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Material Genome for Engineering Applications

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Abstract *:* Existence of different human genes is due to the different combinations of 4 basics gene codes. In the same way new materials can be obtained by combining elements in the periodic table in possible different ways which is called materials genome. Materials genome is the invention of new materials from existing materials in periodic table by combining them in required proportions and controling their phases transitions. New compounds can be obtained by combining different elements in periodic table. But our main objective is to find the optimal combination with desired properties. Finding the desired compounds by conducting experiment on each and every combination involvs a lot of time and money. Thus a computational tool has to be developed where the properties of a material can be known before a compound is ever made

INTRODUCTION

Materials available to us now-a-days does not meet the requirements of engineering applications and technological advancement. Thus new materials with desired properties are required in the fields where the mechanical and chemical properties of the existing materials are to be advanced and in the fields where the existing materials are scarce in nature and alternative materials are to be found. The demand for new and advanced materials keeps on increasing since past decades.

New materials or new ways of combining and using existing materials is required for the human welfare and sustainable, clean energy. Major technological advancement is lead by the discovery of new materials. From the prehistoric discovery of bronze and steel to the twentieth century invention of synthetic polymers, new materials have been responsible for vast transformations in human civilization. Today, materials innovations also hold the key to tackling some of our most pressing societal challenges, such as global climate change and our future energy supply.

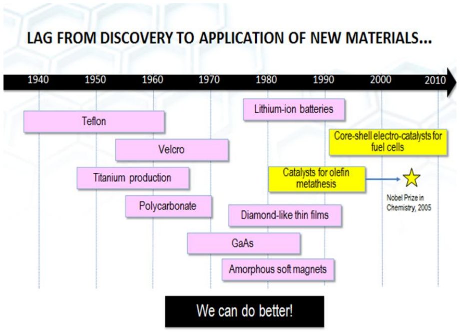


Figure 1 : Lag from discovery to application of new materials

However, materials discovery today still involves significant trial-and-error. Many experiments have to be performed traditionally to detect the properties of the materials which involves a lot of time and cost. It can require decades of research to identify a suitable material for a technological application, and longer still to optimize that material for commercialization. Thus a computational tool has to be developed by integrating theoritical,experimental and computaional fields by which properties of the materilas can be computed analysed and displayed easily.

In the summer of 2011,US President Obama announced the “Materials GenomeInitiative(MGI)”For Global Competitiveness.The Materials Genome Initiative is announced to develop an infrastructure to accelerate advanced materials discovery and deployment. This new initiative calls for major efforts to significantly advance three areas of research: multiscale computational materials science, open source cyber infrastructure for data management, and an integrated approach combining computation and experiments to accelerate the development of advanced materials.The ultimate goal is to generate computational tools that enable realworld materials development, that optimize or minimize traditional experimental testing, and that predict materials performance under diverse product conditions.

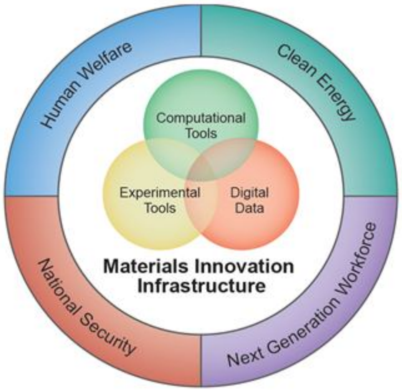


Figure 2 : Materilagenome initiative for global competitiveness

An early benchmark will be the ability to incorporate improved predictive modeling algorithms of materials behavior into existing product design tools. For example, the crystal structure and physical properties of the materials in a product may change during the product's processing, due to varying conditions. It could be disastrous to the performance of a product if, for instance, the tensile strength of its bolts changed during manufacture. The ability to model these morphology and property changes will enable faster and better design.Many important materials properties can be predicted by solving equations based on the fundamental laws of physics using quantum chemical approximations such as density functional theory (DFT).

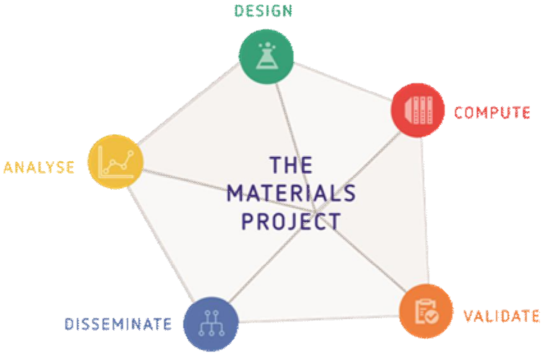


Figure 3 : Overview of material project thrusts

Computed data are validated, disseminated to the user community, and fed into analysis that is ultimately used to design new compounds for subsequent computations.This high-throughput computational approach has been used to screen up to tens of thousands of compounds for potential new technological materials. Examples include solar water splitters, solar photovoltaics, topological insulators, scintillators, CO2 capture materials, piezoelectrics, and thermoelectrics, with each study suggesting several new promising compounds for experimental follow-up. In the fields of catalysis, hydrogen storage materials, and Li-ion batteries, experimental "hits" from high-throughput computations have already been reported using Materials Project.The Materials Project (www.materialsproject.org), is a core program of the Materials Genome Initiative that uses high-throughput computing to uncover the properties of all known inorganic materials. This open dataset can be accessed through multiple channels for both interactive exploration and data mining. The Materials Project also seeks to create open-source platforms for developing robust, sophisticated materials analyses. Future efforts will enable users to perform ''rapid-prototyping'' of new materials in silico, and provide researchers with new avenues for cost-effective, data-driven materials design.he integration of computational materials science with information technology (e.g., web-based dissemination, databases, data-mining) to go beyond the confines of any single research group. This development has expanded access to computed materials datasets to new communities and spurred new collaborative approaches for materials discovery.

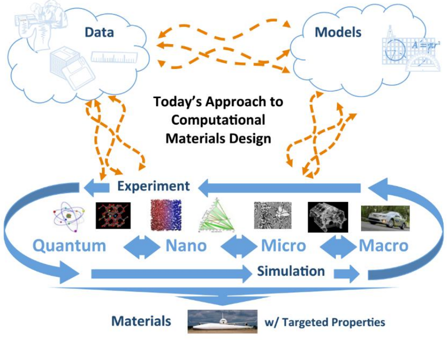


Figure 4 : An overview of workflow process of materials genome

Phase field method for materials genome initiative:

Materials usually exhibits different physical and chemical properties as they undergo phase transformations. Thus phase transformations and microstructure evolution plays an important role in materials genome. Materials undergo structure and morphological changes during processing and manufacturing of the materials, due to varying external conditions and exhibit different physical and chemical properties. These structure and morphological changes refer to the phase transformation and microstructure evolution. A microstructure contains a wide variety of structural features such as phases of different compositions and crystal structures, grains of different orientations, domains of different structural variants, domains of different electrical or magnetic polarizations, as well as structural defects such as interphase boundaries, grain boundaries, twin walls, cracks, surfaces, and dislocations. Thus microstructures evolve during materials processing or in service due to change in process variables like temperature, composition, heating or cooling rates. Microstructures may also evolve under the influence of external fields such as an applied stress or electrical or magnetic field. Thus our main goal is to capture the optimum microstructure with desired properties and to minimise its degradation in service. Finding an optimum microstructure requires to conduct long and costly traditional experiments on each and every element for different compositions and process parameters. To avoid this computational tools integrated with data sources have to be employed to accelerate the time and number of materials deployed by replacing lengthy and costly empirical studies with mathematical models and computational simulations.

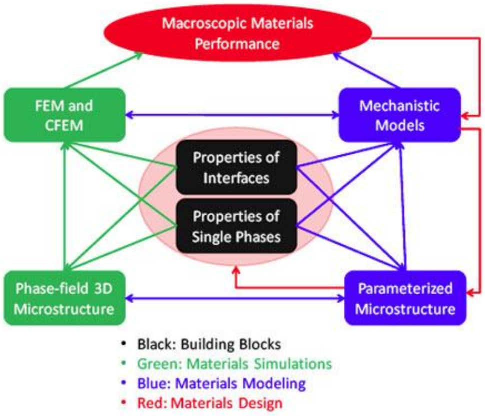


Figure 5 : An overview of phase field method

Pymatgen : (Python Materials Genomics)

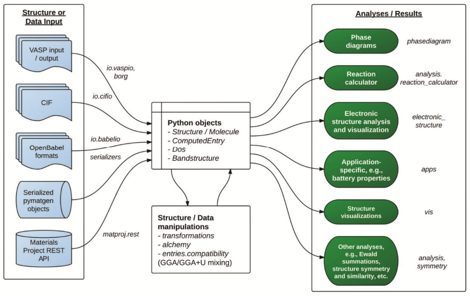
The possibilities for designing new materials based on quantum physics calculations are

rapidly growing, but these design efforts lead to a significant increase in the amount of computational data created. A software infrastructure that supports the collection, storage, retrieval, analysis, and sharing of data produced by many electronic-structure simulators is required to face this challenge. Pymatgen addresses this challenge by implementing a modular framework in Python that provides tools for collecting, storing, grouping, searching, retrieving, and analyzing data generated by many modern electronic-structure simulators. Pymatgen is a robust open source python library of materials and their properties. It is the result of a collaboration under the Materials Science Project (www.materialsproject.org), which aims to establish the core technology for integrated computational materials design. Thus a computational tool is developed with the integration of data base pymatgen and python.

The aims of pymatgen are as follows:

1. Define core Python objects for materials data representation.

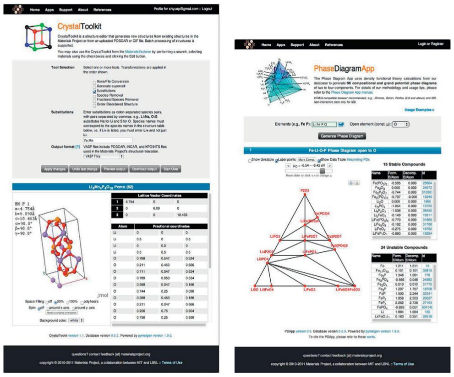
2. Provide a well-tested set of structure and thermodynamic analysis tools relevant to many applications.



3. Establish an open platform for researchers to collaboratively develop sophisticated analyses of materials data obtained both from first principles calculations and experiments

Figure 6 : An overview of the typical workflow for pymatgen

Pymatgen consists of many packages in which data is stored and is addressed by different codes assigned to them. Using these codes required data can be imported into python software to compute and analyse material properties. By using phase diagram package phase diagram of any materials can be generated and plotted. The phase diagram package is currently used in the Phase Diagram App of the Materials Project to generate phase diagrams from calculated materials data.



(a) CrystalToolkit (b) PhaseDiagramApp

Figure 7 : The CrystalToolkit and PhaseDiagramApp in the Materials Project, utilizing pymatgen's alchemy and phase diagram packages respectively

Pymatgen is an open source and is free to use. One can also contribute their research data to it. Thus pymatgen is continuously being improved.

Materials genome for graphene-cement nanocomposites:

Graphene nanoplatelets have unique mechanical, thermal, and electrical properties that render them ideal reinforcing materials. The attractive properties of graphene have led to intensive research on graphene-polymer nanocomposites. During the last several decades, the need for high-performance structural materials and components has led to the rapid development of new classes of materials. The essence of nanotechnology is the ability to work at the molecular level, atom by atom, to create large structures with fundamentally new molecular organization. New classes of nanomaterials such as carbon nanotubes, nanofibers, nanowires, and quantum dots need to be assembled atom by atom with various high-tech applications in mind, e.g., electronics, biomedicine, energy, and the environment. For applications in civil infrastructure (e.g., bridges, dams, and buildings), these materials are still very expensive and can only be produced in relatively small quantities, which limits their applications.

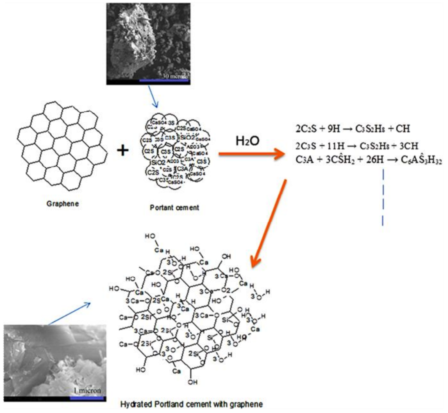


Figure 8 : Schematic of hydrated graphene-cement composite and possible nanocomposite structure

Genome of C-S-H:-

The understanding of the fundamental building blocks of materials is termed material genome.The strength of concrete originates from hydration products. The major portion of the hydration products is usually in the form of a rigid gel termed C-S-H. In other words, C-S-H gel is responsible for the strength and cohesion of concrete structures. Graphene is a single-layer sp2-bonded carbon sheet that forms a honeycombed crystal lattice.

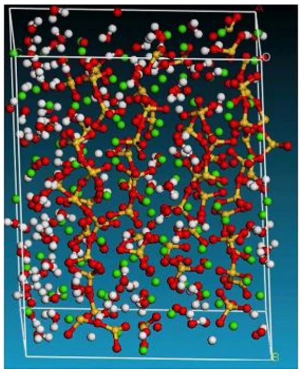


Figure 9 : Atomic model for C-S-H

NEED FOR RESEARCH ON ADVANCED MATERIALS

Research on advanced materials will improve solar energy materials efficiency:-

More energy from sunlight strikes the Earth in one hour (13 terawatts) than all the energy consumed by humans in one year. Sunlight is an important carbon-neutral energy source and continues to grow at a rapid pace.

Materials scientists and engineers can provide materials-based solutions to efficiently capture the unlimited and free energy from sunlight to address the world's energy needs

- Unlimited, free and renewable energy source
- Produces maximum energy during the day during periods of greatest demand
- Energy payback is less than 3 years
- Power output can be tailored to match requirements
- "Off Grid" installation possible for energy self-sufficient communities
- Low carbon footprint (less than 35 grams CO 2 /kilowatt-hour)
- Materials used can be recycled

Photovoltaics (PV)

PV directly converts sunlight into electrical power. There has been significant growth in PV over the past decade, greater than 40% per year, and the cost of electricity from PV continues to decrease. The recent growth of PV has been driven by lower costs due to increased efficiency, primarily from advances in four main types of PV materials including: crystalline silicon; thin films such as cadmium telluride (CdTe), copper-indium-gallium-diselenide (CIGS) or amorphous silicon (a-Si); multifunction systems with solar concentrators; and organic flexible molecular, polymeric or nanoparticle-based cells. Materials R&D challenges for PV technologies include the need to continue to increase solar cell efficiency by improving material properties and cell designs. This can be achieved by

- Identifying or developing alternate materials that are abundant, nontoxic, low-cost
- Developing novel nanoscale surfaces to reduce reflection and increase capture of the full spectrum of sunlight
- Extending the lifetime of photovoltaic systems by addressing materials aging issues • Reducing manufacturing costs and creating efficient, high volume methods to recycle solar system materials at end-of-life • Closing the gap between research and commercial cell efficiencies to reduce the cost of power from modules Concentrating Solar Power (CSP) CSP uses reflectors to concentrate sunlight to generate high temperatures to heat fluids that drive steam turbines to produce utility-scale electric power. Three main CSP types are parabolic trough, dish and power tower systems. Each makes use of reflective mirrors to focus sunlight on fluid such as oil, water, gas or molten salt. Materials research is needed to
- Improve optical materials for reflectors with greater durability and low cost
- Enhance absorber materials and coatings with higher solar absorbance and low thermal emittance
- Develop thermal energy storage materials with improved heat capacity

- Improve corrosion resistance of materials in contact with molten salts. The future
- Convergence of PV and nanotechnology to capture and convert solar energy more efficiently
- Inexpensive plastic solar cells or panels that are mounted on curved surfaces
- Unique forms of PV driven by the imagination of materials scientists: silicon nanowires, nanotubes, flexible plastic organic transparent cells, ultra-thin silicon wafers

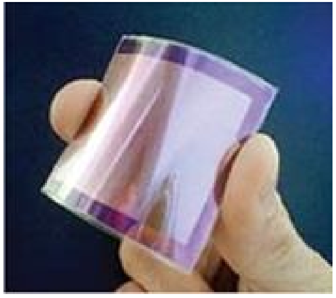


Figure 10 : Flexible Solar Cell

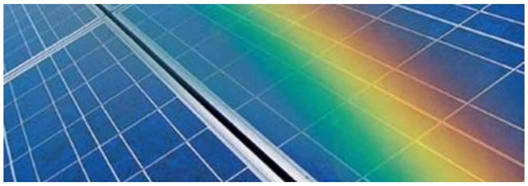


Figure 11 : Silicon PV Module

Challenges for materials genome:

New hard materials for drilling hard rock for deep geothermal wells

New piping materials that resist the extreme hot corrosion conditions of fluids used to transfer heat in geothermal systems.

Sensors included in turbine blades to continuously monitor fatigue damage and signal the need for repair

High strength materials that resist corrosion and fatigue

Need for advanced materials:

New materials, or new ways of using and combining existing materials, are being required to meet tomorrow's engineering applications. This need is compounded by pressures to stay competitive by keeping costs reasonable while continuing to make new material technologies available the world. The main challenges created by today's environment include the understanding and assimilation of the rapid technological advances being made by industry, the integration and application of these advances to customer needs, and preparation for the next set of requirements and applications made possible by maintaining a leading technical edge.

Although many inventions represent innovative design concepts, it is the materials and the advanced processes of making and combining materials that increasingly help turn these concepts into reality. The ability to quickly and reliably lay down multiple conductive layers with ultrafine resolution has led to the miniaturization and low cost of most microelectronic components. Consider, for example, computers that used to take up an entire room and cost hundreds of thousands of dollars that have been replaced by inexpensive handheld calculators. Also, the advent and continued development of synthetic fibers have led to low-cost clothing and bulletproof vests. The combination of fibers with advanced polymer resins (modern day composite materials) has resulted in dent-resistant automotive panels, lightweight fighter aircraft, and golf clubs with tailored flexibility. Things that could not even be conceived of a few decades ago are becoming a reality owing to the advances being made in materials.

NEED FOR ENERGY RESOURCES:

Since ancient times, advances in the development of materials and energy have defined and limited human social, technological and political aspirations. The modern era, with instant global communication and the rising expectations of developing nations, poses energy challenges greater than ever seen before. Access to energy is critical to the wealth, lifestyle and self-image of every country. The global use of electricity captures the triumph and the challenge of energy. Since past decades electrical technology has undergone many revolutions. From its initial use exclusively for lighting, electricity now symbolizes modern life, powering lights, communication, entertainment, trains, refrigeration and industry. In the past century, world has gained access to this most versatile energy carrier. Such changes in our lives do not come from incremental improvements, but from groundbreaking research and development on materials that open new horizons. Tremendous opportunities currently exist for transitioning from carbon-based energy sources such as gasoline for engines to electric motors for transportation, as well as from coal-fired electric power generation to renewable, clean solar, nuclear and wind energy sources for electricity. These advances will require a new generation of advanced materials, including

- Battery materials for massive electrical energy storage
- High-efficiency and low cost solar cells
- Corrosion-resistant alloys for high-temperature power conversion
- Strong, lightweight composites for turbine blades
- Superconducting power distribution cables
- Advanced power handling electronics, and more

Modern transportation, by air, land and sea, is also an essential part of our lives. Advancements in materials for lightweight aerospace alloys, high-temperature engine materials and advanced composites, have been a critical part of improving the capability, safety and energy efficiency of our transportation vehicles. As we look to transportation options that further improve energy efficiency and safety and move us beyond the current fossil fuel paradigm, forefront materials research is needed for

- Improving combustion efficiencies
- Batteries for electric and hybrid vehicles
- Fuel cells
- Hydrogen storage
- New tire compounds and manufacturing processes
- Biofuel production, and more

Despite these technological triumphs, a large part of the world lives without adequate energy. Many people have no access to electricity, and the electricity grid is woefully inadequate in many other areas of the world. Furthermore, the current reliance on fossil fuels puts substantial strain on the world's resources, with significant implications to the economic and national security of many nations, and leads to greenhouse gas emissions that threaten climate change. There is no "silver bullet" to solve the daunting energy requirements of the developed and developing world—twice the energy use in the next half-century—while simultaneously addressing environmental impacts. We must use and innovate across the full spectrum of the energy options available to us.

Finding Substitutes for Critical Minerals:

Minerals are important components of many products civilians use in daily life (e.g., cell phones, computers, and automobiles), as well as crucial military applications (e.g., avionics, radar, precisionguided munitions, and lasers).Manufacturing industries go on consuming minerals but does not mine or process them.This may result in the scarcity of minierals in the near future. A critical mineral is one whose supply chain is at risk, for which the impact of a supply restriction would be severe. Many materials are referred to as "critical" because supply is highly concentrated in either one country or by a few corporate interests, and because they are used in the production of goods that are important economically or for national security. Today, there is particular concern about materials like platinum, tellurium, and certain rare earth elements because they are essential to the manufacture of products in key high-growth sectors, including clean energy, consumer electronics, and defense, among others. The discovery and development of technology substitutes that deliver the same functionality but replace critical minerals, like the rare earth elements, with those that are more earth-abundant is one strategy that would have the dual benefit of protecting our military capabilities while also addressing the growing dependence on any mineral resource, domestic or foreign, that are unstable or subject to supply disruptions. The infrastructure created by this initiative could assist researchers and engineers to rapidly discover and develop substitutes for technologies and applications that are currently dependent on these critical minerals for which no known alternative is available today. Such applications will range from personal electronics to missile guidance systems.

MATERIALS FOR HUMAN HEALTH AND WELFARE:

There are many applications for advanced materials to address challenges in human health and welfare — from biocompatible materials like prostheses or artificial organs to protective materials designed to prevent injury. Advanced materials designed to prevent traumatic brain injuries are one example with potential benefits across diverse user groups including athletes and military

CONCLUSION

Thus new materials are needed for the human welfare and advancement of our technology to meet present days demand. Materials genome concept plays an important role in the discovery of new and advanced materials by developing a computational tool to accelerate the discovery and deployment by reducing time and cost involved.

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