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Grand Challenges in Soft Matter Science Campaign: Prospects for Microgravity Research

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Executive Summary

In response to the National Academy of Sciences call for White Papers, we propose the following Research Campaign to create a Soft Matter Institute (SMI) that will support and enable the creation of innovative materials––some of which have yet to be imagined––and expand our understanding of the dynamic molecular mechanisms of life itself. Soft matter, based on materials derived from organic living organisms, has gone from studies of inanimate materials to active particles, devices and systems that cross the barrier from inanimate to life-like. The present and future of the field is quite astonishing: materials and machines that self-assemble, sense and react to their environment and each other, self-replicate and grow exponentially, walk, swim, flock, chase and avoid each other, store and transduce energy, and respond to and emit light, sound, and temperature and chemical gradients. Further ahead, these synthetic materials will even think and communicate. These systems not only inform our understanding of life as we have observed it, but foretell what it could be elsewhere or in the future. They also introduce new technologies at the nanometer and micron scales, important for businesses from photonics to medical applications. Crucial to all of this is microgravity. It not only facilitates these investigations by eliminating extraneous effects but frees these systems from sedimentation to the floor and opens the door to the third dimension.

Engineering and biological applications of this soft matter research on 3D non-equilibrium systems are introduced in the **Science Priorities** section below. To coordinate enough resources to find transformative solutions we must initiate collaboration between leading scientists and engineers. We must also provide the necessary tools and the microgravity research environment essential for this work. The SMI will operate in phases as shown in Table 1.

The **New Technologies and Platforms** section provides additional detail. From its inception, and as the program evolves, the SMI will initiate research activities to attract recognized scientists, serve the next generation of STEM students, and provide researcher development. Initial activities will include scientific workshops, ground-based research and developments, and computer modeling and theory. This will support a portfolio of microgravity proposal announcements, for research and microgravity flight experiment opportunities. SMI activities will enable access to: an enhanced drop tower at NASA Glenn Research Center (GRC), the microscope capabilities listed below on the ISS and the ISS National Lab, and the emerging commercial LEO destinations (CLD) platforms and suborbital facilities that will continue when the ISS is retired in 2030.

1 **Science Priorities**

The March 2021 APS/NASA report entitled "Grand Challenges in Soft Matter Science: Prospects for Microgravity Research" [3] helped bring in several hundred signatories for soft matter topical white papers submitted to the present Decadal Survey [4-14]. In that workshop report, eight chapters highlighted themes that promise to change life in the 21st century. Each of the eight chapters stresses the importance of microgravity for its topic, and how revolutionary changes may be realized by the 3D measurements made possible by the microgravity environment, which overcomes the 2D constraints imposed by ground-based experiments.

Great enthusiasm emerged at the workshop for the breakthroughs in the past two decades: in materials; in experimental, simulation, and theoretical techniques; and in technologies and phenomena discovered. As emphasized in other reviews of the soft-matter research challenges [Nagel 2017][15] and [van der Gucht][16], these advances have significantly changed the vision and direction of this field and portend an exciting future.

These enabling developments include, (i) advances in machine learning, artificial intelligence, big data, and simulations that have changed not only the way data are currently analyzed but also how experiments are being conceived and executed, (ii) new material building blocks that have been developed, which include designer particles and materials that can sense their surroundings, change shape, communicate, self-assemble, self-replicate, and respond specifically at remote distances (e.g., as in allostery in proteins), and (iii) the discovery of new symmetries, symmetry breaking, and topological protection.

Taken together these advances allow us to address more complex fundamental and technological challenges involving **far-from-equilibrium phenomena, complexity and cooperativity**, and to envision life-like materials and machines of technological importance. In section 1.2, we highlight three overarching themes, distilled from the eight workshop chapters[3], for inclusion in a Decadal Campaign, which will accelerate and transform the field of soft matter.

1.1 Soft Material with Life-like Properties

As the field of soft matter has evolved, the ingenuity of physicists, chemists, and material scientists has imbued soft materials with more life-like properties. These building blocks now have properties such as activity, recognition capability, chemical-, temperature-, and/or light-sensitivity and the ability to change shape. One theme that arose in the workshop was – why not go a step further and let them 'think' and communicate? A basic question then is how to understand, control, and use such a complex dynamical system so that it doesn't destroy itself chaotically. This is also the aim of much of 21st century science. The resulting 3D structures, whose component interactions are unmasked in microgravity, will allow us to understand these fundamental and technological problems.

SMI will pursue the following grand challenges:

1.2 Grand Challenges, Toward Artificial Life

1.2.1 *Machines Made out of Machines*: Every living thing is a machine made of machines [Needleman 2017][17]. One goal is to create materials that behave in the same way. Imagine an interacting network of active elements each with its own power source and which is connected to its neighbors chemically or physically. What we know from network theory and from preliminary experiments is that interesting phenomena occur as soon as the network nodes are nonlinear. We expect such machines to be able to self-repair, self-replicate, micro-compartmentalize, specialize, operate as distributed engines, compute, and learn. Aside from the clear utility of intelligent machines they also demand an understanding of complex dynamics and cooperativity that we sorely lack and which are hidden in a gravitational environment. These machines would have the potential to impact technologies from smart fabrics to soft robotics. These relationships can be teased apart in microgravity, providing needed understanding for engineering capabilities.

1.2.2 *Scalable Self-sustaining Ecosystems*: Systems which recycle their building material using only an external power source are found in cells and on the planetary scale. With the advent of 3D printing of structures, one challenge is to create such devices and clothing, which can be recycled, for example, during a space voyage. As an example, biology uses metastable polymers that can draw energy from themselves. Designing self-sustaining ecosystems with similar properties has become a major challenge. Processing materials is intrinsically a nonlinear and non-equilibrium process and requires understanding gravity effects; rheology; friction; and dynamical self-assembly in systems that are glassy, granular, disordered, or suspended particulates. This challenge aims at understanding fundamental dynamical organizational principles and advancing technologies in space such as hierarchical additive manufacturing, recycling, conservation, pharmaceuticals, and biomedical applications.

1.2.3 *Active Materials and Metamaterials*: Attractive active particles can condense into a liquid phase with unusual properties that are only beginning to be understood or explored. They can be engineered to have 'negative' viscosity — they output power into useful work rather than intake power and dissipate it. Spinning particles and other parity-violating systems that break time-reversal symmetry give rise to dissipationless 'odd' viscosity coefficients. New types of order and phase transitions are dynamically accessible as in active liquid-crystal phases. The elasticity of active solids is even less explored. It entails the presence of 'odd' elastic moduli absent in continuum theories constructed from energy-minimization. Metamaterial realizations of active solids have already revealed exciting macroscopic optical, magnetic, and mechanical properties induced by the interplay between designed microscopic structure and activity, whose 3D properties, which are accessible in space, offer knowledge not available under gravity, with only 2D capabilities and limitations due to layering from sedimentation and jamming.

In addition, other workshop topics addressed by the SMI include:

- *Intelligent processing and machine learning*: The pursuit of such challenges requires new ways of doing science. The explosion in the amount of data now generated from experiments and ever-more-sophisticated simulations requires intelligent processing. Machine learning is used not only in analyzing experiments and simulations but in designing and running experiments on Earth and in space, recognizing, categorizing and discovering new phenomena and even formulating theories. Experiments may, in turn, inform an understanding of how machine learning works.
- *The role of Microgravity*: Dissecting complex phenomena requires isolating individual phenomena, activity and function, building up the knowledge of how many parts work together. Gravitational sedimentation limits the experimentalist to two dimensions or systems with gradients. Gravity subjects the systems to external uncontrolled forces and enhances the often-unwanted effects of friction and transport due to thermal convection. Active processing in microgravity will differ from that on earth and we must study both environments to control each separately and to observe the nonlinear and dynamic phenomena at time scales that afford us insights into how such phenomena may be controlled and understood.
- *Instrumentation that would facilitate such dynamic non-equilibrium experiments*: This would include microgravity experiments that allow magnetic, electric[18, 19], and optical fields flow, shear, and other activation, some of which is implemented in the European Space Agency's FLUMIAS, NASA's KERMIT, and sophisticated future microgravity microscopy facilities, see Table 2.

2. New Technologies and Platforms, including Commercial Platforms

To address the challenges listed above, we propose the following deliverables:

- Form the microgravity SMI – a multi-disciplinary institute with on-line and physical participants. It will evolve with the continued addition of significant people through rotating appointments with university positions, a great opportunity for senior staff on sabbaticals. The SMI will also incorporate a University Consortium to support STEM and workforce development. Conduct soft matter-focused workshops and conferences at a regular cadence.
- Increase the NASA complex fluids / soft matter ground-based program by a factor of five, which removes the risk of a single critical path, and facilitates a much larger advocacy group.
- Coordinate ISS microscope facilities in collaboration with NASA and others to enable reduced gravity studies of colloids, granular media, foams, liquid crystals, polymer solutions, etc. The microscopes will have the capability of including external fields, see Table 2. Flow and external field control can serve a dual role in driving/activating the samples and changing their properties. The proposed Light Microscopy Suite (LMS) will replace the Light Microscopy Module (LMM) that was on the ISS from 2009–2021 with a state-of-the-art Physical Sciences Microscope (PSM) facility. In addition to the staged capabilities listed in

Table 2, the proposed PSM with its sample containment and manipulation will include laser tweezers to allow different forms of activation, automatic sample changing, and positioning, temperature-controlled objectives to control Soret diffusion, phase contrast, dark field, simultaneous multi-color fluorescence microscopy, and other standard scientific microscope capabilities. The total LMS should be cloned for use on commercial LEO destination (CLD) platforms and suborbital facilities to both increase science throughput and retain these microgravity research capabilities after the ISS retires in 2030.

- Provide access to one flight-qualified and four functionally identical ground-based microscopes that will be shared by Institute members a few months at a time – with the usual overhead of loaning, shipping, receiving, and alignment being streamlined through the SMI.
- Prepare both new and existing classes of colloidal samples in quantities available to Institute members; Profs. Andrew Hollingsworth (NYU) and Stefano Sacanna (NYU) have agreed to participate in supporting SMI in this way. Samples include micron-sized particles with controllable shapes, size, polydispersity (or lack thereof for creating photonic crystals in microgravity), DNA coatings, mixtures, light activated samples with multiple fluorophores. The ability to create core-shell fluorescently tagged particles should enable us to create optical transistors from 3D colloidal crystals[17].
- Design and test a variety of sample containment methods for confocal (3D) microscopy. Microfluidic, droplet microfluidic and other high throughput devices allow present or modified microscopes to process thousands/millions of samples rather than a few. Start on Earth with the development of improved temperature-controlled, leak-free sample containers and then acquire the understanding of sample instabilities experimentally and computationally. Then add fields for active control (see Table 2), and the ability to manipulate and place any type of particle at any location in the 3D sample. Test initial design capabilities with a 'mag-rail' drop-tower at NASA GRC to understand how to make sample containers without bubbles, nonuniformities, and/or instabilities on Earth, and increase microgravity times[20] for reproducibility, repeatability, and metrology (control), for the production of photonic crystals in commercial quantities. Sample cells for crystal manufacture must allow recovery of the product without damage or deterioration.
- Pursue transformative science (Section 1.2) and manufacturing. For example, fabricate large 3D photonic crystals, as shown possible on the ISS with the recent ACE-T11 (hard spheres) [21]. Add fields and designer particles. Recent results growing single large 3D colloidal crystals with no obvious defects on ISS should brighten "The three-dimensional counterparts are still far from commercialization but may offer additional features such as optical nonlinearity required for the operation of optical transistors used in optical computers, when some technological aspects such as manufacturability and principal difficulties such as disorder are under control." [22]
- Provide access to major computational facilities (neural net and large data processing) that can be shared by all members of the SMI.
- Provide group meetings and colloquia to include both virtual and in-house brainstorming to address issues of science, theory, computation, design, and logistical implementation.

3. Interagency Partnerships and International Partners

We plan to build upon the successful collaborations of the NASA complex fluid/soft matter program, which included ESA/ESTEC, the Canadian Space Agency, the Republic of Korea, the ISS National Lab, NASA ARC, MSFC, JSC, GSFC, and KSC. We propose to leverage resources by building upon interagency collaborations and international partnerships.

Solutions to Grand Challenges identified in the Soft Matter workshop report[3] will be achieved by the microgravity SMI, while minimizing the administrative burden for NASA.

Notes	Year	2023	2024	2025	2026	2027	2028	2029	2030	2031	2032	Total Value	SMD Cost
												$(M)	$(M)
1	Soft Matter Institute	7	7	10	10	12	12	14	14	12	12	110	110
2	Ground Program	2	3	3	2	1	1	1	1			14	14
3	Flight Microscope		5	10	12	5						32	32
4	Sample Modules		5	5	2	1	1	1	1	1		17	17
5	Flight Operations					3	3	3	3	3	1	16	8
6	Sustaining Engineering					2	2	2	2	2		10	
7	Data Analysis/Publication	1	1	2	2	2	2	2	2	2	2	18	12
8	Grants (Flight)	2	3	3	3	3	3	3	3	3	2	28	20
9	STEM	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	5	5
	Total Year	12.5	24.5	33.5	31.5	29.5	24.5	26.5	26.5	23.5	17.5	250	218
*1	Includes ground-based grants, 25 grants a year starting in 2023 with each at $200K/year for 5 years												
*2	Drop towers, low-gravity aircraft, particle synthesis, experiment development												
*3 & *4	See Below												
*5 & *6	Cost Sharing with JSC/OZ and JSC/OB, plus other LEO Platforms, Sustaining Engineering for supporting Flight Systems												
*7 & *8	Cost Sharing with International Partners & Industry. 8 flight experiments a year in 2023 and 2032; and 12 flight												
	Hardware Cost	exp./yr. 2024 – 2031, with grants each at $250K/year, funded one year past flight for publication											
*3	Flight Microscope Cost ($M)		5	10	12	5							
	Note: Flight + Engineering Model (EM)/Ground Simulator + Four Shared + Supporting Hardware												
	Flight: Build/Launch 2024-2025, EM: Build 2023-2024, Shared: 2025-2026												
*4	Sample Modules Cost ($M)		5	5	2	1	1	1	1	1			
Major accomplishments (below):		Note (above): Four Sample Module Varieties (Temperature, Electric, Magnetic, Flow)											
2023 - Start SMI, capture requirments, develop select capabilities; 2023 – 2025 - Flight experiments with existing on-obrit capabilties;													
2026 - Exp. using remote active manipulation; 2027 - Exp. using autonomous active control; 2028 – 2031 - Conduct non-equilibrium													
experiments with laser tweezers, fields, and active control that validate the modelling and organizing prinicples of soft matter;													
2032 - Conduct capstone experiments driven by serendipitious results - repeat great things that were unexpected.													

Table 1. Schedule and Budget for Light Microscopy Suite (LMS): microscope and sample development.

Comparison of ISS Microscope Capabilities
Past, Present, and Proposed

	LMM (2009-2021)	LMS (Phase 1 - 2023)	LMS (Phase 2 - 2024)	LMS (Phase 3 - 2025-2026)	KERMIT (2019 -)	FLUMIAS (2018 -)
Traditional Microscopy (transmission, reflection mode, immersion optics, etc.)	●	●	●		●	●
Confocal Microscopy	●	●	●		X	X
Laser Tweezers	X	X	X	●	○	○
Dynamic Light Scattering	○	○	●		●	○
Rheology (flow, shear etc.)	X	X	X	●	X	X
High-Speed Video Capability	●	●	●		○	○
Macro Imaging	●	●	●		○	X
Micro rheology - Interactions at Microscopic Level	○	○	○	●	○	○
External Stimuli - Temperature Control/Gradient	●	●	●		●	●
External Stimuli - Magnetic Field	●	●	●		○	○
External Stimuli - External Force	X	X	○	●	○	X
External Stimuli - Electric Field	●	●	●		○	○
External Stimuli - Mixing	●	●	●		○	●
Larger number of samples	○	○	○	●	X	X
High-speed data, acquisition and transfer	○	○	●		○	○

● Capability; ○ Some capability or needs mods; X No Capability

Data for KERMIT and FLUMIAS taken from: Equipment & Alignment with Complex Fluid Research Presentation 11March2021 Ray, McQuillen, Sprunger; LMM – Light Microscopy Module, LMS – Light Microscopy Suite – used with permission from ZIN Technologies, Inc.

Table 2. Light Microscopy Suite (LMS) and other microscopy capabilities on ISS.

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Acronym list:

ACE – Advanced Colloids Experiment (2016-2021)
APS – American Physical Society
CLD – commercial LEO destinations
FLUMIAS – (ESA ISS microscope, launched SpX-15, 2018-)
GRC – Glenn Research Center
ISS – International Space Station (1999-2030)
KERMIT – KEyence Research MIcroscope Testbed (launched 2019, ISS Inc. 63, 65, 64, …)
LEO – Low Earth Orbit
LMM – Light Microscopy Module (2009-2021, ISS Inc. 19-65)
LMS – Light Microscopy Suite (proposed launch 2024, ISS and other platforms)
PSM – Physical Sciences Microscope
SMD – Science Mission Directorate (NASA HQ)
SMI – Soft Matter Institute