THE WHITE HOUSE
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AI ASPIRATIONS

An AI Aspiration for Sustainable Materials

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IMAGINE IF…

… in just years rather than decades, we could develop new generations of high-performance materials for semiconductors that alleviate concerning environmental and health problems. Imagine if this advance could enable U.S. semiconductor manufacturers to sharpen their edge in a fiercely competitive global industry that is essential for American economic and national security.

Today

U.S. semiconductor manufacturers are on track to regain a strong global position thanks to President Biden's landmark CHIPS and Science Act, which recognizes how critical semiconductors and domestic production are to American jobs, supply chains, and national security and intelligence. In this fast-changing technology, maintaining a globally competitive position will require overcoming many more hurdles in the years ahead. One of those significant hurdles is a daunting materials challenge.

Each new generation of semiconductor technology requires more and more complex stacks of disparate materials to realize advances in performance. It currently takes decades to design, synthesize, and adopt these new materials. But because today's materials and chemistries to produce chips come with environmental, health, and safety problems, new regulations will require materials changes in a few short years. Companies face the difficult challenge of meeting regulatory requirements with new materials that also achieve higher performance at acceptable cost and with robust supply chains—on a time scale that has never been achieved before.

New materials must meet the many unique challenges of semiconductor manufacturing. Material characteristics such as thermal, chemical, electronic, and mechanical properties must be considered alongside sustainability and reliability. Sustainability includes health, environmental, economic, and societal impacts. Ease of synthesis and integration into the semiconductor fabrication process also factor in, as well as potential requirements of new manufacturing equipment and metrology tools. The parameter space for material design, synthesis, and integration into the manufacturing stream is daunting. Optimization across possible materials typically takes 10-20 years from concept to production and requires extensive capital for experimentation and validation.

Per- and polyfluoroalkyl substances (PFAS), often termed "forever chemicals" due to their long lifetime before breaking down, are known health hazards with high global warming potential, but play many critical roles in semiconductor fabrication. A radical change in semiconductor R&D efficiency and speed is needed.

AI opens the door

A paradigm shift in materials innovation has been brewing over the past decade, fueled by exponential advancement of AI and Autonomous Experimentation (AE), with the express goal of accelerating design and synthesis for new materials with custom-engineered properties. First, AI is emerging as a powerful tool to open up the design space of new materials for targeted properties using physics-based materials models. Second, with orders-of-magnitude more potential materials to meet critical needs, AI also accelerates downselection to a small subset for experimental verification. Third, the combination of AI and labs using robotic equipment allows for continuous feedback from experiments into physics-based models of the materials, which the AI system uses to refine further experiments in an iterative cycle. This dynamic re-planning of experiments cuts down dramatically on unhelpful iterations, arriving at the optimal materials much more quickly and efficiently.

Large-scale computational materials databases and repositories have been amassed over many years and can now seed AI-based planning, experiments, and analysis for dramatic acceleration of material innovation. Continuing to build and share data will be important to the scope and accuracy of the materials accelerator. The methodology for physical and virtual infrastructure to support AE has also built up over the past decade. These advances offer promise for the materials challenges of semiconductor manufacturing. But no current AE capabilities directly address the complex needs of co-optimization across so many different kinds of materials and chemistries.

The work ahead

The sustainable material AI Aspiration will mobilize stakeholders and provide resources across the semiconductor value chain to create platforms for materials design, synthesis, validation, and adoption of chemistries and materials: a Materials Accelerator that can reduce the time to deploy advanced materials from 10-20 years down to 1-3 years.

Research and Development
Accurate physics-based models of the wide variety of materials and processing chemistries composing semiconductor manufacturing must be developed and refined to inform experiments. This should include failure points to facilitate verification, validation, and certification by the industry. R&D into efficient merging of physics-based models with data-driven inference and decision-making is required, particularly in the case of small to moderate datasets generated by experimental synthesis and characterization. AI will also need to be developed for the co-optimization of materials across all the constraints including sustainability and reliability. As external factors change in the future, the industry could quickly adapt its material solutions to accommodate, remaining agile and competitive under dynamic conditions.

Community Infrastructure
One of the first steps necessary to execute on this platform will be to expand and connect autonomous robotics to create AE labs capable of undertaking the particularly complex semiconductor materials challenges. This includes both physical facilities and digital toolsets. A unified materials and processing database must also be established to enable widespread access with IP protection, considering the extensive datasets amassed by semiconductor companies across the entire value chain. AI training on proprietary data will be important to refine the broad range of material and process models.

Workforce Development
A strong talent pool across multiple disciplines will be required to implement this Materials Accelerator. We will call on sectors from industry, government, and academia to work together toward an accessible and widespread curriculum in AI/AE for materials to educate and upskill a talented and diverse workforce. We will leverage existing collaboration networks for opportunities with dissemination, mentorship, and internships and coops.

Prototype Capability Demonstration
A national transformative capability for materials acceleration will require a phased development approach, with aggressive goals at each phase. Given the diversity of semiconductor technologies, each carrying unique material and processing requirements, researchers will need to define appropriate metrics for each production process. A three-year phase 1 effort is envisioned at the end of which a complete prototype is demonstrated incorporating AI/AE-generated sustainable material(s) and/or fabrication processes. As one

example, a heterogeneously-integrated advanced logic chip may be realized with 90% reduction in PFAS emission. Another example may be the realization of an ultra-high-density interconnect interposer with ethically-sourced materials and 50% reduction in water consumption during fabrication. In all cases, AI/AE platform and database infrastructure will be erected to support an adaptive framework for accelerated materials innovation. After prototyping, a 2-year duration is anticipated for validation and verification alongside new tools and metrology, where appropriate, to enable high-volume production. At the end of this phase, a full transition of the new material, chemistry, or process into manufacturing is expected.

Benchmarking and Assessment
Materials acceleration platforms will be evaluated for their degree of autonomy, new material test throughput, experimental precision, material usage per experiment, accessible demonstrated and theoretical parameter space (including attainable measurement techniques), and optimization efficiency. Ultimate validation of the effort will be assessed based on the demonstration of the new material or process in production with the performance and sustainability metrics defined in the first phase.

Major hurdles and societal risks

Because no one has yet used AI to deliver robust materials design for the level of complexity we face here, an important hurdle to achieve our objective will be scientific and technical validation of the AI models that will be used to seed AE experiments. Building in adaptive models and focusing efforts on early-stage metrology to converge on and validate accurate models will be critical. Another major hurdle will be rapid adoption of technically successful results, because companies necessarily have a high bar for introducing new materials and processes. Industry stakeholders will be engaged from the beginning.

These AI and AE advances will come with some new and potentially important risks: risks of safety if these systems lead to toxic or otherwise dangerous new materials and chemistries; risks to manufacturers' infrastructure if new materials cause contamination or destruction of equipment. Rigorous standards for vetting outputs will be set up and implemented into the AI models defining materials design. This will include toxicity, environmental effects, sustainability, and compatibility through the entire manufacturing process.

A transformative national capability

A dramatic acceleration for implementing new materials for semiconductor manufacturing can simultaneously address a critical safety and health challenge, enable higher performance chips, and help keep American industry competitive. It can become possible to eliminate almost all PFAS emissions much more quickly. This accelerated time for next-generation materials can also contribute to energy, water, and waste abatement. The resulting contribution to the semiconductor innovation ecosystem will boost continued U.S. leadership in this critical field.