WHITE PAPER ON POTENTIAL MPS/NSF INITIATIVE:

"MATTER BY DESIGN"

Supporting Integrated Experiment,Computation, and Theory to Transfrom Science

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Fundamental science addressing matter spans length scales from atomic and molecular to planetary and intergalactic. While great progress over the last decades in theory, simulation, synthesis, characterization, instrumentation, and processing has created a wealth of novel materials, the ability to make a material starting from designed building blocks and aimed at specific target properties continues to be one of the "holy grails" of scientific research.

But matter is more than materials: it may be a quantum object, a condensate, a superfluid phase, a molecule, an assembly of objects, a hierarchical system, conceivably even an organism! Imagine complex matter that is responsive, adaptive, programmable; matter that could be self-healing or even self-replicating; matter inspired by nature or even designed to circumvent what we thought of as the laws of nature (e.g., a "metamaterial"). The ultimate vision would be to be able to design and create any type of matter for any combination of properties, ideally from first principles.

The MPS vision for “Matter by Design” emphasizes research activites that contain integrated experiment, computation, and theory. In this crucible the tremendous advances experienced in each area alone will fuse into a new and transformative way to discover and create new matter.

An MPS initiative on “Matter by Design” should lead to theoretical and modeling breakthroughs, powerful experimental and cyber-enabled tools, transformative developments in synthesis, assembly, characterization, and processing, and ultimately to the integrated optimization of matter at any of its length scales. This initiative would bring innovation to fundamental science and engineering, build connections among NSF disciplines, catalyze interdisciplinary education, and enhance US global competitiveness.

- **<u>What is new</u>**

Transformative advances in theory, modeling, computation, optimization, data mining, and mathematics, aided by the explosive growth of cyber tools are now offering a foundation for the rational design of matter from electrons, atoms, molecules, their assemblies at nano and meso scales, all the way even to devices. For example, at the smallest length scales, density-functional-theory is now used routinely for high-throughput screening of a wide array of compounds, ranging from pharmaceutical molecules for hitherto untreatable diseases, to novel catalysts aimed at reducing reliance on fossil fuels. Screening of compounds for multifunctional behavior and combinations of properties (e.g., chemical sensing and detection, biological activity, biomedical compatibility, thermoelectric performance, optical anisotropies) is now attainable. And while still nascent, a better understanding of out-of-equilibrium interactions, models, and methods has the potential to lead to hitherto unattainable states of matter.

In parallel to the advances in theory and simulations, revolutionary developments in chemical synthesis and molecular self-assembly are creating new types of supramolecular nanostructures. For example, multifunctional molecules can be programmed or coerced to self-assemble into intricate nano-scaffolds whose surfaces are biochemically functionalized to initiate growth of nerve cells, blood vessels, or bone-like analogues. It is now conceivable that such scaffolds could be used to grow sophisticated ultra-small circuits capable of performing at unprecedented speeds, novel high-efficiency catalysts for advanced, high-density energy harvesting, or revolutionary systems for energy or data storage. Similarly, the dream continues of rationally creating new crystalline materials that provide the electronic environment to induce new states of quantum electronic matter at low energy to transmit energy without loss, and to enable new devices that manipulate quantum states for their operation. Beams of laser light can lock atoms into cold crystals of light mimicing correlated states of matter and providing the basis of a new atomtronics technology. At the same time we now have at hand powerful and sophisticated characterization techniques aimed at complex structures ranging from assemblies of ultracold atoms and many-body systems to membranes, interfaces, composites, living organisms – and all the way to matter at the cosmic scale.

Recently "metamaterials" have been realized whose properties are alien to the natural world and depend on their structure and not just their composition. Exotic and potentially transformative advances have resulted from these, including negative refractive-index compounds, optical modulators, and "cloaking devices". The world of electronics and photonics has been undergoing a revolution as the limits of Moore's Law are pushed and new paradigms emerge beyond it. Single-molecule electronic devices (such as diodes and transistors) have recently been demonstrated, although they are still in their infancy in terms of overcoming problems of power control, robustness, and device integration. Great strides are being made in designing new photovoltaics and other alternative-energy components. Correlations of electronic and photonic behavior can now be engineered in homogeneous or heterogeneous materials, yielding new and exceptional electro-optic and acousto-optic properties, transport, and thermal conductivity.

At the same time, revolutionary strides have also been made in processing of matter at all scales. Intricate electronic devices can be printed on flexible polymers, leading to widespread adoption of "electronic books" and to the vision of entire computers on a foldable plastic sheet. Elaborate circuit elements can be created by directed assembly of polymers, and complex plasmonic devices by directed assembly of nanoparticles. Nano-stamping techniques have recently been developed that enable matter of essentially any shape to be "printed" in unlimited copies at the nanoscale all the way down to the size of individual macromolecules. One can stamp out artificial analogues of bacteria and viruses – or of shaped "lock-and-key" nanostructures that might block their pathogenic activities. The “lock-and-key” interactions of biomolecules can be exploited to mediate the self-assembly of complex large scale nanostructures.

- **<u>Why now</u>**

Despite the progress achieved in recent years, there are major technical challenges to surmount in this area. A number of recent NSF workshops (e.g., on polymers, solid-state chemistry) and NRC studies (e.g. on condensed matter, integrated computational materials) have identified the extraordinary relevance and timeliness of this emerging endeavor.

Largely enabled by major cyber-infrastructure developments, the spectrum of synthetic, characterization, and theoretical/modeling capabilities are converging such that “matter by design” in a rational, predictive, and processable way is now attainable. Our ever-increasing experimental sophistication in synthesizing and interrogating matter at all levels is now taking place under the guidance of elaborate predictive models whose solution and simulation has been enabled by powerful cyber-capabilities and sophisticated mathematical and computational algorithms.

A variety of critical societal problems would benefit from an interdisciplinary, hand-in-hand design of matter using these new capabilities and the continuous feedback among experimentation, theory and computation. Successful outcomes may lead to unique systems for efficient harvesting of the sun's energy; enzyme mimics to guide and hasten reactions converting biomass into fuels; targeted drug-delivery vehicles for "silver-bullet"-like disease treatments; and even nature-inspired functional materials with programmable properties. Fulfilling the promise of molecular electronics and photonics, practical alternative-energy sources, and sensing/identification of potentially harmful or dangerous substances, (ranging from toxins to explosives) may depend on a paradigm shift in our approaches toward design of matter for such purposes.

Spanning the length scales from quantum to cosmos, one can conceive of designed sub-atomic systems capable of performing quantum computations; hierarchical, programmable morphing, or even self-replicating matter; and new materials that may make possible detectors and instrumentation with transformative capabilities for probing the universe. Perhaps more intriguingly, one can also foresee the tantalizing prospect of discovering new matter that no one has ever imagined. At the same time, such an initiative may fuel the development of new mathematical algorithms, modeling techniques, and cyber-tools that might lead to integrated theories of matter accounting for electron, spin, chemical-bond and spramolecular aspects, thus leading to prediction of structure and all equilibrium and out-of-equilibrium properties.

- **Potential for MPS-or NSF-wide initiative**

Matter by Design rests on the integration of new theoretical concepts and modeling, powerful mathematical and computational tools, and novel chemical, physical, and materials sciences approaches. Concerted interactions between theoreticians and experimentalists, including mathematicians, physicists, chemists, and materials scientists, through a continuous feedback loop is necessary to achieve the full potential of “Matter by Design.” Thus such an inititative would find a natural home across MPS.

At the same time, such an initiative requires the critical aspects of engineering, processing, manufacturability, and larger-scale integration; chemical, electrical, biological and mechanical engineers would find a rich set of opportunities here. Needed tools will rely on computer and cyber-enabled discoveries – thus on the strengths of computer scientists and engineers. Of course, inspiration and paradigms from nature and biology are a central driver, providing fertile ground for the contributions of biologists, bioengineers, and environmental scientists.

Interdisciplinary education would also be a critical ingredient of such an initiative. Not only the creation of interdisciplinary courses, but also cross-disciplinary internships for students, postdocs, and even faculty would be highly desirable. The educational opportunities across the boundaries of the now traditional three pillars of science – experiment, computation, and theory are extraordinary. “Matter by Design” will produce a new generation of scientists and engineers that are uniquely qualified to address the grand challenges facing the US and the world.

Thus, an initiative on “Matter by Design” should resonate not only across MPS, but through much of NSF. Because of the wide diversity of disciplines necessary to address this challenge optimally, and the need for intimate collaborations between experimentalists and modeling experts, a Center-mode of funding might be the preferred approach; a large-group-mode would be another alternative. The breadth of this area would make it advisable for any solicitation to be focused on a narrower sub-topic to avoid overstimulation of the community, inordinate numbers of proposals, and success rates in the single digits

- **Other Agency investments**

DOE/BES has identified this area as one of its Grand Challenges. AFOSR has had an active program on "Complex Materials and Structures". The NRC has highlighted the importance of advanced materials in several studies. A number of the recent "NAE Grand Challenges" hinge on advanced materials by design. Foreign funding agencies have this area within their priorities. Many aspects of this research area are in the "Implementation Agenda" of the 7th Framework Program of the European Union. The current "National High-Tech R&D Program" of the Chinese Ministry of Science and Technology includes new materials and advanced manufacturing technologies as an item of "strategic importance" in its current 5-year plan. Japan also considers advanced materials a priority area and recently established its National Institute for Materials Science (NIMS).