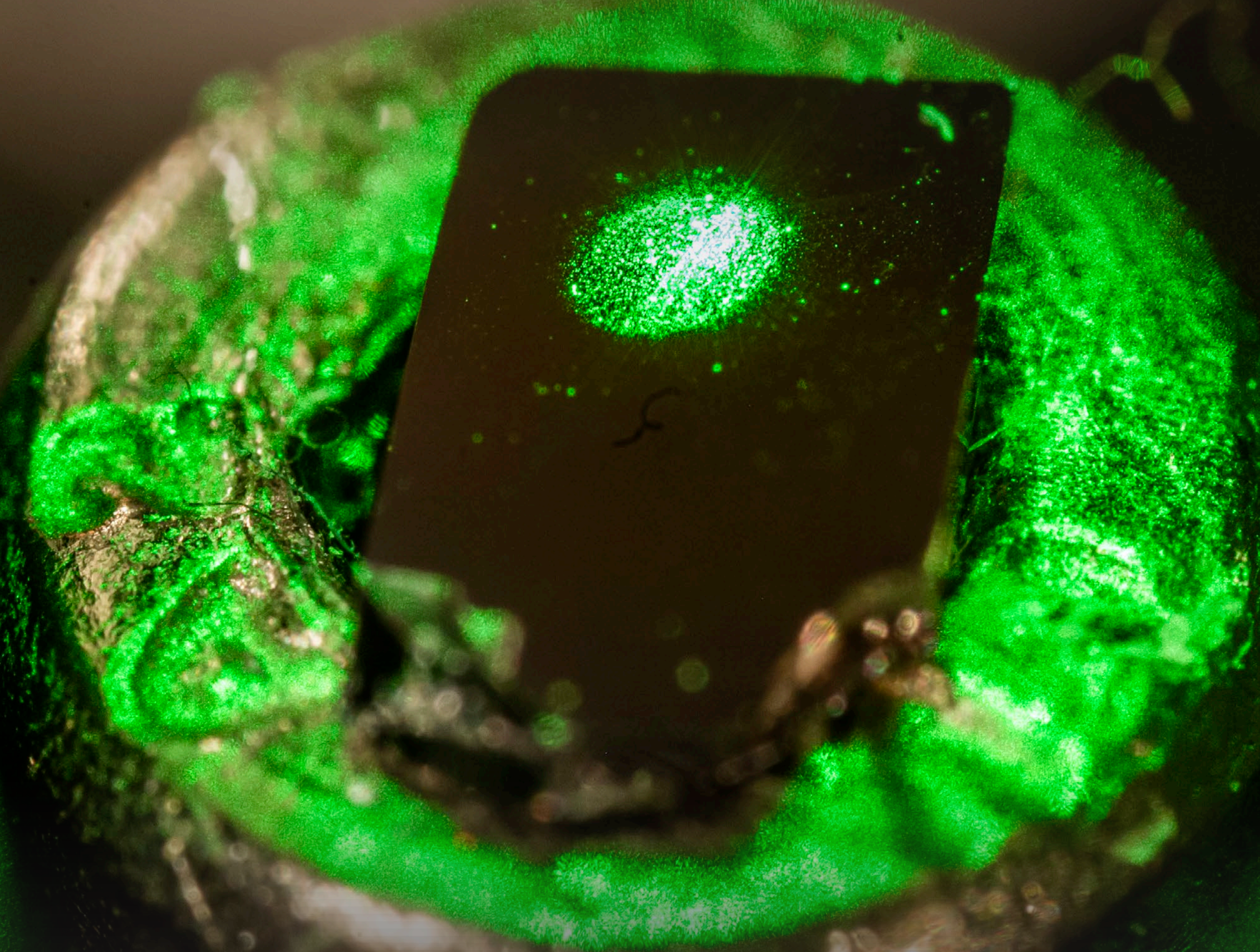
Wallenberg Initiative
Materials Science for
Sustainability

Materials science that enables a sustainable world



CHALMERS UNIVERSITY OF TECHNOLOGY

KTH VETENSKAP OCH KONST

LINKÖPING UNIVERSITY

Knut och Alice Wallenbergs Stiftelse

LUND UNIVERSITY

Stockholm University

UPPSALA UNIVERSITET

Wallenberg Initiative Materials Science for Sustainability

A research program to enable sustainable technologies with impact on our society by understanding, creating, and controlling complex materials with a precision down to the single atom level.

Authors

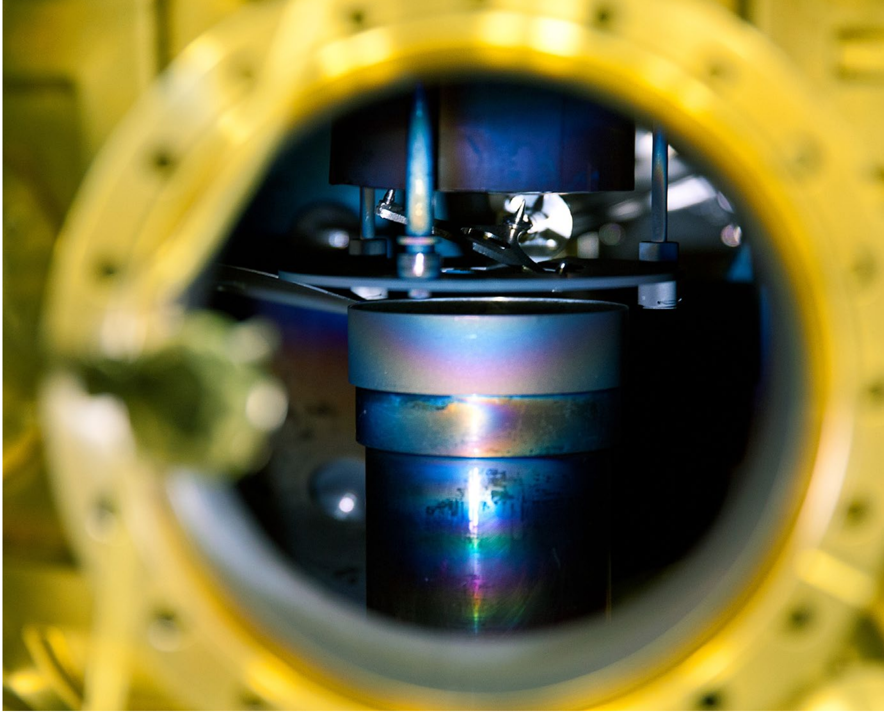
Magnus Berggren (director, LiU)
Olle Eriksson (co-director, UU)
Pontus de Laval (KAW)
Lars Kloo (KTH)
Heiner Linke (LU/LTH)
Anders Palmqvist (Chalmers)
Jan-Erling Bäckvall (SU)
Johanna Rosén (LiU)

Contact

Magnus Berggren, Director – magnus.berggren@liu.se
Olle Eriksson, Co-director – olle.eriksson@physics.uu.se

Website

wise-materials.org



Contents

Materials science for sustainability: Vision and mission

Materials provide the physical and structural basis for our highly advanced society. Major efforts conducted during the past centuries in materials science and engineering have led to complex and high-performing products, construction, and technologies. This development has enabled a society where healthcare, communication, infrastructure, and digitalization perform in a highly sophisticated and effective manner. However, the facilitating components, made from advanced materials, require energy and are traditionally derived from non-recyclable origins. The associated pollution and over-consumption of natural and mined resources has driven humanity and society into a state of imbalance versus nature, including the atmosphere, hydrosphere and biosphere. New, fundamental knowledge is thus needed to derive materials that reroute civilization onto a pathway towards a sustainable society that lives in balance with our valuable and limited resources.

WISE will address these tasks by understanding, creating, and controlling complex materials with a precision down to the single atom level. In order to accomplish this, WISE will evolve the state of the art in the design, synthesis, structuring, and characterization of properties and performance of materials and devices. Within this context, materials are here classified as both hard and soft materials in the broadest manner (*e.g.,* alloys, semiconductors, ceramics, polymers, oxides, metals, and hybrids thereof) and will be investigated and explored in WISE, excluding the fundamental studies and engineering of materials derived from the forest (already being conducted in WWSC).

Specifically, efforts will be devoted to identifying new or significantly improved materials, which provide a distinct advantage in physical, chemical, biological, or functional performance when compared to existing materials and technologies. This relates to materials that demand less resources, are less environmentally hazardous, and enable sound and efficient recycling processes. WISE will also explore materials that, when used in energy technology, generate less negative climate impact under operation, while offering high performance and efficiency when in action at large scales.


Vision

Materials science that enables a sustainable world.

Mission

To perform basic and need-driven materials science at the international forefront, to empower sustainable technologies with positive impact on society, and to train future leaders in society, industry, and academia in Sweden.

Goal

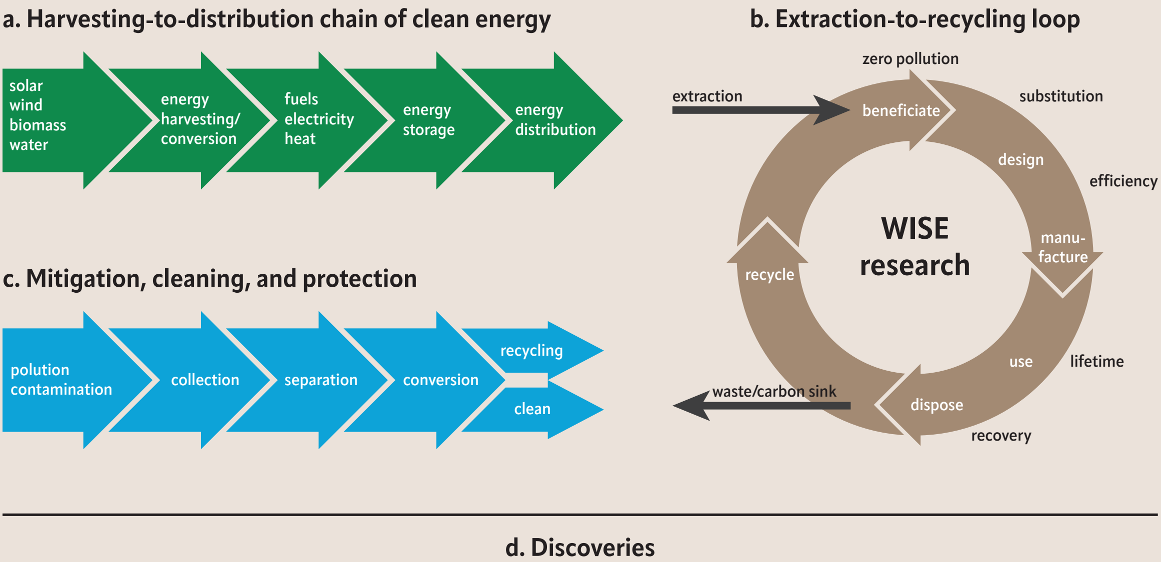
WISE will promote and activate a transition towards a sustainable society, while pushing the scientific frontier in materials science to new vistas that firmly establish Sweden as a leading nation in the field. WISE aims to explore and research advanced, functional materials targeting the following thematic areas:

- Conversion, storage, and distribution of clean energy
- Circular materials replacing rare, energy-demanding, and hazardous materials
- Mitigation, cleaning, and protection of the atmosphere, soil, and water
- Discovery of materials for novel sustainable technologies and applications


Materials and sustainability

Materials derived from renewable or non-renewable resources have profoundly affected the development of our society. The utilization of materials from natural resources in production and consumption processes can be linked to many environmental, economic, and social consequences that spread beyond national borders. The global annual use of resources amounted to nearly 90 billion metric tons in 2017 and is forecasted to double by 2050. This increase will mainly be caused by a shift in materials extraction from Europe and America to Asia and Africa[1]. Today, 60% of all materials are already extracted in Asia, and the primary production of materials accounts for a quarter of all global greenhouse emissions[2]. The repertoire of materials derived from natural resources are predominantly represented by metals, construction minerals, fossil energy carriers, and biomass[3]. The prime production of metals alone exploits about 8% of the global energy production. In addition, our dependence on raw materials from all parts of the world is associated with severe environmental, human rights, and global political issues.

Although the production and extraction of materials are connected to environmental strain, their use is paramount in transforming our world towards a sustainable society. Functional materials are simply the most important parameter in the ambitions to accomplish green growth, since they form the physical components of future, greener technologies and circular economies. An agenda is being carved out in the materials science community and in relevant industries to aid such a transformation and to promote future business and society settings.



This spearheading agenda is fully aligned with the major efforts undertaken by the international community in recent years. In 2015, the United Nations General Assembly adopted the Resolution “Transforming our world: the 2030 Agenda for Sustainable Development”. This resolution is based on five values (People, Planet, Prosperity, Peace, and Partnership) and the associated seventeen Sustainable Development Goals (SDGs) were generated to give explicit guidance for the future. In December 2015, 196 countries signed the Paris agreement which states that the rise in global mean temperature should be maintained below 2 °C, preferably <1.5 °C. With this legally binding international treaty on mitigating and combating climate change, individual countries should undertake the necessary actions to outline adequate protocols. Materials connect to nearly all the SDGs (page 28) and materials science is certainly critical for energy technology and the materials circularity of the future. The urgency in undertaking fast and firm measures was further confirmed by the recently published IPCC report[4].

The materials science community must now research and develop the performance of sustainable material technologies along the entire harvesting-to-distribution chain of green energy, throughout the complete loop of extraction-to-recycling, and for mitigation, cleaning, and protection, see figure above (parts a-c). In addition, scientific discoveries and breakthroughs in materials science (figure part d, underlying all others) are needed to make the necessary large leaps in knowledge that enable future innovations for novel sustainable technologies and applications, especially targeting improved energy efficiency. The scientific community is already on task and performing, as exemplified by several recent important breakthroughs, such as engineered living materials to manufacture bioplastics[5], near complete depolymerization of polyesters using enzymatic systems[6], electrocatalytic production of hydrogen peroxide fuels using all-organic electrodes[7], identification of new classes of superconductors with critical temperatures approaching room temperature[8], and the discovery of materials with reduced dimensionality for solar cells[9].

Overview of materials science

Materials science defines the area of research encompassing discoveries and design, along with characterization, of novel materials. All forms of materials are embraced in the field and basic science of hard and soft solids together with fluids are conducted, with activities also found in molecules in the gas state. Materials science originally stems to a large extent from metallurgy and from studies of minerals and ceramics. A proven strategy of materials research over the last few decades stands on the five pillars for combined operations of (*i*) design and modelling, (*ii*) synthesis and processing, (*iii*) structures, (*iv*) properties, and (*v*) performance. However recent high-tech materials discoveries have led to an extended classification, represented by semiconductors, functional materials, biomaterials, heterostructures, materials with reduced dimension, topological materials, and nanomaterials. With WISE, sustainability in the design, operation, and decommissioning will be integrated, thus avoiding material science based on the classical trial and error approaches.

When reviewing recent international conference calls and publications covering trends in materials science, the area can be seen to stretch out in several specific directions. Sustainability and energy technology are by far the strongest driving forces in the field today, followed by novel and high-performing materials for technology, healthcare, biotechnology and constructions. See major focus areas in the box on the next page.

The evolution of materials science, as a solitary research field, can be monitored and compared based on the total number of scientific publications gener-

Major efforts in materials science are currently focused on

- Advanced theoretical studies of materials by high-throughput calculations and artificial intelligence, combined with massive computation power, for the design of new functional materials,
- Exploring sustainable energy-enabling materials based on abundant elements and components,
- Developing green chemical and physical processes to achieve materials and nanostructures, optimizing transport and reactions of matter (gas and liquids), to improve the performance of energy technologies (e.g. batteries, photovoltaics and fuel cells), and
- Combining several advanced characterization techniques to gain deeper insights to, and validate the performance of energy and circular materials, in situ and in operandi.

ated globally. One finds that materials science currently represents close to 7% of the total output of scientific publications and the area increased by ~140% during the period 2002 to 2016. This makes materials science one of the fastest growing research areas worldwide[10]. Regarding the annual number of published articles, China, USA, and Japan hold the first, second, and third positions, respectively. They are followed by five European countries: Germany, France, England, Italy, and Spain, that position themselves within the top-20 globally[10].

Several outstanding and revolutionary discoveries have been made in materials science with immense impact on science and society. The Nobel Prizes awarding discoveries in Physics 2007 (magnetic data storage), 2009 (optical fibers), 2010 (discovery of materials with reduced dimension), and 2014 (light emitting diodes) serve as good examples, as do the Nobel Prizes in Chemistry 2007 (catalysis), 2011 (quasicrystasl), and 2019 (Li-ion batteries). Equally important discoveries are found in techniques that are crucial for characterizing materials, *e.g.*, X-ray photoelectron spectroscopy (Nobel Prize in Physics 1981), transmission electron microscopy and scanning probe microscopy (Nobel Prize in Physics 1986), and density functional theory (Nobel Prize in Chemistry 1998). These and other advances have led to an unprecedented ability to control, characterize, and understand materials.

For the tech-industry in general, functional materials for sustainability and energy applications are well represented as frontier trends of established companies as well as for start-ups. For instance, next-level process automation, future biomachines, next-generation smart materials, and clean technologies all rely directly on high-performing advanced and sustainable materials[11]. We also identify trends that typically include responsive materials, nanotechnology, additive manufacturing, light-weight materials, material informatics, and advanced composites.

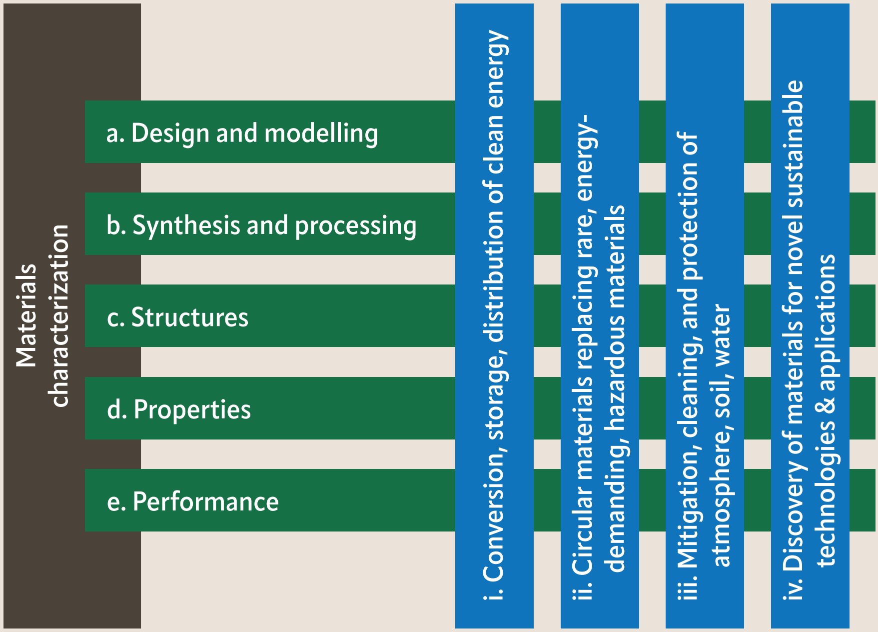
Program areas

The WISE program will address the most challenging scientific questions in materials science, as schematically illustrated in the figure on the next page. Advanced materials science must necessarily rely on design combined with simulation/theory, synthesis, nano-structuring, processing, characterization, and evaluation of properties. From a sustainability point of view, it is also highly relevant to assess the materials flows from reactants to waste, *i.e.*, how process waste and energy needs can be minimized in the recycling of critical materials, how mining of materials can be achieved with minimal detrimental environmental impact, and how to identify greener routes from mineral to material. Many challenges of our society are coupled to the transformation, storage, and distribution of energy. Technologies with small environmental impact primarily operate by the conversion of sunlight and wind to electrical power. Electrification of transport demands advanced batteries and fuel cells based on non-fossil fuels, with the ability to efficiently store energy. Hydrogen and other energy carriers are likely to contribute more to society and industry in the future, which calls for materials for reliable conversion, transport, and storage of energy.

For the reasons outlined above, four thematic areas are identified in WISE: (*i*) conversion, storage, and distribution of clean energy; (*ii*) circular materials replacing rare, energy-demanding, and hazardous materials; (*iii*) mitigation, cleaning and protection of the atmosphere, soil, and water; and (*iv*) discovery of materials for novel sustainable technologies and applications. These thematic areas overlap with five research areas, as detailed below, and will be investigated with the goal of securing technologies that support our energy and materials demanding society in an environmentally friendly fashion.

Research areas

a. Design and modelling. Theoretical methods that allow the design and modeling of new materials have matured and are used in all fields of materials science. This involves electronic structure methods based on density functional theory, molecular dynamics simulations, and Monte Carlo techniques. Lately, this field also involves data-filtering methods of huge databases, where hundreds of thousands of compounds listed – for instance in the Inorganic Crystal Structure Database (ICSD) and Cambridge Structural Database (CSD) – and screening tools are designed to extract materials with specific properties. High throughput electronic structure calculations have been a key ingredient in this development. Furthermore, machine learning methods are increasingly being used in theory-guided materials science. Although the methods used in theoretical materials research are to some extent sufficiently accurate and efficient in many areas, there is still need for major improvements in this field. As an



example, it can be noted that theoretical calculations of X-ray and electron spectroscopy pose a significant problem for existing methods.

b. Synthesis and processing. In a wide perspective, synthesis can involve many levels of sophistication from the extraction and recovery of specific elements or materials components to the designed synthesis of specific molecular motifs and materials with predicted properties, also involving composites, hybrid materials, and materials with specific topology or multi-scale ordered structures, as well as low-dimensional materials and atomic scale control. Synthesis is performed in the vapor, liqui,d or solid states. For materials to ultimately become useful in large-scale applications, aspects of sustainable and efficient post-synthesis processing and upscaling are important, *e.g.*, by heat treatments to drive secondary phase transformations.

c. Structures. This involves architectures of matter ranging from Ångström dimensions, via nanostructures and mesoscopic sizes, to macroscopic constructions and include materials-defined functions at different dimensional levels. Materials structures represent the crucial instrument to introduce specific properties and performance parameters that together form desired advanced functions for a resulting material targeting specific applications. Structures are formed, *e.g.*, via synthesis, interface engineering, self-organization, etching, and additive manufacturing. Electrode and membrane materials for fuel cells are archetypical examples of complex structures, which enable transport of reactants and components, in gas and liquid phases, along with charge transport.

d. Properties. Materials are designed and produced for a special purpose and thus target specific properties. For instance, light-harvesting materials in solar cells must provide efficient conversion of the energy of light to electric energy, with subsequent fast conduction of the energy-rich charge carriers produced, while minimizing recombination losses for ultimate high yield for usage or storage. Materials properties depend on the composition, as well as the structure and topology at different length scales. Therefore, detailed characterization of properties in relation to the structure and physical mechanisms is essential for enabling targeted applications.

e. Performance. Performance investigations represent the benchmark of a material or a device with respect to the requirements of an intended application. Examples involve investigations of high-frequency capabilities, energy consumption, and lifetime of electro-optical devices; the energy density, rate of loading/unloading and cyclability of energy storage materials; hardness, toughness, and temperature tolerance of materials for industrial tools;

and the weight, load, and durability of structural materials. Materials are also used in catalytic applications, *e.g.*, in the synthesis of organic compounds and fuels based on hydroge, and in various sustainable applications. These performance parameters must also be coupled to the environmental impact of the materials that are being used.

Materials characterization will be essential to, and integrated in, all the five research areas above. Characterization includes chemical, physical, electrochemical, spectroscopic, imaging, as well as diffraction techniques that provide an insight into the materials structure, composition, and properties, from the atomic level up to macroscales. Characterization will require everything from lab-scale instrumentations via accumulated local or regional resources, such as technology platforms, to national laboratories like MAX IV. Further, recent advances of *in situ* and *operando* methods ensure that scientists can investigate materials and couple their fundamental characteristics to performance under operation.

Thematic areas

i. Conversion, storage, and distribution of clean energy. Renewable energy from intermittent sources, such as solar and wind power, needs to be harvested and converted into suitable energy-rich carriers that can be readily used or efficiently stored and transported. In this context, hydrogen produced from water electrolysis and fuels produced using CO_2 as source are examples that pose significant materials challenges. In order to handle the lack of balance in supply and demand of energy and power, energy storage solutions are critically needed and, in this aspect, low-cost materials with high energy storage capacity are required. This includes batteries and supercapacitors for storage of electricity. It also involves catalytically active materials for the conversion and storage of energy in chemical forms, such as hydrogen and redox-active molecules, including the storage of thermal energy, *e.g.*, using the energy embedded in molecular isomerization. Many of the existing materials used in these applications include noble, rare, and non-sustainable elements that rule out implementation on a global scale, with the consequence that there is a significant need for the exploration of sustainable alternatives. Functionalized, porous, structured materials have recently seen significant progress regarding for instance enabling the replacement of noble metals as fuel cell catalysts. Finally, energy must be distributed and used as efficiently as possible. Higher quality, wide band-gap semiconductors will help to reduce losses in power conversion, and novel electronic materials will allow efficient use of electricity in computing, data transfer, and appliances, breaking the current rapid growth in global electrical power consumption.

ii. Circular materials replacing rare, energy-demanding, and hazardous materials. Many commercial actors rely on technologies that operate by use of materials associated with challenges in terms of sustainability, *i.e.*, materials that involve critical or environmentally hazardous elements, that are extracted under dubious mining conditions, or cause a negative environmental impact in other ways. Emphasis will be devoted to investigating metals, ceramic materials, and other construction and engineering materials from a clean energy point of view, in particular targeting new materials systems formed under CO_2 neutral conditions (*e.g.*, green steel). This thematic area also involves research on bioplastics, developed materials systems from the forest, and light composites and their applications. Further, examples under this thematic area involve cobalt, a critical element that for instance is used in hard metals (tungsten carbide in a cobalt matrix) and cobalt oxide-based materials used as electrode materials in the best performing Li-ion batteries. Permanent magnets used in wind power plants highlight another example, where primarily controversial mining, extreme Chinese dominance of the world market, and the price of rare-earth metals pose major challenges. Therefore, new technologies based on sustainable materials and processes for materials recycling represent key targets for sustainable development.

iii. Mitigation, cleaning and protection of atmosphere, soil, and water. Emissions to the environment from human activities represent the main source of pollution problems. Over the past decades, materials science has provided technical solutions to efficiently abate emission of, for instance, volatile organic compounds, SOx, and NOx by conversion over catalytically active, nanostructured, and porous materials. Now, the global concern is focused on strategies for the collection and conversion of CO_2 to mitigate the anthropogenic global warming effects. Designed materials for selective absorption and chemical conversion are central to such strategies, for instance involving versatile energy carriers, such as methanol or hydrogen, obtained from renewable energy sources. In this area, both photocatalysts and enzymatic conversion have shown progress, but challenges remain, and more efficient materials are needed. Mitigation of point source emission will also demand novel materials, for instance regarding the capture of CO_2. Existing polluted sites in soil, at sea, or in the air will require further development of cleaning processes based on materials optimized for specific separation or extraction of targeted pollutants from the exposed matrix. In the long-term perspective, replacement of existing technologies giving rise to environmental hazards will rely on the discovery of completely new materials.

iv. Discovery of materials for novel sustainable technologies and applications. Discoveries will be an integral component in thematic areas i to iii. However, in this fourth thematic area we want to emphasize the importance of breakthrough research. Over the next fifty years, we can be certain that new technologies and applications will and must emerge, enabled by breakthrough discoveries of materials with novel and advanced performance and properties. Such discoveries will typically be unforeseen, unplanned, and emerge from side-projects to larger programs. A scientific freedom for the unforeseen discoveries of new materials must therefore be a significant ambition of a visionary scientific program. For this reason, we propose to devote 20% of the budget to high risk and high reward research, with a 10+ year perspective regarding sustainable applications. It is foreseen that research within WISE will explore and advance the understanding of materials for information technology systems and high-tech devices that use orders of magnitude less energy; affordable solar cells with power conversion efficiency near the theoretical limit; design of implicit properties in technology, construction, and consumable materials that can be converted and disassembled into desired units and precursors allowing a conversion from today's linear to sustainable circular materials flows; upscaling and processes for advanced functional materials to enable large scale sustainable technologies; superconductivity at room temperature, which alone would solve a series of energy-related challenges; and high energy density storage far beyond existing limitations. Ever since the industrial revolution, large scale production of chemicals via catalysis has enabled affordable products and increased the standard of living, where the catalytic production of ammonia for ultimate use in fertilizers may be the clearest example of societal impact. Materials play a key role in catalytic processes enabling sustainable chemical synthesis of base- and fine chemicals, as well as fuels that in the future can become sustainable.

Needs in society and industry

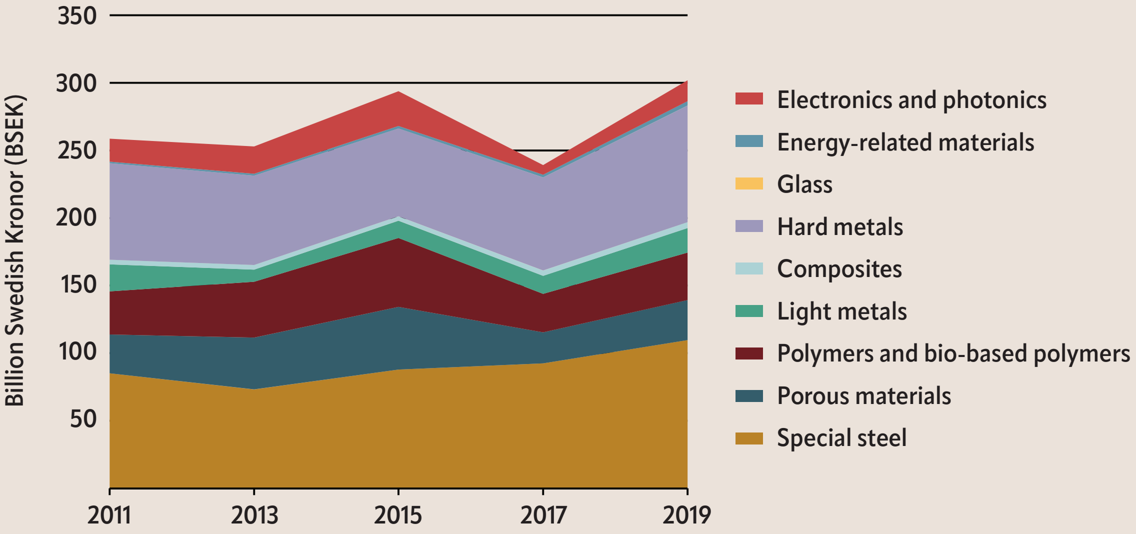
Advanced materials play a significant role in Swedish society, with forest, mining, steel, and chemical industries playing a vital role in building our nation's wealth. Advanced materials and materials science and technology will also play a decisive role for our transition to a sustainable society, *e.g.*, for electrifying transport, decarbonizing steel production, and giving us new sustainable materials from the forest. Examples include the Hybrit and H2GS initiatives with direct reduction of iron ore using hydrogen, Northvolt's large investments in new battery technology, and AB Volvo's investment in fuel cell technology for heavy transportation.

Industry has a long tradition of collaboration with academia through joint projects, sharing technology platforms and laboratories, as well as recruitments. Three examples of the latter are ABB with their electrical insulator laboratory in Västerås, Testa Center (a testbed for biological production) in Uppsala, and Swerim, the steel, metal, and mining industries joint research center in Luleå and Kista.

The Swedish industries working with advanced materials have recently been investigated by Faugert & Co on behalf of the Swedish Association of Advanced Materials (SAAMs) and funded by the Swedish Foundation for Strategic Research (SSF). Their findings were published in a report[12]. Data and insights in this section originates primarily from this report. Here, "advanced materials" are divided into nine categories: electronics and photonics, energy related materials, glass, hard materials, composites, light metals, polymers including biobased polymers, porous materials, and special steel.

Special steel and hard materials (primarily hard metals for metal cutting and mining) are the dominant areas for industry with roughly two thirds of the total revenue. The industries in glass are small, only 90 MSEK 2019, but show the strongest growth since 2011 together with energy related materials. In total, Swedish industries with a direct dependance on advanced materials have an aggregated revenue of approx. 300 BSEK. This should be compared with a total revenue of 9500 BSEK for Swedish industry (3.2% industry with advanced materials). However, the indirect coupling of advanced materials to other industry sectors should not be underestimated.

Electronics and photonics. Sweden had a significant semiconductor industry with both Ericsson and ABB operating their own silicon foundries. However, during the late 1990s and early 2000s these foundries were closed as both Ericsson and ABB could more efficiently source their semiconductor needs



Reproduced from Ref. 12

from external vendors. In the aftermath of these shutdowns several small niche companies emerged producing a wide range of semiconductor related products (sensors, lasers, RF electronics, etc.) and process equipment. A brief survey has been made by Electronic Products & Systems identifying more than 80 companies with a total revenue exceeding 5 BSEK. Research interests from industry are in various semiconductors (Si, SiC, SiGe, GaN, etc.) but also new materials for heat transport (graphene etc.). Recent semiconductor shortages in industry have emphasized the importance of the area and the need for a national competence base.

Energy related materials. This area includes materials for batteries, fuel cells, and solar cells, as well as production and handling of hydrogen. The industry in these fields is today small but shows substantial growth. Interesting examples include Northvolt that develops and produces Li-ion batteries, the Hybrit project (LKAB, SSAB, Vattenfall) using hydrogen for direct reduction of iron ore, and Powercell producing fuel cells. The revenue from this industry is estimated to 3.2 BSEK in 2019. Examples of research interest from this industry relate to new battery material combinations, membranes, bipolar plates, catalysts for fuel cells and electrolyzers, materials for storing and handling hydrogen, and more efficient materials for solar cells.

Glass. The main developments in the industry involve chemically hardened glass and multifunctional glass. Hardened glass is used in mobile devices, cameras, car windows, etc., while multifunctional glass is used for instance in smart windows and eyeglasses. This industry is quite small in Sweden, with approx. 90 MSEK revenue in 2019, but exhibits a fast growth. The main industrial R&D efforts are focused on controllable glass (*e.g.*, PDLC, SPD), adaptable glass (*e.g.*, photochromatic, thermochromic), and hardened glass.

Hard materials. Hard materials in industry consist of sintered powder metallurgical composites of tungsten carbide particles (>80 vol%) and binding materials such as cobalt. They are used in applications where strength and durability in harsh conditions and at high operating temperatures (800–1000 °C) are important, *e.g.*, in metal cutting and mining/rock drilling. Swedish industry is traditionally very strong in this field with several world leading companies, *e.g.*, Sandvik, Epiroc, and Seco Tools with revenues exceeding 85 BSEK. Examples of industrial research in hard materials include hard metals with new macro-gradients and/or self-hardening properties for rock drilling, metal cutting inserts with alternative binders, and hard metal coating properties for machining of metals, as well as new wear-resistant coating materials. In this sector (metal cutting and rock drilling) polycrystalline diamond materials, as well as new processing techniques such as additive manufacturing of hard metals, are also studied.

Composites. Composites in this context are represented by fiber-reinforced polymers where fibers are primarily made from carbon or glass. Examples of applications in industry are high performance carbon fiber composites for aeronautics and space and low-cost glass fiber composites for leisure boats. Swedish industry showed a revenue of approx. 4 BSEK in 2019. Examples of industrial research in this field involve composites with very high surface accuracy (laminar flow in aeronautics), nanomaterial reinforced composites, and conductive composites.

Light metals. The most industrially relevant light metals are aluminum, magnesium, titanium, and their alloys. Characteristics are light weight, high strength, and stiffness often combined with good corrosive properties. Another important light metal is lithium for batteries. Swedish industry is strong in both mining, producing, and processing the required minerals for these light metals with an estimated revenue of 18 BSEK in 2019. Examples of industrial R&D in this field is concentrated to new alloys, additive manufacturing in, and reduced CO_2 footprint of the production processes.

Polymers and bio-based polymers. Polymers can be divided into three areas: bulk polymers for consumer goods (*e.g.,* bottles, clothes, plastic bags), high performance polymers for industrial use (*e.g.,* insulators, bearings, implants), and bio-based polymers where the raw materials come from bio-based processes. Swedish industry is strong in the field with a total revenue of 35 BSEK in 2019. Examples of industrial research in this field are bio-based polymers, additive manufacturing, polymers for electrical applications, and recyclable polymers.

Porous materials. Porous materials are materials that contain voids and pores for various functionalities. These voids are created, by nature or artificially, using a molecular or supramolecular assembly as structure-directing agent. A wide variety of materials are found in this category, ranging from synthetic zeolites, metal-organic frameworks and metal oxides, to activated and synthetic carbons, as well as polymers and paper. Typical applications of porous materials include filtration or absorption of fluids and gases and catalytic conversion. Swedish industry is strong in this field with an estimated revenue of 30 BSEK in 2019. Examples of industrial research are in nanocellulose, nanopores, catalysts, and membranes.

Special steel and powder metallurgy. Special steel encompasses steel alloys designed for special purposes, *e.g.,* stainlessness, heat resistance, or desired magnetic properties. The Swedish steel industry has over the years become more and more focused on such special steel niches with considerable achievements – in many cases reaching a world leading position. Metal powder is used in a wide variety of applications, such as additive manufacturing, soldering, magnetic composites, and surface treatments. The revenue from the Swedish steel industry exceeded 100 BSEK in 2019 with a steady growth over the last years. Examples of large R&D efforts in this industry include the ambition to make the production process CO_2-free by using hydrogen for direct reduction of the iron ore (*e.g.,* Hybrit, H2GS), high-strength steels, and high-entropy alloys.

"This is a powerful, hands-on initiative for a more sustainable world"

"This is a powerful, hands-on initiative for a more sustainable world. Knut and Alice Wallenberg Foundation is allocating just over SEK 3 billion over an twelve-year period to build knowledge contributing to the achievement of the targets set under UN Agenda 2030 and the Paris Agreement.... This long-term research initiative is intended to make possible a more sustainable future, to make the Swedish forest sector more competitive, and to pave the way for new enterprises based on innovations in this field."

PETER WALLENBERG JR
Chair, Knut and Alice Wallenberg Foundation

"Industry needs to transition towards sustainability at a swifter rate"

"To meet climate and environmental targets industry needs to transition towards sustainability at a swifter rate. For this reason, the research program will be conducted in collaboration with Swedish industry in the form of industrial PhDs and postdocs, and also via research arenas allowing an exchange of knowledge and problems between academia and private enterprises. Industry acquires knowledge generated by research in materials science, and researchers gain insights into the technological and application challenges faced by companies."

SARA MAZUR
Chair, WISE Board and Director of Strategic Research, KAW

Faculty & research constellations

WISE includes six universities, which together form a complete and complementary knowledge base to successfully execute the core activities in research and education. Below, a summary of the key environments are outlined.

Chalmers. Research contributes to the program areas and all methodological aspects of the WISE program, outlined in the figure on page 11). Notable activities relate to materials for energy conversion and storage, and cover solar cells, molecular solar thermal, thermoelectrics, batteries, supercapacitors, fuel cells, and electrolysis and catalysis. Other areas of expertise include advanced theoretical modeling, synthesis and characterization including use of large-scale synchrotron and neutron facilities. The research is carried out at the departments of Chemistry and Chemical Eengineering, Physics, MC2, and IMS. Researchers active in these areas are also supported by, *e.g.*, the SFOs in Materials Science, Nanoscience and Energy, and the European Graphene Flagship hosted by Chalmers.

KTH. Materials science is virtually organized under the KTH Materials Platform and represents a wide spectrum of scientific areas involving more than 80 research groups and in total over 1000 researchers at different levels, spread over all five schools and several departments. Much research can be linked to existing applications or industry, such as mining, electronics, and forest industry. However, studies on fundamentally new materials are also pursued, involving synthesis, characterization, and theoretical modelling. The materials research can be divided into six thematic areas: polymer materials, emerging materials, materials for energy applications, sustainable material, engineering materials, and materials for information and communication technologies.

LiU. Materials science, including the perspective of sustainability, involves more than 400 scientists. Thematic areas comprise theoretical modelling, synthesis and characterization (spectroscopy, microscopy) of advanced functional ceramics, inorganic and organic semiconductors along with soft functional materials, including thin films, mixed ion-electron conductors, nanoparticles, low-dimensional materials, organic electronics, and photonic materials. Activities are found in the divisions of the Laboratory of Organic Electronics, Semiconductor Materials, Thin Film Physics, Materials Design, Theoretical Physics, Electronic and Photonic Materials, Nanostructured Materials, and Mechanical Properties of Structural Materials. Application targets of the materials science at LiU include large area energy harvesting, internet-of-things and massive scale energy storage and conversion, hard and lightweight technological materials, and high-power components.

Lund University

Stockholm University

Uppsala Universitet

LiU is home to the SFO Advanced Functional Materials.

LU. Materials science is a strong strategic focus of LU, which also hosts MAX IV, and has decided to establish a significant part of its research and education in physics and chemistry in the immediate vicinity of MAX IV. With this major investment, LU will help realize the Swedish government's ambition to establish a leading international centre for materials sciences in Science Village. The university's Centre for Nanoscience (NanoLund) has a strong core competence in semiconductor and metal nanostructures and comprises around 400 scientists, including almost 150 PhD students. Application areas include sustainable information technology, energy conversion devices, safety of nanomaterials, and devices for personalized medicine. LU research groups also have key competences in biomaterials, fuel cells, energy research, structural and building materials, and in circular material flows.

SU. Research within material science at SU has a strong focus on developing new materials for a sustainable society, employing green synthesis, and sustainable processing routes. Materials Chemistry and Catalysis in Organic Chemistry are two of the profile areas at SU. There is a strong expertise in polymers, porous materials, energy-related materials, and composites with focus on developing sustainable catalytic processes for organic synthesis, renewable materials, CO_2 and biomass conversion, and materials recycling. Studies are also done on surface reactivity relevant for catalysis to move the chemical society towards sustainable hydrogen feedstocks from fossil sources to water electrolysis. The research is found at the Departments of Materials and Environmental Chemistry, Organic Chemistry, and Physics. The materials development and applications are strongly coupled to methodologic developments of advanced characterization techniques with synchrotron facilities (including ultrafast characterization of surfaces) and cutting-edge electron microscopy and diffraction.

UU. Research is focused on materials for light harvesting (artificial photosynthesis and semiconducting solar cells), energy storage (batteries and metal hydrides), as well as magnetic materials for energy conversion. Expertise exists in advanced theoretical modeling, synthesis, and characterization as well as development and use of large-scale facilities (*e.g.,* Tandem lab and MAX IV). Studies in assessing the flow of critical materials required for a sustainable energy transition are also pursued, in particular, when and why this can be a problem, and how this can be avoided through measures such as substitution and recycling. The research is found at the departments of Engineering Science, Physics, and Chemistry, all hosted at Ångström Laboratory, and at the Department of Geoscience. Curiosity driven materials science, *e.g.,* in spintronics, that can only have impact for green technologies in a longer perspective, are also pursued in experimental and theoretical groups. Excellence markers of this activity can be identified, *e.g.*, in that UU is the host of the flagship program Battery 2030+ and SNIC (the National Infrastructure of High-performance Computing).

Across the six universities, and within the areas of materials science described above, in total 12 scientists have been selected as Wallenberg Scholars, 30 scientists have been selected as Wallenberg Academy Fellows, and 76 scientists have been awarded an ERC starting, consolidator, advanced, or synergy grant.

Science and technology platforms

Technology platforms represent important enabling facilities for the progress of science. WISE aims to fill the gap between individual instruments and large-scale national or international facilities. An inventory of existing technology platforms of relevance to sustainable materials is shown to the right. As noted, rather few labs of instrumentation, aiming at the synthesis or characterization of materials for sustainability, presently qualify in the platform scope window defined, and thus such resources need reinforcement driven by both the universities and WISE in concert. Support to the individual universities may involve both the further development of existing labs and/or the investment in instrumentation for new ones. A large part of the support should be offered early in the program. Already in the first year of the program, the universities should be offered the possibility to define their needs in terms of one or a few coherent labs for sustainable materials with the ambition to serve a significant and well-defined researcher community at local, regional, or national level. A clear added value for the synthesis or characterization of materials for sustainability represents a must requirement. Further, state-of-the-art technology platforms should also attract international young and established scientists.

MAX IV, MyFab, Tandem Lab, and supercomputer centers represent research infrastructures essential to many materials researchers at the Swedish universities. The universities should be able to apply for dedicated instrumentation at these facilities as a part of the technology platforms.

A fundamental requirement in the proposals from the universities should be a guarantee for base support to the existing or planned technology platforms (including machine workshops, lab space, electrical/gas/water connections, and research engineers/staff), so that the outcome of the KAW investment can be maximized.

	Existing platforms	Proposed new platforms
CHALMERS UNIVERSITY OF TECHNOLOGY	– Mass-spectrometry – Materials Analysis Laboratory – Nano Fabrication Laboratory – SEEL-batteries and fuel cells	– [T.B.D.]
KTH VETENSKAP OCH KONST	– Albanova Nanolab – Hultgren Lab (metals) – Odqvist Lab (engineering)	– [T.B.D.]
LINKÖPING UNIVERSITY	– Additive processing – Soft functional materials – Advanced functional ceramics – Electron microscopy	– Scanning probe for soft functional materials – *In situ* and *operando* electron microscopy
LUND UNIVERSITY	– In-situ electron microscopy – Semiconductor nanofabrication – *Operando* scanning, electrical, and optical probes	– Nanolab Science Village: equipment enabling synthesis, structuring, and characterization of sustainable materials
Stockholm University	– Green chemistry – Electron microscopy – Lab on porous materials – Heterogenous catalysis for the synthesis of fine chemicals	– *In situ* and *operando* liquid phase electron microscopy and cryo-EM for soft matter – [T.B.D.]
UPPSALA UNIVERSITET	– Solar Cell Laboratory – Tandem Lab – SuperADAM (ILL)	– Compact X-ray source – Sustainable synthesis

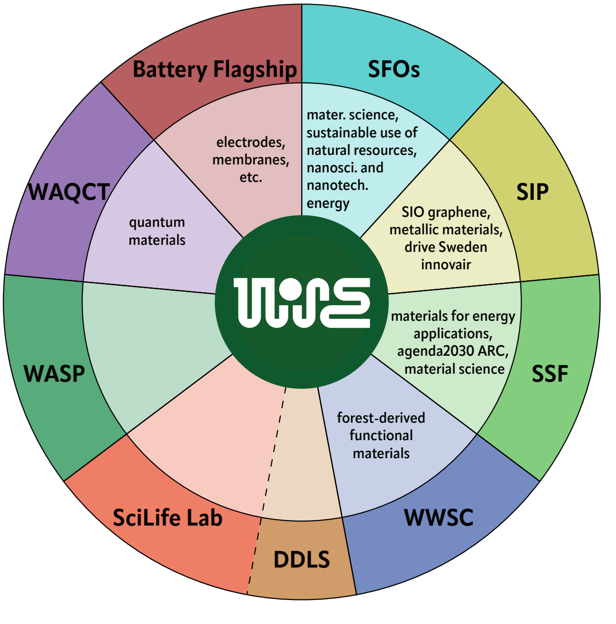
– Interoperable lab booking system(s) (cleanroom facilities for micro- and nano-structured advanced materials)
– SNIC, Berzelius, MAX IV

Relation to other program initiatives

WISE will stand on its own regarding excellence of materials science for sustainability. However, materials science, just as science in general, will benefit from cross-disciplinary collaborations. Major excellent research programs in other areas are currently in operation in Sweden, which are financed by KAW, as well as by other funding agencies (see figure on this page). As sustainability is critical in all aspects of society and science, and where cross-disciplinary activities can be justified by the outstanding research to be conducted, there is an opportunity for WISE to reach out to identify interfaces for collaborations and complementary activities. Several opportunities for joint projects are foreseen with the existing KAW programs, where interfacing or significant complementing activities can be identified. For instance, in the Wallenberg Wood Science Center (WWSC) biomaterials from the forest are researched, with several activities leading to advanced materials for consumer, technology, and energy materials. Further, in SciLifeLab, within the Data Driven Life Science (DDLS) program, research is conducted with the use of the Berzelius Supercomputer initiative at NSC in Linköping, where materials science relevant to green chemistry, medtech, and diagnostics is also included.

For these reasons, several opportunities for joint activities with WASP, WWSC, and SciLifeLab will be justified and possible. The activities in the quantum technology program WAQCT are also relevant for WISE, specifically targeting quantum materials. The national landscape of relevance to materials science also includes the Vinnova SIPs, the well-established SFOs, and different SSF initiatives in materials science and sustainability.

Further, the science generated in WISE will be evaluated for start-up and commercialization activities, which mandates that the program will reach out to innovation support offices, investment funds, and for support to patent.



Strategic recruitments

Sweden is at the international forefront in various research areas of importance for WISE. The profiles of the universities complement each other, which means that planned strategic recruitments will evolve around different research topics, all providing a unique possibility to strengthen and renew competence.

The aim with new recruitment is to attract outstanding international candidates that increase the competence level of universities participating in WISE. There are two main strategies: either to couple to and to strengthen existing research areas, or to establish entirely new research areas by recruiting world-class researchers. Both strategies will include recruitment of researchers at the level of Assistant or Associate Professor, targeting "rising stars". Recruitment strategies will be flexible and allow, if needed, for the recruitment of full professors or part-time guest professors. The successful candidates are expected to place their absolute majority of time in residence at a campus in Sweden, rather than holding honorary appointments from distance.

The budget of the packages allows for 25 strategic recruitments, each comprising a recruitment package of two PhD students and two post-doctoral fellows. Moreover, the WISE environment will also provide state-of-the-art infrastructure. The recruitment process will be aligned with the strategic recruitment plans of the university, to ensure additional, long-term, faculty funding.

All partner universities will make a strategic plan for faculty recruitment within WISE. The process for recruitment (including choice of research area) will be defined by the WISE Steering Group (see page 27).

+25

Postdoc and PhD recruitment and graduate school

The aim is to establish a joint postdoc and graduate school in 2022, which will reaches full capacity in 2023, when all of the first 50 PhD students and 50 postdocs will have been enrolled. In addition to the 50 PhDs and 50 postdocs recruited through the strategic recruitment packages (page 23), WISE will enable recruitment of 130 PhDs (30 of which industrial) and 130 postdocs (also 30 of which industiral). The research topic of each individual position will be defined through an application process, to which senior researchers of the environments above (page 18) will be invited to take part. Projects of relevance in this process are those outlined in the figure on page 11, and all project proposals will be evaluated critically to assess scientific quality and relevance with respect to the mission of WISE. Announcements and evaluations will be coordinated and executed by the WISE Steering Group (see page 27). Supervision of PhD students and postdocs will be performed by the main applicant, together with co-supervisors within the hosting university, and ideally, also with co-supervision residing at other universities nodes in the WISE program.

The organization of the postdoc and graduate school will consist of a director and assisting local support at the partner universities. The school director will be responsible for operating the school, organizing seminars, and outreach activities, where the latter will involve engagement of the recruited postdocs to organize events. These events will include hosting prominent lecturers, workshops at the different partner universities, visits and training at technology and industry research platforms, as well as study visits to relevant industries and institutes.

The postdoc and graduate school will provide a multi-disciplinary academic arena for PhD students, industrial PhD students, and postdocs. The intent is to stimulate research collaboration and networking among the young scientists in the WISE program, both within academia and industry. Further, there will be flexibility allowing double-degree programs for PhD students, involving Swedish universities beyond the partner universities as well as international universities.

+180

+180

"Functional materials [are] the key component in developing green energy technologies"

"I see functional materials as the key component in developing green energy technologies of the future, enabling us to achieve circular solutions to the challenges we face. The aim of the program is to understand, create and control complex materials systems right down to atomic level so we can develop sustainable innovative technologies."

MAGNUS BERGGREN
Director of WISE and
Professor at LiU

"An incredibly important initiative for research in materials science in Sweden"

"This is an incredibly important initiative for research in materials science in Sweden, and the focus on new functional materials is particularly exciting, being the foundation for new technologies for a sustainable society. A strength of the WISE program is its cross disciplinary nature that encompass the three pillars modern materials science stands on: synthesis, characterization, and simulation."

OLLE ERIKSSON
Co-director of WISE and
Professor at UU

WISE Research Arenas (WIRA)

In order to assure that the mission of WISE is relevant for the challenges of our society and environment, industrial prerequisites must be considered. Those include producibility, up-scaling, tech-parameters, system design, lifetime, and stability, along with standardization, regulatory, and other crucial protocols. Research arenas (WIRAs) will therefore be identified and established in WISE, into which materials scientists and engineers from academia and industry jointly explore materials science for sustainability, aiming at bridging fundamental science with societal/industrial needs. A WIRA is defined as a research or development setting (the area of production and design may also apply), established in industry or in any other organization outside academia. A WIRA will serve as a laboratory or development resource where research results can be explored, evaluated and positioned in the context of industrial applications and societal needs. In addition, WIRAs gives access to industrial infrastructure and knowledge, promoting a successful implementation of novel materials in technologies. WIRAs will also give industry a straight avenue to express needs, identify challenges, and explore opportunities, in dialogue and collaboration with researchers at academia. In this collaboration, the aim will be to spark new scientific topics, identify new high-tech activities and establish collaboration between industry and academic partners. In addition, industry will contribute with resources and expertise to evolve science into materials technology systems for applications.

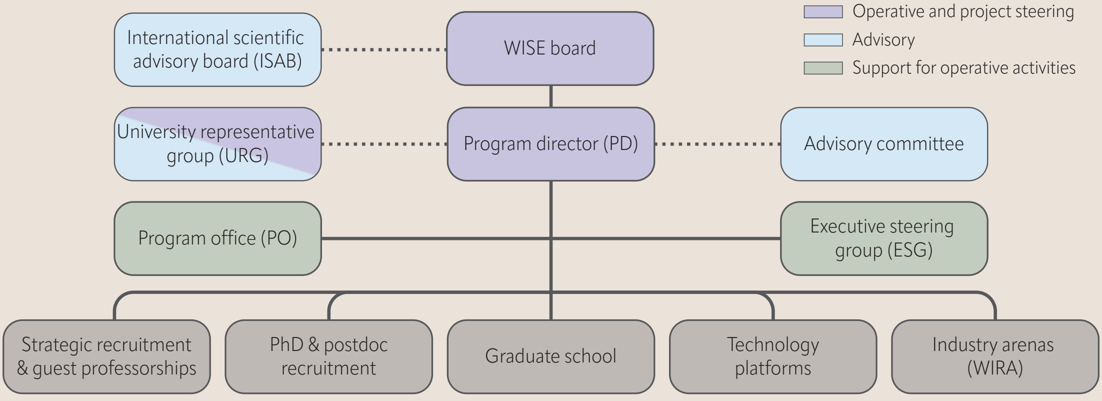
WIRAs are suggested to be defined as a platform, composed of several materials science disciplines and technologies, combined with several industrial techniques and platforms, targeting one specific sustainability theme, positioned in one the four thematic areas (see pages 11–13). WIRAs could, for example, include (*i*) recyclable bioplastics for the manufacturing industry, involving synthesis, structuring, additive manufacturing processes, etc., having industry members from plastic, recycling and food industries onboard; (*ii*) electrical energy storage for mobility, involving theory, modelling, synthesis, and structuring of novel electrode and membrane systems for green energy storage and materials for power transfer, also comprising automotive, power, and grid industries; (*iii*) energy-efficient information processing, involving materials enabling energy efficient data storage, handling and transfer, AI and autonomous systems (*e.g.*, neuromorphic computing) including electronic and automotive industries; and finally (*iv*) high-performing green steel materials, twinning theory, metallurgy, characterization, and adaptive processing (heat treatment, forming, welding, cutting, coating, etc.) with the steel, construction, and automotive industries.

Organization

The structure of the steering and management organization is shown below. The WISE Board consists of a chair (Sara Mazur), a vice chair, six host university representatives (Chalmers, KTH, LiU, LU, SU, and UU) and four industry representatives (*e.g.*, from areas focusing on manufacturing, recycling, high-tech, energy, and/or steel). The board will have the overall responsibility for the center and will be advised by an International Scientific Advisory Board (ISAB).

The Executive Steering Group (ESG) will be led by the Program Director (PD, Magnus Berggren, LiU) and co-Director (Olle Eriksson, UU) and will include input from six host university representatives (URG). The ESG will report directly to the WISE Board. The PD/ESG will perform executive tasks decided by the board, such as decisions on the conditions and criteria of funding calls, the structure and composition of evaluation panels, appointment of the Director of the Graduate School, and funding decisions based on the recommendation by the panels. A Program Office (PO) will aid with coordination, accounting, reporting, event management, and communication.

The basis for funding decisions will be prepared by evaluation panels, tentatively one panel for strategic recruitment and guest professors, one for PhD student and postdoc positions, and one for funding of technology platforms. The panels will consist of members from the participating universities, as well as external members.



UN Sustainable Development Goals (SDGs) from a materials science perspective

1 NO POVERTY	Affordable materials able to be produced and recycled, enabling economic advancement
2 ZERO HUNGER	Materials for safe and increased productivity of food, at the same time reducing food waste
3 GOOD HEALTH AND WELL-BEING	Materials enabling good health and protection against hazardous compounds
4 QUALITY EDUCATION	Affordable low-tech and high-tech materials for life-long learning and education
5 GENDER EQUALITY	Materials enabling affordable security technology empowering women
6 CLEAN WATER AND SANITATION	Materials to capture, clean, transport, pressurize, filter, purify, store, and detoxify water
7 AFFORDABLE AND CLEAN ENERGY	Green materials for efficient technology and infrastructure to harvest, transport, store, and convert energy
8 DECENT WORK AND ECONOMIC GROWTH	Resource-efficient use of materials for processes enabling an increased value of (raw) materials
9 INDUSTRY, INNOVATION AND INFRASTRUCTURE	Construct and operate infrastructure from sustainable functional materials
10 REDUCED INEQUALITIES	Improved extraction and ennobling methods for rare raw materials and developing replacement materials
11 SUSTAINABLE CITIES AND COMMUNITIES	Settlements built up from materials that are safe, resilient, and sustainable
12 RESPONSIBLE CONSUMPTION AND PRODUCTION	Efficient (re)use/recycling of (natural) materials for sustainable production/ consumption with lower chem release into soil, air and water
14 LIFE BELOW WATER	Materials to protect and develop oceans, targeting marine ecosystems and food production
15 LIFE ON LAND	Materials promoting reforestation, enrichment of soil, and restoration/ maintenance of biodiversity

Glossary

BSEK Billion Swedish Kronor
CSD Cambridge Structural Database
DDLS Data Driven Life Science
ERC European Research Council
GaN Gallium Nitride
H2GS H_2 Green Steel
ICSD Inorganic Crystal Structure Database
IEI Department of Management and Engineering
IFM Department of Physics, Chemistry and Biology
IMS Department of Industrial and Materials Science
IPCC Intergovernmental Panel on Climate Change
ISAB International Scientific Advisory Board
ITN Department of Science and Technology
KTH Royal Institute of Technology
Li-ion Lithium ion
LiU Linköping University
LU Lund University
MC2 Dept. of Microtechnology and Nanoscience
MSEK Million Swedish Kronor
NOx Nitrogen Oxides
NSC National Supercomputer Center
PDLC Polymer Dispersed Liquid Crystals
RISE Research Institutes of Sweden
SAAMs Swedish Association of Advanced Materials
SFO Strategic Research Areas (*Strategiska Forsknings Områden*)
SDG Sustainable Development Goals
SIP Strategic Innovation Programs
SiC Silicon Carbide
SiGe Silicon Germanium
SOx Sulphur Oxides
SPD Suspended Particle Device
SRA Strategic Research Areas
SSF Swedish Foundation for Strategic Research (*Stiftelsen för Strategisk Forskning*)
SU Stockholm University
UN United Nations
UU Uppsala University
WAQCT Wallenberg Center for Quantum Technology
WASP Wallenberg AI, Autonomous Systems and Software Program
WIRA WISE Research Arenas
WISE Wallenberg Initiative Materials Science for Sustainability
WWSC Wallenberg Wood Science Centre

References

1. Olivetti and Cullen. Toward a sustainable materials system. *Science* **360**, 6396 (2018)
2. Pauliuk, *et al*. Global scenarios of resource and emission savings from material efficiency in residential buildings and cars. *Nature Communications* **12**, 5097 (2021).
3. Green Growth Strategy, OECD Report 2021.
4. Intergovernmental Panel on Climate Change (IPCC) Report. Climate Change 2021: The Physical Science Basis.
5. Elshkaki. Sustainability of emerging energy and transportation technologies is impacted by the coexistence of minerals in nature. *Communications Earth & Environment* **2**, 186 (2021).
6. DelRe, *et al*. Near-complete depolymerization of polyesters with nano-dispersed enzymes. *Nature* **592**, 558 (2021).
7. Vagin, *et al*. Negatively-doped conducting polymers for oxygen reduction reaction. *Advanced Energy Materials* **11**, 2002664 (2021).
8. Drozdov, *et al*. Conventional superconductivity at 203 kelvin at high pressures in the sulfur hydride system. *Nature* **525**, 73 (2015).
9. Wallentin, *et al*. InP nanowire array solar cells achieving 13.8% efficiency by exceeding the ray optics limit. *Science* **339**, 1057 (2013).
10. Hadagali, *et al*. Scientometric analysis of materials science research. *Library Phiolosophy and Practice* (2019).
11. McKinsey & Company. The Top Trends in Tech, Executive Summary (2020).
12. Swedish Association of Advanced Materials (SAAMs). Kartläggning av aktörer inom avancerade material i Sverige (2021).

PHOTO CREDITS

Cover (semiconductor spintronics, Weimin Chen group): Thor Balkhed, Linköping University
Crystals (perovskites for photovoltaics, Feng Gao group): Thor Balkhed, Linköping University
Table of contents (vacuum chamber): Magnus Bergström
Steel pipes: Jatinsanghvi, License CC BY-SA 3.0
Solar panels: Michael Foertsch, License CC BY-SA 4.0
Wind turbines: Matthew T. Rader, License CC BY-SA
Roll-to-roll machine (chemical-free manufacturing of flexible circuit boards): DP Patterning AB
Peter Wallenberg Jr: Samuel Unéus
Magnus Berggren and Olle Eriksson: Magnus Bergström
Sara Mazur: Investor AB

Document version 2022-07-10

Wallenberg Initiative Materials Science for Sustainability

For more information, contact:
Magnus Berggren, Director – magnus.berggren@liu.se
Olle Eriksson, Co-director – olle.eriksson@physics.uu.se

Or visit:
wise-materials.org