four benchmarks ranging from Benchmark 1 (chemicals of high concern) to Benchmark 4 (safer chemicals).

Group	Endpoint		Hazard level
GROUP I HUMAN	Carcinogenicity		*L*
	Mutagenicity		L
	Reproductive Toxicity		L
	Developmental Toxicity		M
	Endocrine Activity		*M*
GROUP II AND II* HUMAN	Acute Toxicity		L
	Systemic Toxicity	single	L
		repeated	L
	Neurotoxicity	single	vH
		repeated	*H*
	Skin Sensitization*		L
	Respiratory Sensitization*		DG
	Skin Irritation		L
	Eye Irritation		L
ECOTOX	Acute Aquatic Toxicity		H
	Chronic Aquatic Toxicity		H
FATE	Persistence		vL
	Bioaccumulation		L
PHYSICAL	Reactivity		M
	Flammability		L

HAZARD LEVEL

- vL (very low)
- L (low)
- M (medium)
- H (high)
- vH (very high)

CONFIDENCE LEVEL

HIGH LEVEL (BOLD)

LOW LEVEL (ITALIC)

Chemical of High Concern (CoHC) Criteria

Consistent with GreenScreen Benchmark 1 criteria, and aligned with Globally Harmonized System for the Classification and Labeling of Chemicals (GHS)

- Carcinogen, mutagen, or reproductive toxicant (CMR), or
- Persistent, bioaccumulative and toxic substance (PBT), or
- Any other chemical for which there is scientific evidence of probable serious effects to human health or the environment that give rise to an equivalent level of concern, or
- A chemical whose breakdown products result in a CoHC that meets any of the above criteria

CoHC/GreenScreen Benchmark 1 Criteria are compared with chemicals on authoritative lists developed by:

- California Environmental Protection Agency
- European Chemicals Agency
- International Agency for Research on Cancer
- MaK Commission of Germany
- OSPAR Convention
- UN Environment Program
- US Centers for Disease Control
- US Environmental Protection Agency
- US National Institutes of Health

CFP CoHC Reference List

- Roughly 2,200 chemicals and chemical groups identified on lists developed by authoritative bodies as meeting CoHC criteria
- Consistent with GreenScreen List Translator-1 (LT-1) chemicals
- Identifies chemicals that are measured in an organization's quantitative chemical footprint metric
- Includes many chemicals commonly used to manufacture and produce renewable energy technologies, including solar systems

Solar panel manufacturers face increasing market and regulatory pressure to meet new corporate performance standards that specify safer chemical use and disclosure of chemicals of high concern, and thereby reduce their chemical footprint.

- NSF 457, the new Sustainability Leadership Standard for Photovoltaic Modules and Photovoltaic Inverters, requires disclosure and elimination of toxic chemicals to receive "gold" level product certification. CFP provides critical metrics and data for key performance indicators in NSF 457's section on "Management of substances."
- The Silicon Valley Toxics Coalition (SVTC) Solar Scorecard ranks companies in part due to their chemical use reduction plans.
- The European Union has two major directives that affect chemicals and materials use in the solar industry: REACH and the Restriction of Hazardous Substances (RoHS) Directive. The REACH Candidate List of Substances of Very High Concern (SVHCs), which all manufacturers are required to track for products sold in Europe, is one of the authoritative lists in CPA's GreenScreen List Translator™ and the chemical footprint metric.

For close to two decades, CPA has worked with manufacturers and technology leaders like Hewlett-Packard, Apple, and Seagate to pilot and implement new approaches to chemicals management in their supply chains, emphasizing hazard assessment and safer substitutions of toxic chemicals. For example, Apple uses CPA's GreenScreen for Safer Chemicals to work with their suppliers to replace chemicals of high concern to human health with safer alternatives in its final assembly facilities worldwide.[17] GreenScreen not only defines criteria for chemicals of high concern, but also defines criteria for safer chemicals.

GreenScreen List Translator

Organizations use the GreenScreen List Translator tool to quickly identify Chemicals of High Concern (CoHCs). The Chemical Footprint Project (CFP) uses List Translator to specify the 2,000-plus chemicals on CFP's CoHC Reference List.

Impact

Partnering with the Solar Scorecard to set new sustainability milestones

In 2020, the Silicon Valley Toxic Coalition's (SVTC) Solar Scorecard celebrated its 10th anniversary. SVTC and CoRE partnered on the release of the 2018–19 Solar Scorecard to ensure that investors, nonprofits, and procurement leaders could assess industry performance on key sustainability attributes. In addition, SVTC and CoRE are spearheading a process to create new content for the Solar Scorecard version 2.0. Enabling development and release of the scorecard allows us to benchmark the progress solar companies are making to improve their performance on critical sustainability metrics.

SVTC and leading investors, representing $1.5 trillion US in assets under management, use the Solar Scorecard to benchmark corporate performance on business practices that value the environment, social justice, and sustainability. It is a guidepost for solar companies committed to pioneering a sustainable path forward and measuring improvement.

In addition to improving their scores, Jinko, Trina, and SunPower have also demonstrated leadership in developing innovative environmental programs. They have participated in Cradle to Cradle Certified™, helped to develop industry-wide recycling initiatives, and are establishing stronger chemicals management programs.

Unfortunately, the solar industry's overall environmental performance is very uneven. Although more than 50 companies have responded to the scorecard since its 2010 launch, only a small number of companies have consistently earned top ranking. More than half of the companies scored do not provide the public with any information regarding their sustainability practices.

Solar Scorecard: Version 2.0

CoRE and the Silicon Valley Toxic Coalition (SVTC) will set new chemical reduction and elimination benchmarks in version 2.0 of the Solar Scorecard in accordance with principles outlined in SVTC's Green Jobs Platform. This includes using the Chemical Footprint Project framework to measure corporate chemicals management programs and define new survey questions for the scorecard, and leveraging CPA's GreenScreen for Safer Chemicals as a best-in-class benchmarking tool.

The solar industry is frequently branded as a "green technology." However, the disparity in performance in the Solar Scorecard across companies that have clearly committed to sustainability programs and those that have not highlights the need to align industry practices with leadership and performance metrics that qualify green technologies.

Solar Scorecard Results

Out of a field of 40 solar companies that comprise more than 85% of the solar marketplace, top respondents in the 2018–19 Solar Scorecard made considerable progress and earned exceptionally high scores. For example, in 2011 Jinko Solar earned a "0" and had limited experience in chemicals management and manufacturing.[18] Every year since, through 2018–19, the company improved its score. This progress shows that it is possible to address the climate crisis with clean technology that is better designed for people and the planet.[19]

Building on a successful start, and planning for a productive future

CoRE has achieved good results since its inception just a few short years ago.

Today, we are poised to continue our groundbreaking work, and keep serving our stakeholders as we add to our impressive list of accomplishments.

Moving forward

As we align a net positive carbon economy with safer chemicals and sustainable materials, CoRE's ongoing impact stems from its emphasis on a multi-perspective, multi-organizational approach—the importance of bringing together people and resources in new, more effective ways, to drive innovation and the power of community involvement for transformational and sustained impact in the renewable energy economy.

Since 2017, CoRE has:

Brought together leaders from different sectors and organizations who are committed to building regenerative material economies that are healthier and more equitable for the industrial communities that support the development of renewable energy technologies.

- Built a stakeholder network (including SVTC and WNY SBR) to advance the CFP Survey and new pathways in the solar sector to impact procurement, supply chain management, and eventually, the industry's lifecycle.
- Convened signature workshops for partners to share, learn, and explore ideas and solutions across silos, and consider systemic changes in the use and development of materials in the solar sector; these programs provide a forum for melding science and social innovation as a catalyst for change.
    - The Erich Bloch MDI Symposium brings together leaders from universities, industry, and national labs to share approaches to developing data-driven materials and technological innovation for sustainability, with a focus on community health.
    - The CoRE Summit follows the Erich Bloch MDI Symposium and brings together solar manufacturers, installers, procurement entities, NGOs, businesses, investors, foundations, and academia, to explore issues of a regenerative solar economy.

Developed strategies to improve chemicals management, toxic chemical reduction, and sustainable materials development for solar technologies, through an approach rooted in defining, developing, implementing, and disseminating the process for measuring and reducing chemical footprints.

- Building on CPA's relationships with Apple, HP, and other technology leaders, we demonstrated how solar manufacturers can measure and reduce their chemical footprint in manufacturing, supply chains, and products.

Partnered with business, nonprofit, government, and academic leaders in the assessment, analysis, diagnosis, development, and implementation of new solutions and strategies through data-driven, materials innovation frameworks.

- Introduced Tesla, Panasonic, SunPower, and WNY SBR members to chemical footprinting.
- Advanced the Clean Production Action (CPA) Chemical Footprint Project (CFP) Annual Survey, which provides a robust framework for evaluating corporate chemicals management, including measuring a company's overall chemical footprint.

Produced a new genre of research development and engagement models for AI-driven chemistry design for sustainable solar manufacturing, using multifaceted data and tools to study the impact of solar technologies and identify pathways for wide-scale inclusion of environmental and human health considerations at the front end of high-performance materials development.

- Created a PFAS Atlas to track molecular data fingerprints for hazardous chemicals and inform safer selection.
- Established AI and machine learning tools to accelerate the material discovery phase for lead-free perovskite solar cells.

> "Clean energy is critical to solving our climate crisis. But we need to consider the full environmental and human health impacts of solar energy generation across its entire lifecycle, including mining, manufacturing, use, decommissioning, and recycling."[20]

Learn more about our progress and our outreach activities at CoreBuffalo.org

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