

## Summary of Research Center Project

\* Compile in English within A4 3 pages.

**Center name:** International Institute for Sustainability with Knotted Chiral Meta Matter (SKCM<sup>2</sup>)

**Host institution:** Hiroshima University (HU)

**Head of host institution:** Mitsuo Ochi, President and Professor, Hiroshima University

**Prospective Center director:** Ivan Smalyukh, Professor, Univ. Colorado Boulder & Hiroshima Univ.

**Prospective Administrative director:** Manabu Abe, Exec. Vice President & Professor, Hiroshima Univ.

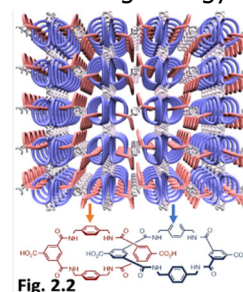
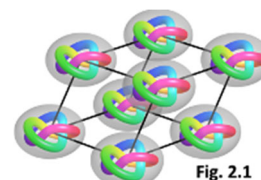
### (1) Overall Framework of the Center Project

The proposed WPI introduces the paradigm of "**knotted chiral meta matter (KCM<sup>2</sup>)**". Everything we see around us, ourselves included, is ordinary matter. Antimatter can exist too, but no macroscopic amounts of antimatter have ever been observed, albeit antiparticles are generated at accelerators and in processes like cosmic ray collisions. Our **KCM<sup>2</sup>** will have its own analogs of fundamental particles/antiparticles and physical principles for designing new materials based on them; it will offer profoundly deep insights ranging from the inner workings of the World to the origins of life, as well as fundamental breakthroughs capable of enabling green technologies needed to sustain it. Aiming to create entirely new embodiments of everything, from fundamental (anti)particles to quasi-atoms and quasi-molecules to both liquid & solid crystals of knots and to materials with highly unusual properties, our WPI's **KCM<sup>2</sup>** paradigm will deepen fundamental understanding of natural phenomena through creating their pre-designed analogs, as well as will solve the knotty Global problems of growing energy demand & climate change by designing matter with highly desirable material properties.

### (2) World-Leading Scientific Excellence and Recognition

#### 1) Research content

Einstein proved the existence of atoms while explaining Brownian motion & introducing the notion of so-called "colloidal atoms". This later led to using colloids to gain insights into the behavior of atomic crystals and glasses, and recently to the large variety of optical, mechanical and other types of metamaterials made from pre-designed, artificial "quasi-atom" building blocks. However, the meta-matter-like behavior of known metamaterials made from such man-made building blocks is limited to only certain types of properties, like the refractive index or mechanical behavior. We envisage creation of the "**knotted chiral meta matter**", the **KCM<sup>2</sup>** paradigm that builds on particle-like quasi-atom properties of topological knot solitons, knotted vortices and knots in colloidal or (bio)polymer molecular strands. Our **KCM<sup>2</sup>** is anticipated to share and explain many properties of ordinary matter and antimatter, but also overcome their fundamental limitations. For example, Fig. 2.1 shows a knot crystal that Smalyukh developed through the self-assembly of topological solitons in the order parameter field [*Science* 2019]. Such knot crystals of quasi-atoms show ~50% anisotropic electro-strictive strain [*Science* 2019], more than two orders of magnitude larger than that known for crystals in conventional matter. While knotted solitons can have chiral nature, the key role played by chirality is in enabling the energetic stability of such particle-like objects. A different **KCM<sup>2</sup>** example is a crystal made of interlocked molecular rings (Fig. 2.2) developed by our PI Sato & colleagues [*Nature* 2021], where topological linking leads to interesting physical properties that may potentially enable carbon dioxide capture and transparent thermal superinsulation often needed for boosting energy efficiency. Like in these examples, the World of **KCM<sup>2</sup>** that we design and create will help to overcome the perceived limits of the World around us. In implementing this vision, we will take advantage of the recent developments in topology in both physical and momentum spaces, and in a large variety of order parameter spaces ranging from chiral liquid crystals to colloids, magnets, (bio)polymers, gels & other condensed matter & biological systems. Within the **KCM<sup>2</sup>** paradigm, we will gain insights into the nature of fundamental building blocks of (anti)matter & origins of life & will create foundations to address global problems of growing energy demand, climate change & human health vulnerability.



#### 2) Interdisciplinary research

The proposed International Institute for Sustainability with Knotted Chiral Meta Matter (**SKCM<sup>2</sup>**) will interknit mathematics, physics, chemistry, material science, biology, cosmology & planetary science to create entirely new research fields & to enable a sustainable future. While **KCM<sup>2</sup>** intrinsically requires collaborations between researchers with different preparation backgrounds, we will assure that the WPI shared laboratories are set up to facilitate interdisciplinary collaborations of researchers recruited globally. One way to promote collaborations

is through co-mentoring of young researchers, the doctoral students and postdocs, where these researchers will have primary, secondary and international co-mentors with whom they will jointly publish while supported by the WPI grant. Having collaborative publications will be an important aspect of performance evaluations. Establishing the primary function of the WPI under one roof of a new building will promote discussions and scientific exchanges between researchers from different fields. Moreover, we intend to organize various tutorials and short courses for teaching key concepts from the fields different from one's primary training. Besides the formal seminars, the WPI will have an informal discussion forum of early outcomes of research, to which all WPI members will be invited. While engaging our international PIs and their teams, we will take full advantage of online meetings, short- and long-term stays of overseas PIs and young researchers in Japan and vice versa.

### **(3) Global Research Environment and System Reform**

#### **1) International research environment**

The *SKCM<sup>2</sup>* network of PIs will involve the very top global centers, including MIT, Cambridge U., Max Planck Inst., CU-Boulder, etc. We will strive to increase the time foreign PIs spend at HU beyond 2-3 months through sabbatical, cross-appointment, consulting & other agreements. Shared laboratory space & equipment from the WPI funding will be provided to foreign PIs as the top priority at the very beginning of the project. Foreign PIs will be the primary advisors for postdocs hired at HU, who will spend 50% time abroad in labs of these PIs & 50% at HU. In addition to HU-based mentors, all WPI-supported PhD candidates will have foreign PI co-mentors, spending ~50% time abroad. Joining research groups is like becoming a family member, so that the foreign & HU PIs will be all inter-knotted with family-like links via their young researcher group members.

#### **2) Center management and system reform**

Our institute will have a level of autonomy envisaged by the MEXT for WPI centers. The director will make all key decisions related to personnel, hiring, budget, etc. His leadership team will assist with the implementation of vision and goals of the proposed project. The current group of PIs at HU and other nodes of the WPI involves a majority of research leaders in the emerging *KCM<sup>2</sup>* field & will be strengthened further through new hires of top young researchers via open international searches, where 5-10 new PIs will join within the 10-year implementation period, including potential new joint hires with RIKEN & AIST. To help implement ambitious WPI-enabled reforms within the entire HU, Abe will initially combine his current role of HU's Executive Vice President with the role of WPI's Administrative Director. Afterwards, Abe will devote himself to the role of the WPI's Administrative Director as soon as possible. Out of three Deputy Directors, two are women: Yabuta will be a Deputy Director for Science, Kotorii for Outreach & Dissemination & Inoue for Education. Women will be in majority on the Executive Board. Moreover, Yabuta & Kotorii will form a strategic planning group and, together with Abe, will help the Director oversee daily operations of the WPI. The overall administration of the center will achieve a balance of gender representation, experience, young energy & the need of both using the WPI to seed reforms and maintain its administrative autonomy, per the vision of MEXT. Kotorii, Senyuk, Yabuta & Inoue, will lead the four research thrust areas of the WPI. Director & PIs will plan and implement education and system reforms at WPI as a seed to reform HU, with strong support from President Ochi. Director will meet with the President on a monthly basis. Once the WPI is launched, research and educational activities will be evaluated within the concept of "meritocracy" introduced under the leadership of Director. To stimulate ground-breaking research with corresponding publications in top-ranked international journals, a cumulative annual impact factor of publications of PIs will be systematically monitored as a summation of impact factors of journals in which individual articles are published, serving as a guide for Director in distributing resources & salary bonuses (this strategy will account for field-specific differences, e.g. between materials science and pure math); additional external grants, international awards, outstanding service to WPI missions & other major successes will be similarly rewarded too. This concept does not exist at HU; once this new system is validated by the WPI, it will be implemented throughout HU as an improvement to the existing system. In addition, by adopting the best practices of administrative procedures learned by the WPI's foreign researchers at their respective institutions, we will pursue reforms, which will lead to the improvement of the administrative system at HU.

### **(4) Values for the Future**

#### **1) Generating and disseminating the societal value of basic research**

Through high-impact publications & outreach, we will convey to both scientific communities & the general public how our fundamental research helps address many knotty problems that Japan & the entire World face, like the growing energy demand & its impact on climate change. For example, buildings consume 40% of all generated energy for cooling and heating; 20% out of it lost through windows, the least efficient part of the building envelope. Could one maintain the desired environment within a building interior without energy consumption, like in a thermos? Sato & Smalyukh will collaborate to develop such transparent super-insulating materials by

cost-effective fabrication of novel aerogels via knotting/linking molecules. Jointly with Vignolini, they will also develop materials for the building envelope inspired by gold and silver beetles that use porous chiral structures for thermal regulation (silver/gold reflections play a role like silver coatings in a thermos, though instead noble metals beetles use the emergent power of chiral self-assembly of chitin fibers). Learning from nature, we will develop low-cost energy-efficient materials from nanocellulose. From yet another perspective, further developments of electronics require miniaturization, which is limited by quantum effects at small scales. These limits can be overcome by our chiral magnetic spin systems and topological insulators. For example, the racetrack memories can utilize topologically protected multi-dimensional solitons like hopfions as information carriers to design entirely new principles of future electronic devices, where topological objects like knots in fields can serve as information carriers. From the standpoint of biomedical applications, changes of chirality & knotting in proteins can cause protein metamorphosis diseases, such as Alzheimer's disease, so the ability of detecting and controlling these processes may aid in developing biomedical treatments. Knots are also found in the viral RNA genome of coronavirus whereas the spike protein coat that changes with mutations of coronavirus may be responsible for vaccine inefficiency, as studied by our PI Hsu. These examples show how our research may help to address pressing problems that the World faces, also achieving missions of Japan's Society 5.0. We will pursue a vast variety of outreach activities designed to elevate public awareness of our sustainability enabling *KCM<sup>2</sup>* research & to attract talented young people to science careers, led by Kotorii, Deputy director for outreach & dissemination. WPI's summer/winter schools & conferences will have public lectures & outreach designed to interest the public in Japan in science for sustainability. Mimicking US NSF's guidance for dissemination of research outcomes to the public, PIs will develop their own unique outreach components of the WPI-related activity to broadly share the excitement about the research we do. Public lectures by Peace Nobel Laureates will complement the science programs at WPI schools, as a reminder of the important roles that need to be played by scientists to sustain global peace. The WPI will seed reforms & boost global reputation, making HU like the Harvard of Japan, educating a new generation of researchers with a global perspective, enabling energy demand reduction, climate change mitigation, Japan's society 5.0 missions & economic growth.

## **2) Fostering next-generation human resources linked with higher education**

Over 50% of the WPI grant funds will be dedicated to supporting young scientists, including PhD students. To promote highly interdisciplinary research, we will introduce a system of co-mentoring young talented researchers, doctoral students and postdocs, who each will have three or more co-advisors with different backgrounds. For example, a doctoral student in Physics at HU might be co-advised by HU PIs in chemistry or math & by a PI from an international node. Specialized graduate coursework will be co-designed and taught by the WPI PIs. Our strategy will take advantage of the top international research centers in this research area, allowing students and postdocs from HU, TokyoTech and RIKEN to spend extended periods of time at the other WPI nodes, such as MIT, Cambridge & CU-Boulder. Conversely, Japanese institutions will host young researchers & PIs from the international nodes of the WPI, all co-mentored by foreign & domestic PIs. These arrangements will allow doctoral students to take specialized courses at the partner institutions. Furthermore, to help reform graduate education, we will introduce cross-disciplinary coursework, along with international research exchange, schools, conferences & forums to bring the broader interdisciplinary community together. The WPI will pay PhD students' salary, like in USA graduate programs, as well as will sponsor student/postdoc exchanges between Japanese & international nodes. Using matching funds, 5-10 new young PIs will be hired within the implementation period, striving to attract the most talented young researchers & achieve gender balance & diversity. Our WPI will seed reforms of education & research at HU, in other institutions of the large Chugoku-Shikoku geographic area and throughout Japan. Our Center will promote internationalization and gender balance in academia, will mobilize and reinforce the global research efforts for a sustainable, peaceful future. The WPI will strive to hire women PIs, young researchers & administrators. Out of 5-10 faculty hires, we will recruit 50:50 male-female, Japanese-International, achieving gender balance & a stimulating cross-disciplinary & multi-cultural environment. Young researchers will connect HU with top global centers & will erase disciplinary boundaries between the fields by working with co-mentors having different backgrounds.

## **3) Self-sufficient and sustainable center development**

In addition to the WPI grant, PIs will pursue multiple individual grant applications in Japan, in countries of participating PIs & globally. Our ability to attract such funding will be enhanced further by the international network of collaborations & visibility of research outcomes of the *SKCM<sup>2</sup>*. Besides these conventional funding sources, we will pay attention to private foundations (like the Simons, Templeton & Moore foundations in the USA) & will establish Endowed Chair positions & student/postdoc fellowships jointly with philanthropists and industry in Hiroshima/Japan/globally, as well as local governments of Hiroshima prefecture/city. While HU's support will be sustained past 10 years, the external funding will grow with each success, making the *SKCM<sup>2</sup>* an independent permanent center of research excellence at HU, self-sustained after the implementation period.

## Research Center Project

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Appendix 1: "Biographical Sketch of Prospective Center Director" (attached)

Appendix 2: "Reference (recommendation) for prospective center director by world's distinguished researcher(s) in the center's target field" (7 letters attached)

**Prospective Administrative director:** Manabu Abe, Exec. Vice President & Professor, Hiroshima Univ.

Appendix 3: "Biographical Sketch of Prospective Administrative Director" (attached)

### 1) Overall Framework of the Center Project

\* Clearly and concisely describe your center's mission statement as a WPI center, its identity, and its goals toward achieving the objectives of the WPI program.

A **short slogan** that embodies the vision for our Center and its missions is "Building a sustainable World, knot by knot," conveying the notion that our fundamental interdisciplinary research on knotted matter not only expands the bulk of scientific knowledge but also strives to contribute to achieving a sustainable, peaceful future.

**Missions of the SKCM<sup>2</sup>** center are the following:

- Establish a new research field of knotted, chirality-enabled meta matter
- Develop solitonic knots as new, designable quasi-atoms & quasi-molecules
- Cross-pollinate topology & chirality knowledge across disciplines & scales
- Create foundations for technological innovation to solve global knotty problems
- Become a magnet to attract & a knot to inter-connect young talent globally
- Create a testbed for research-based education reforms within & beyond Japan
- Inter-link natural & social sciences for sustainability & global peace

The **SKCM<sup>2</sup>** center will be uniquely identified on the global stage by the following **key identities**:

- The only center globally that integrates multi-dimensional knot topology & chirality research
- Differing from centuries of pre-existing research on matter that nature gave us, this Center strives to create its own (anti)matter and materials from pre-designed fundamental (anti)particles
- Leveraging our experience as a Global research institute "without walls", spanning from HU to Tokyo, MIT, Boulder and Cambridge, we will lead the World in reforming education in Japan and abroad
- Leveraging its international and interdisciplinary scope, the SKCM<sup>2</sup> center will conduct research collaborations at an unparalleled level while fostering the next generation of young talent
- The SKCM<sup>2</sup> center will be the only WPI conducting highly fundamental research that also enables a sustainable future by boosting energy efficiency to slow down climate change, as well as contributing to the Global Peace and Japan's human-health-related Society 5.0 goals

Guided by the above missions and unique identities, **the main goal** of the proposed WPI is to introduce the paradigm of "knotted chiral meta matter (**KCM<sup>2</sup>**)", with its own analogs of fundamental particles and antiparticles, with profoundly deep insights ranging from the inner workings of the World to origins of life and to fundamental breakthroughs capable of enabling green technologies needed for sustaining it. Aiming to **create entirely new embodiments of everything**, from fundamental (anti)particles to quasi-atoms and quasi-molecules to both liquid & solid crystals of knots and to materials with highly unusual properties, our WPI's **KCM<sup>2</sup>** paradigm will deepen fundamental understanding of natural phenomena through creating their pre-designed analogs, as well as will solve the knotty Global problems of growing energy demand & climate change by designing matter with unusual, highly desirable material properties. While cross-pollinating and fusing research fields that rarely interact, from pure math to material science and both subatomic and cosmological-scale physics, the ambitious goals of our center may lead to field medals and Nobel Prizes, as well as other WPI-scale recognitions. More importantly, our research will allow for the

Hiroshima University-1

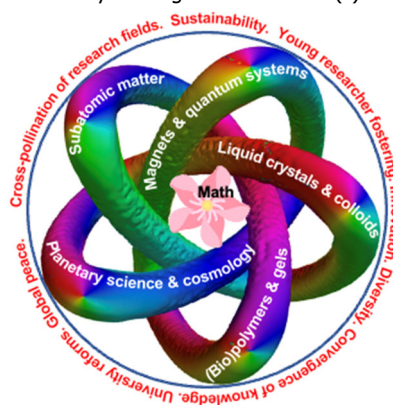
International Institute for Sustainability with Knotted Chiral Meta Matter (SKCM<sup>2</sup>)

deeper understanding of the World around us and will create the means for making it more sustainable by introducing fundamental breakthroughs that enable new technologies & improve quality of life.

## 2) World-Leading Scientific Excellence and Recognition

### 2) -1 Research fields

\* Write in your target research field(s)



Our WPI center's activity (Fig.3.1) is mainly centered within the field of mathematical & physical sciences, while integrating pure math with soft & quantum condensed matter physics, subatomic & biological physics, chemistry, as well as planetary sciences & cosmology. The new **KCM<sup>2</sup>** paradigm introduced & developed by this center will lead to a new level of fusion of these research fields. The center will collaborate with social scientists to better serve the needs of young researchers and to elevate the awareness of the general public in Japan & globally about the need for sustainability-focused research & the role that scientists can play in securing global peace.

**Fig.3.1.** Diverse research fields & natural hierarchies are inter-knotted by the **KCM<sup>2</sup>** paradigm while reforming education & yielding great values for a sustainable future.

\* Describe the importance of the target research field(s), including the domestic and international R&D trends in that research domain and neighboring field(s), and describe the scientific and/or social significance of the field(s).

The new interdisciplinary research field and paradigm will allow for non-incremental, substantial advances in multiple branches of science and technology. The proposed WPI will establish a research paradigm of "**knotted chiral meta matter (KCM<sup>2</sup>)**", with topological knot solitons in physical fields & knotlike molecules acting as its fundamental building blocks. While individual papers in the research areas associated with **KCM<sup>2</sup>** have emerged already, many of which are published by members of our team, the WPI will allow for establishing the **KCM<sup>2</sup>** as a new, internationally visible interdisciplinary research field. Our **KCM<sup>2</sup>** research will range from fundamental concepts of symmetry breaking and mathematical descriptions of solitons and knots, will benefit from experimental realizations and in-depth studies of such structures in condensed matter and biological systems, will explore the role of knot chirality in the origins of life and fundamental particles, will establish the means of controlling material properties and physical behavior and will culminate with the creation of foundations for new technologies & other sustainable future values. A large network of interdisciplinary collaboration with top participating researchers within Japan and in other countries around the World will enrich this effort. The outcomes of our interdisciplinary fundamental **KCM<sup>2</sup>** research will lead to breakthroughs and key developments in pure math, physical, biological, planetary and other sciences, as well as will be of transformative importance for future technologies and humankind's ability to address global challenges like climate change; we expect that our WPI research efforts will lead to both Fields Medals and Nobel Prizes. The centuries of prior research focused on understanding and using the ordinary matter around us, but we intend to go well beyond this approach by creating our own, pre-designed meta matter based on the notion that knots can act as its building blocks. Our WPI Center will integrate chirality- and knot topology-focused research in math, different branches of physics, chemistry, biology and material science while using fundamental breakthroughs to develop foundations for future new technologies. We will explore and exploit the power of emergent knots and chirality to bring benefits for a sustainable future and human health.

\* Describe the value of carrying out research in the field(s) as a WPI center (e.g., Japan's advantages in the subject fields, the project's international appeal as an initiative that challenges world-level science issues, and the future prospects of the research)

Through cross-pollinating topology and chirality knowledge across disciplines & scales, we seek to deepen understanding of ordinary matter around us by creating its artificial analogs, including counterparts of conventional crystals, glasses, liquids and liquid crystals. This fundamental research will form foundations to enable metamaterials with pre-designed properties not found (& not anticipated) in naturally occurring systems but that are highly desirable to address global challenges like growing energy demands and climate change. The combination of topology and chirality will form an interdisciplinary basis for the new field of **KCM<sup>2</sup>**, which we believe is ideally suited for the WPI mission. Indeed, the WPI is a unique program



not just in Japan, but globally, & a very attractive opportunity to pursue paradigm-changing research. Japan is famous for world-class chirality research, with multiple chirality-related Nobel prizes in chemistry & physics, with truly outstanding discipline-specific chirality research in cosmology, biophysics, quantum matter and material science. The Mizuhiki artforms reveal how not only the top, world-leading scientists but also the general public in Japan are truly fascinated by aspects of topology, most notably related to knots. Hiroshima University (HU) excels in what we define as the science of knots, ranging from mathematical knot theory (here we have 4 mathematicians focusing on this topic from the pure math standpoint) to multi-dimensional topology in physical, chemical, biomedical and planetary sciences. This creates a fertile ground to establish our **center on “knotted chiral meta matter (*KCM<sup>2</sup>*)”**, here, in Japan, with the headquarters at HU. It is also symbolic and timely for us to have the goal of pursuing this **fundamental *KCM<sup>2</sup>* science for sustainability**. A sustainable future requires global peace, slowing down climate change and addressing the challenges related to human health. In the middle of the global COVID-19 pandemic, in a city that suffered from atomic bombing during the World War II, with 3 PIs (including the prospective Director) originally from Ukraine that suffers from Russia’s war, with the global warming accelerating with every day, we feel & hope that our knowledge & creativity in doing fundamental science can serve to address global challenges for a sustainable future.



As a host institution, HU is located in the peace memorial city Hiroshima & is the leading university in the Chugoku-Shikoku area (Fig. 3.2), a large part of Japan that so far has not benefited from the reforms-enabling WPI program. With a large fraction of international students, HU is aspiring to become a major international sustainability-focused research center, with high visibility that is only possible to achieve with the help & partnership of the WPI program.

**Fig. 3.2.** The new WPI will bring MEXT-envisaged reforms to HU & the entire Chugoku-Shikoku region.

\* List up to 5 centers either in Japan or overseas that are advancing research in fields similar to the center’s field(s), and evaluate research levels between your center and those centers.

Our proposed Center is going to be in many ways a unique Center globally, envisaged as a home for fundamental research on knotted chiral meta matter, as well as the birthplace of the ***KCM<sup>2</sup>*** paradigm. The proposed highly fundamental research aims to prioritize fundamental science, helping to make our World sustainable through enabling new insights, technologies & materials needed to reduce the growing energy demand and climate change, as well as to overcome human health-related challenges. While there are many Research Centers, National Labs, Institutes & other organizations globally that define sustainability among their key missions, most of these institutions focus on technologies and approaches that are much more traditional & mature in terms of their development. For example, prospective Director Smalyukh is a Founding Fellow of the joint institute of CU-Boulder and the National Renewable Energy Laboratory (NREL) in the USA, the Renewable and Sustainable Energy Institute (RASEI). Both NREL and RASEI focus on the development of technologies based on renewable energy generation from solar, wind and other renewable sources, with the research being rather applied in nature and based on broadly accepted approaches also pursued by dozens of other institutions around the World. One of the existing WPIs, the International Institute for Carbon-Neutral Energy Research (I<sup>2</sup>CNER), also aims to accomplish goals very important for a sustainable future, but their approach is to improve materials, processes and technologies in order to accomplish this goal. Differently from NREL, I<sup>2</sup>CNER and many other institutions with similar goals, our proposed WPI will enable approaches for addressing the energy demand and climate change problems that so far nobody has thought about because even materials that they would require do not exist. Using the ***KCM<sup>2</sup>*** paradigm, we will develop these unusual materials from knots to have properties that have been never possible before. As an example, if Sato and Smalyukh succeed in using inter-linked/knotted molecules for making highly porous materials with thermal super-insulation and high optical transparency, these materials could be used in windows and other parts of building envelopes to save about 40% of all energy generated globally that is wasted by commercial and residential buildings to maintain the comfortable indoor environment through heating and conditioning. Instead, the future buildings built using the materials we envisage would be capable of maintaining a comfortable indoor environment without energy consumption, like a thermos maintains a desired temperature of its contents without consuming energy. Looking back into history, one can find analogies of how we dream our approach can help solve the pressing modern problems of energy demand and climate change. Some 200 years ago, quickly growing cities like New York worried about the limitations of horse-based transportation, with the sad projections that cities could be literally covered by horse waste if no better ways of cleaning it were invented. However, the horses were replaced by automobiles,

an invention that the conventional thinking at that time did not foresee, eliminating this horse-related challenge. In a similar way, we hope that the pre-designed metamaterials enabled by knotting could one day help reduce the energy consumption to the extent (note that 40% of all generated energy is consumed by buildings) that all the needed energy could come from renewable sources alone. This example shows the out-of-the-box thinking and philosophy of our WPI in relation to sustainability: invent materials thought to be impossible, so that energy would not be wasted when it does not have to be wasted, and so that the sources of the climate change problem related to the generation of this energy are simply eliminated. To the best of our knowledge, no institution globally has such vision, but this is what it may take to save our planet.

Beyond sustainability, which is what largely motivates and sets goals for our research, knot topology and chirality are key concepts that also help to uniquely distinguish our proposed WPI from other institutions. Although topology is recently very popular in solid-state physics, and there are many institutions globally where such research takes place, this existing research is discipline-focused, combining topology knowledge with materials physics within a relatively narrow subset of systems. Furthermore, the aspects of topology in the momentum space of solid-state materials typically involve low-dimensional physical and order parameter spaces, which is different from the knot theory aspects that we will pursue and apply in the interdisciplinary context of our WPI's missions.

The knot theory research, a subfield of pure math, is typically pursued by individual researchers scattered globally, typically one per department/university. Uniquely, HU has 4 talented mathematicians in this research area (including the PI Kotorii, but also professors Teragaito, Nozaki and Koda). A notable example of a Center with strongly inter-linked pure math and theoretical physics research is the Institute for Advanced Study (IAS) in Princeton, USA, with one well-known example of its success related to the Fields Medal awarded to Ed Witten for providing deep insights into the mathematical knot theory based on quantum field theories; Witten is the only physicist to be awarded the Fields Medal, the highest honor for mathematicians. However, this cross-pollination within IAS so far had no experimental components and did not go beyond math and theoretical physics.

At the University of Birmingham, Prof. Mark Dennis (one of the supporting letter writers) leads a rather inter-disciplinary Topology Center with a rather broad scope. The Prospective Director Smalyukh actually participates in this international network; he often hosts PhD students from Birmingham in his lab at CU-Boulder. While the scope of our Center is even broader, is built on the fusion of topology with chirality research, still the experience of the University of Birmingham center will be valuable in implementing the vision for the **SKCM<sup>2</sup>** center. Arrangements will be made for collaborations and mutually beneficial student exchanges between the centers, which are rather different but can be partners.

While there are many Chirality-focused research centers and centers of excellence globally, including many such centers in Japan (Inst. for Molecular Science, RIKEN, University of Nagoya, Osaka Pref. Univ., AIST, Chiba University, University of Hokkaido, Spring-8, Kyushu Univ., Kyushu Inst. of Technology & many others), they deal with more discipline-specific aspects & we collaborate with them already. Japan is especially famous for the breakthrough research on chirality-catalyzed reactions (Noyori's 2001 Nobel Prize in Chemistry), broken symmetry in subatomic matter (2008 Physics Nobel Prize of Nambu, Kobayashi, Maskawa)... Chirality research efforts in Japan span cosmology, biophysics, quantum matter, material sciences and so on, constituting pervasive, outstanding efforts, with "chiral" found in titles of ~1000 articles/year in Japan. The history of excellence in chirality research creates a fertile ground to establish our new WPI, building on these strengths & enhancing them while integrating math, physics, chemistry & engineering to explore & exploit chiral effects. However, there is no example of an institute or other organization that integrates knot topology and chirality research, apart from the proposed WPI.

With all unique identities of our center accounted for, there are no direct analogs of the proposed WPI in Japan or elsewhere in the World. The assembled team of PIs and their colleagues/collaborators publish over 50% of the highest impact articles that contain "knot" in the titles of articles in Nature & Science journals globally. This team is uniquely poised to establish the new paradigm of **KCM<sup>2</sup>**.

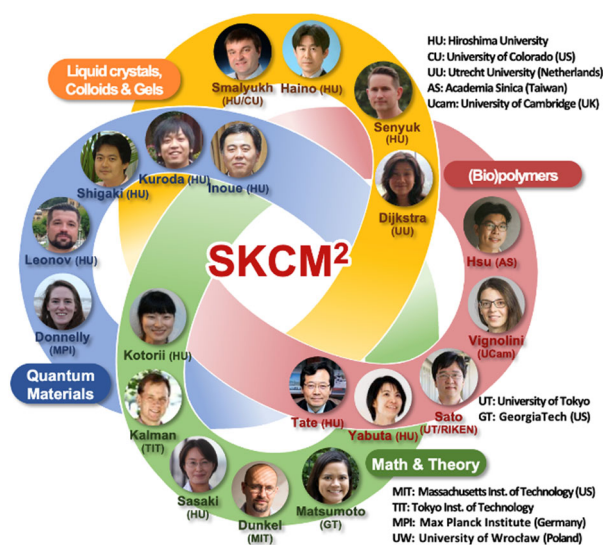
\* Appendix 4: "Up to 10 English-written papers (review papers are also acceptable) closely related to the center's project and their list" (attached)

## 2) -2 Research objectives and plans

\* Describe in a clear and easy-to-understand manner by the general public the research objectives that your project seeks to achieve by the end of its grant period (in 10 years). In that process, describe what world-level scientific and/or technological issues are you seeking to solve, and what will be the expected impact of the scientific advances you aim to achieve on society in the future.

The proposed WPI introduces the paradigm of **KCM<sup>2</sup>**, with its own analogs of fundamental particles and antiparticles, with profoundly deep insights ranging from the inner workings of the World to the origins of life and to fundamental breakthroughs capable of enabling green technologies needed for sustaining it. Aiming to create entirely new embodiments of everything, from fundamental (anti)particles to quasi-atoms and quasi-molecules to both liquid & solid crystals of knots and to materials with highly unusual properties, our WPI's **KCM<sup>2</sup>** paradigm will deepen fundamental understanding of natural phenomena through creating their pre-designed analogs, as well as will solve the knotty Global problems of growing energy demand & climate change by designing matter & unusual, highly desirable materials. This **KCM<sup>2</sup>** paradigm builds on particle-like quasi-atom properties of topological knot solitons, knotted vortices and knots in colloidal or (bio)polymer molecular strands. **KCM<sup>2</sup>** will share and explain many properties of ordinary matter and antimatter, but also overcome their fundamental limitations. As an example, knot crystals of solitonic knotted quasi-atoms [Smalyukh, Science 2019] show ~50% anisotropic electro-strictive strain, more than two orders of magnitude larger than that known for crystals in conventional matter. A different example is a crystal made of interlocked molecular rings developed by Sato & colleagues [Sato, Nature 2021],

where topological linking leads to interesting physical properties that may potentially enable carbon dioxide capture & transparent thermal superinsulation needed for boosting energy efficiency. Like in these examples, the World of **KCM<sup>2</sup>** that we design and create will help to overcome the perceived limits of the natural World.



**Fig.3.3.** Research thrusts, PIs & participating institutions of the Center depicted with the help of a T(4,3) torus knot.

Pursued by our highly interdisciplinary international team of PIs (Fig. 3.3), the fusion of topology & chirality research in this paradigm-changing context will allow for new concepts and material/structural design strategies that may otherwise seem impossible. For example, mathematical knot and homotopy theories motivate our search of topological solitons such as hopfions in different physical systems. The well-known Derrick

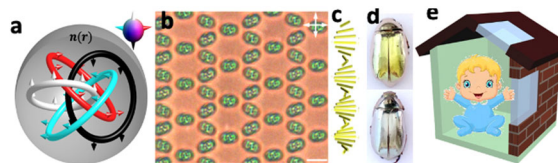
theorem would preclude their stability and their very existence, but these constraints can be overcome with the help of chirality. For example, the chiral terms in the hamiltonians for chiral magnets and liquid crystals (LCs) allow for stabilizing multi-dimensional topological solitons in chiral condensed matter, where Hamiltonian expressions become effectively the same in the one-constant approximations for LCs. Such similarities of mathematical descriptions of physical systems arise across the entire hierarchy of length and time scales as these similarities are related to symmetry breaking in these different systems. The spin texture of a soliton called hopfion is a physical embodiment of the celebrated mathematical Hopf fibration in the order parameter. It now can be studied experimentally in LCs and magnets, and in the emergent magnetic field. Our combined experimental and theoretical studies will reveal what types of topological knot solitons can be stabilized by chirality, providing insights into topologically similar objects in other, experimentally less accessible systems, like particle physics and cosmology. Similarities of Hamiltonians in chiral spin systems & quantum chromodynamics will provide opportunities to establish a unified fundamental understanding of phases, origins and consequences of nonlinearities, universality classes and generalizations, all done in the spirit of historic cross-inspiration between theories of particle physics and condensed matter. Synergistically with these efforts, we will be pursuing discoveries of new phases in soft condensed matter systems like LCs and colloids, where very fundamental questions of co-existence of order, chirality, topological knotting and fluidity also arise and will be addressed by both modeling & experiments.

While the bulk of our research will focus on experimentally highly accessible systems, like LCs, colloids, magnets and biopolymers, our findings will have immediate impacts for the studies of objects and phenomena on less accessible scales, like the still elusive types of elementary particles and cosmic strings, for which even their very existence remains unknown. Conversely, theories of particle physics and cosmology will inspire us to develop a deeper understanding and practical utility of related phenomena



based on these highly accessible condensed matter and biological systems. The potential technological applications that could be enabled by emergent knot chirality research will range from energy-efficient building technologies to thermally insulating materials, to biomedical detection & treatment of diseases, as well as spintronics, electro-optics & data storage.

**Fig.3.4.** Overall vision of the proposed research program that pursues fundamental studies spanning from (a) pure math and theories of particle physics to (b,c) novel materials, solitons and structures, to (d) bioinspired photonics and thermal control, and to (e) enabling sustainable future.



The power of our approach is best illustrated with examples that cross the disciplinary boundaries but have lots in common, calling for cross-pollination of knowledge (Fig. 3.4). Chiral carbon centers of LC molecules mediate emergent self-assembly of micrometer-range crystal lattices of topological Hopf solitons, which were discovered and named “heliknotons” [Tai & Smalyukh. *Science* **365**, 1449-1453 (2019)]. Researchers later theoretically predicted such chirality-stabilized Hopfions and ensuing interesting quantum mechanical effects related to the emergent fields in magnetic solids at tens-of-nanometers length scales [*Phys Rev Lett* **125**, 057201 (2020)]. They then also experimentally found such solitons in cuticles of certain beetles and in chiral self-assemblies of bacteria-made colloidal cellulose nanocrystals. The relation to sub-atomic systems might be not obvious, but particle physicists were the first ones to develop theoretical models based on the celebrated mathematical Hopf fibration and Hopf maps. The so-called gravitational hopfions are related mathematical models associated with cosmic black holes that recently generated a great deal of excitement (curiously, their polarized images resemble ones of LC hopfions, albeit at very different length scales). We will use helical phases of cellulose nanocrystals to template highly porous, thermally super-insulating aerogel materials for applications in building envelopes, including transparent insulation for windows. These examples show how abstract mathematical concepts of the topological soliton (Fig. 3.4a) can materialize in the open crystal lattices of the heliknoton-type Hopf solitons found embedded in synthetic chiral LCs (Fig. 3.4b) and also in that formed by bioderived cellulose nanocrystals and in chiral configurations in cuticles of the *Chrysina resplendens* gold scarab beetle and *Chrysina chrysgyrea* silver scarab beetle (Fig. 3.4c,d). Bioinspired porous photonic materials with designable reflectivity can be used as thermally super-insulating building envelopes to reduce the energy demand and its impact on climate change (Fig. 3.4e). At each hierarchical level, emergent fundamental phenomena define complex physical behavior that can have practical utility & can be controlled by external stimuli, like by magnetic fields for the case of chiral magnetic colloidal LCs. The interdisciplinary study of such effects will generate new fundamental knowledge & will allow researchers from different fields to apply & exchange the concepts developed within their fields effectively. Such inseparable knot-chirality-centered knowledge took decades to “diffuse” across fields to yield not only fundamental insights but also practical utility. Our proposed WPI plans to reduce this time 100-fold by eliminating disciplinary boundaries.

\* Describe concretely your research plan to achieve these objectives and any past achievements related to your application.

**General overview of research plans.** Our center will be structured to optimize our ability to pursue ambitious research goals while using the available resources most effectively. It comprises four research thrust areas shown in Fig. 3.3. Considering the space limit of this document, we first give a brief general overview of the research plans of different research thrusts and the cross-pollinating interactions between them, & then provide additional details in relation to examples of specific efforts. Within the research thrust area on LCs, colloids & gels, the goal is to develop new forms of knotted soft matter. New chiral LCs & nano-colloidal systems will be synthesized by Haino; Smalyukh will use them as host media for novel solitons, vortices and crystals, whereas Senyuk will exploit such solitonic active matter to gain insights into the behavior of knot quasi-atoms in an out-of-equilibrium setting. Additionally, LCs with designable high-dimensional order parameter spaces will be modeled & co-implemented by Dijkstra, Smalyukh, Haino & co-PI Tasinkevych. Sato will synthesize new breeds of knotting-enabled high-porosity gels, like hydrogels & aerogels, & will collaborate with Smalyukh to control & understand properties like infrared reflectivity, visible-range transparency and thermal conductivity, as needed for future building envelope applications.

The research thrust of quantum matter knots will explore multi-dimensional topology in both real and momentum spaces in spin systems and quantum chromodynamics (QCD). Inoue will lead synthesis of new magnetic materials designed to host the multi-dimensional topological solitons and their crystals.

These efforts will be guided by modeling of stability diagrams by Leonov & Smalyukh & will culminate in direct 3D experimental visualizations/mapping by Donnelly. Sasaki & Leonov will collaborate to explore the fundamental synergies between the phase diagrams in spin systems and QCD, and then Shigaki will work with Inoue and Donnelly to experimentally probe these insights from the condensed matter and nuclear physics perspectives. Kuroda will study the momentum-space multi-dimensional topology, once again developing synergies with particle physics related to Weyl and Dirac semimetals in the solid state, working closely with Sasaki, Smalyukh and Leonov.

Within the biopolymer thrust, Yabuta will study the topology of nano-sized organic matter in extraterrestrial materials (e.g. meteorites), as well as will carry out an enantiomer analysis of not only amino acids but a larger suite of organic compounds in extraterrestrial objects to reveal how molecular chirality in Space played a role in chemical evolution toward the origins of life. Tate & Hsu will study the role of knotting & solitonic configurations in biopolymers like RNA & DNA & in defining protein structures in contexts ranging from fundamental properties of biopolymer knotting & linking to Alzheimer's disease & Coronavirus mutations. Sato will synthesize molecules that will be "programmed" for knotting & linking in controlled ways, as well as for the self-assembly into materials with unusual mesoscale structure enabled by chirality-controlled spontaneous knotting/linking. Vignolini & Smalyukh, along with co-PI Matczyszyn, will study how knot solitons can emerge in both the natural photonic structures (like in cuticles of beetles) and in hierarchically self-assembled cellulose nanocrystal based chiral LCs.

We intend to address many fundamental, inter-disciplinary questions on relations between chirality and the different knots (& their crystals) in vortices, colloids, LCs, proteins & so on. This study of various knots & solitons in diverse physical, chemical & biological systems will be integrated through the deep connections with mathematical knot theory modeling by Kotorii, Kalman, Sasaki, Dunkel & Matsumoto & the co-PIs from the entire Hiroshima knot theory group. We intend to expand the current cohort of PIs by bringing in 5-10 new hires at HU, further enhancing & integrating these research thrusts to further boost cross-pollination between the diverse research fields. Considering the size constraints of this proposal, below we provide detailed plans & approaches for only a representative subset of activities to be pursued.

***Pure & applied math insights into the knotted chiral meta matter.*** PI Kotorii & co-PIs Koda, Nozaki and Teragaito will research the pure math aspects of Hopf fibration and topological solitons while collaborating with Smalyukh. Hopf fibration is a continuous map from the 3-dimensional sphere  $S^3$  to the 2-dimensional sphere  $S^2$ , a representative element of a generator of the 3rd homotopy group  $\pi_3(S^2)$  of the 2-dimensional sphere  $S^2$ . The preimage (Fiber) of each point in  $S^2$  by Hopf fibration is a trivial knot in  $S^3$  and a pair of any two fibers is a non-trivial link, called a Hopf link. On the other hand, a 3-dimensional topological soliton (a nonsingular vector field) can be regarded as a continuous map from the 3-dimensional Euclid space  $R^3$  to the 2-dimensional sphere  $S^2$  and so it can be regarded as an element of  $\pi_3(S^2)$  by one-point compactification. Experiments revealed topological solitons which are different from Hopf fibration as an element of the 3rd homotopy group, called heliknotons. Smalyukh described some topological solitons which dramatically change topologies at some point through physical state change tuned by external stimuli. Knot theory researchers will construct mathematical models corresponding to these changes. The team will explore the possibility of new topological solitons & inter-transformations. Extending this further from a pure to applied math perspective, Dunkel at MIT will study the energetic pathways of such solitonic inter-transformations, in order to gain insights about subsets of material systems capable of revealing such behaviors beyond the experimental examples already studied.

The pure math/topology team members at HU, Koda, Kotorii, Nozaki and Teragaito, will research the chirality of Knots and links together with other members in this WPI as follows. A chiral knot is the knot that is not equivalent to its mirror image, that is, it cannot be continuously transformed into its mirror image. The judgement/sensing of chirality of knots is an old problem. Many knots, including well known examples like the trefoil knot, are chiral, which can be revealed by knot invariants, such as Jones polynomial. But we don't have invariants completely sensing chirality yet for all knots and so one cannot systematically identify all knots at large crossings numbers. We will explore how to probe chirality of knots and links in natural sciences. Moreover, we will also investigate chirality of virtual knots which is a generalization of classical knots, adding virtual crossings. Collaborating with chemistry and biological thrust members of WPI, mathematicians will help correlate virtual knots and objects in science, such as substances and phenomena, and will give the object new properties from the viewpoint of chirality. Further, by investigating the chirality of virtual knots, we will establish classification and new possibilities for them.

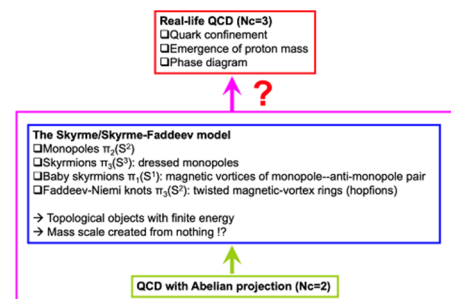
Kotorii at HU and Kalman at TokyoTech will also research physical manifestations of higher-order linking numbers of non-closed curves together with chemical and biological members in this WPI as follows. Shapes of chemical strings like protein and DNA have been distinguished and classified by Knot theory. However, these strings are not loops. Therefore, we have had to close them into loops to use knot theory, which treats loops. Because there is no canonical way to close them, this causes a problem that these classifications depend on the ways of closing. We will introduce indices that directly distinguish strings, including non-pool and pool ones, by generalizing the existing link invariants. In particular, we will generalize the higher-order linking numbers as an expansion of linking number for any component links. Then, together with the (bio)polymer thrust members of this WPI, we will verify the applicability of these indices by using simulations of proteins & DNA, and classify/distinguish these strings.

The combined pure math, applied math & physics perspective on knotted matter will put us in an ideal position to address a series of key fundamental questions with interdisciplinary importance:

- What are the allowed transformations between knot configurations & their physical stability?
- What restrictions do different material symmetries impose on the knot types?
- What knot invariants have physical significance for each (chiral) knotted field realization?
- How do soliton-type and singular knotted fields coexist with each other?
- What new knot-soliton condensed matter phases are possible?
- When knots decay or emerge, what are the topological cascades of knot types in different systems?
- What is the relation between topological complexity and energy landscapes?
- How do knotted structures interact? What types of dynamics of singular/solitonic knots can be realized?
- How topological concepts in dynamic phenomena can lead to entanglement of material properties?
- Is knotting in high-dimensional order parameter spaces, ( $SO(3)=S^3/\mathbb{Z}_2$  &  $SO(3)/D_2=S^3/Q_8$ ) possible?
- Could high-dimensional topological objects  $\pi_4(S^3)=\mathbb{Z}_2$  and  $\pi_4(S^3)=\mathbb{Z}_2$  with dynamic knotting emerge in out-of-equilibrium matter?

**KCM<sup>2</sup> at subatomic-to-Universe scales.** Quantum Chromodynamics (QCD) is the modern theory to describe strong interactions responsible for nuclear forces binding protons and neutrons in nuclei. The mechanism to generate the proton mass has a crucial impact over the formation of matter in the Universe after the Big Bang. Because of the characteristic feature of QCD, called asymptotic freedom, confinement of the elementary particles (quarks and gluons) into composite systems (hadrons) emerges, and the pair of a quark and an anti-quark gets condensed leading to spontaneous breaking of the QCD global symmetry (chiral symmetry), which gives rise to the mass of the hadrons in the ground state as well as a tower of resonances. Yet today, it remains highly challenging to reach a contemporary consensus on the mysterious interplay between the two phenomena. This is one of the central issues in understanding the physics of the early Universe in which the temperature reaches  $10^{12}$  Kelvin (n.b.  $10^7$  Kelvin in the Sun's core) accessible in the present & near-future accelerators, and of compact stellar objects that are much denser than the ordinary matter around us. The ordinary matter composed of hadrons is expected to change into a plasma of quarks and gluons at high temperature &/or high density. Such a phase transition is driven by a drastic change in the strong interaction mediated by the gluons in a hot/dense medium. The main goal is to disentangle the interplay between emergence of massive hadrons & confinement of quarks & gluons in extreme environments, & eventually to establish the intrinsic properties of QCD & its phase diagram. Given the fact that there exists an intriguing similarity to the phase structure of chiral magnetic materials, Sasaki will lead the theoretical thrust research effort aiming at the primary description of complex phenomena related to the underlying symmetry & topology in those systems (Fig.3.5).

**Fig.3.5.** Particle/nuclear physics fundamental insights arising from fusing topology & chirality paradigms by the SKCM<sup>2</sup> Center.



*Topological objects in QCD:* The Skyrme model describes nucleons as static solitons of the theory for pions. Interestingly, the model yields all the topological solutions known in physics: (1) monopoles with  $\pi_2(S^2)$ , (2) skyrmions with  $\pi_3(S^3)$  as dressed monopoles, (3) baby-skyrmions with  $\pi_1(S^1)$  as magnetic vortices connecting monopole - anti-monopole pairs, and (4) Faddeev-Niemi knots with  $\pi_3(S^2)$  as twisted magnetic-vortex rings made of helical baby skyrmions. Thus, the Skyrme model is a model of monopoles that build

up those topological objects carrying finite energies. The Skyrme model can also be deduced from QCD with 2 colors, therefore it has a high potential to describe the topological aspects of the real-life QCD that carries 3 colors through. The proposed project aims to extend the above framework to QCD in various conditions to explore the origin of the proton mass supposed to be generated via strong gauge dynamics as well as various phases of the theory at finite temperature, baryon density and external magnetic fields. *Phases of high-density QCD:* Skyrmion matter crystals at high density are known to be described by a body-centered cubic (BCC) lattice of half-skyrmions. In strongly correlated many-particle systems, 2nd-order quantum phase transitions can be realized because of topological defects - the phase change takes place through "deconfinement" of a skyrmion into 2 half-skyrmions at the boundary and a U(1) gauge field emerges. In quantum field theory such emergent gauge degrees of freedom are naturally expected. When the underlying dynamics can be separated into "slow" and "fast" modes and the latter are integrated out, non-abelian gauge potentials (Berry phases) are induced. It is of particular interest to study the physics of QCD at high baryon density by means of topology. We will also find how its changeover would take place for given external parameters as well as the experimental verification in heavy-ion experiments and in astrophysical observations.

*QCD critical point(s):* Existence of a 2nd-order QCD phase transition at finite temperature and baryon density remains hypothetical, whereas in systems of strongly interacting electrons the methodology to determine the location of a critical point is established. The goal is to employ the method, with appropriate extensions, to predict any critical point(s) in the context of QCD.

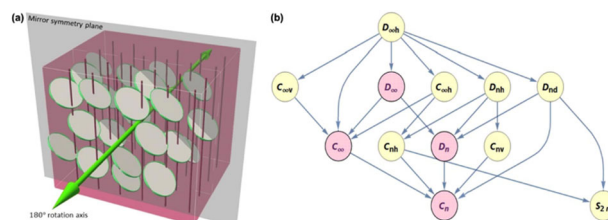
*Experimental insights guided by the theory:* The QCD phase diagram can be probed for at least three parameter axes: temperature, baryon chemical potential (quark density), and magnetic field. The controllable parameters in heavy ion collision experiments are somewhat limited: collision energy, nuclear mass number, and collision geometry (centrality), among which the collision energy has the dominant impact. Collaborating with Sasaki, PI Shigaki will be working to pursue the highest temperature with low chemical potential via the highest collision energy at the LHC at CERN, Switzerland. The regime at finite chemical potential can be accessed via using lower collision energies. It has been considered earlier, but is now attracting a broader interest, e.g. in relation to the equation of state of neutron stars.

*QCD versus chiral spin systems:* The researchers will explore & exploit the similarity between the phase diagram of chiral spin structures in chiral magnetic materials and the phase diagram in QCD. Being related to symmetry breaking, the Hamiltonians of the chiral spin systems in solid-state magnets and in chiral LCs resemble the one describing elementary particles of single chirality. Therefore, the behaviors of elementary particles can be modeled by chiral spins in chiral magnets and LCs. Inoue & Shigaki will be working together with Sasaki & a few other QCD theorists (Kenji Fukushima, Yoshimasa Hidaka, et al.) to find what one can extract from the comparison between the spin systems in magnetic solids & QCD systems. One of the ideas is that an inhomogeneity known in chiral spin systems may emerge in the QCD system. PIs will introduce an experimental approach to look for the proposed phenomenon; they are currently assessing the feasibility of addressing this within the ALICE experiment. The high statistics data at ALICE (2022-2025) will confirm the behavior with improved accuracy to compare with the spin system.

***Knotted phases of soft matter.*** Drawing inspiration from the QCD diagram/phases, Smalyukh, Haino, Senyuk and Sato will collaborate to design & experimentally demonstrate highly ordered, low-symmetry (triclinic & other) fluids with emergent physical behavior not encountered in nature, which will be then used as host media for novel solitons and topological phases based on them. Nematic LCs are states of matter that combine orientational order & fluidity. They are ubiquitous in technological applications & often serve to model behavior of less experimentally accessible systems, ranging from elementary particles to cosmology. While symmetries of crystalline solids are classified in textbooks, diversity of possible LC fluids remains to be explored. Only several (<10) distinct nematic LC symmetries with uninhibited 3D fluidity have been discovered so far. Nanoscience breakthroughs recently allowed Smalyukh & other researchers to introduce molecular-colloidal nematic LCs that combine the thermotropic and lyotropic subclasses (Fig. 3.6) [*Nature* **590**, 268-274 (2021); *Science* **360**, 768-771 (2018)], where rich phase behavior emerges from stimuli-tunable molecular and colloidal interactions at the hierarchy of length scales, from angstroms to micrometers. These LCs promise to reveal unusual order and fluidity, like the monoclinic and orthorhombic symmetries. On the other hand, they are found hosting topological solitons with particle-like behavior manifesting in solitonic crystals & different forms of active/driven matter. Historically, LCs were often discovered accidentally. To increase the odds of discovery, a common recipe was to design building

blocks with symmetries of anticipated phases and hope that interactions between them lead to such phase behaviors. Yet, Smalyukh recently revealed an emergent effect of high-symmetry disc- and rod-like colloidal and molecular building blocks forming orthorhombic & monoclinic nematic phases, where the molecular and colloidal subsystems order along obliquely oriented directions in the latter case (Fig. 3.6a). Hypothetically, the orientational order of colloidal nanoparticles with pre-designed shapes within a molecular nematic host could lead to a large series of symmetry-breaking transformations (Fig. 3.6b), starting from the  $D_{\infty h}$  symmetry of the uniaxial molecular nematic LC host, including chiral & topologically interesting phases, but one needs to find the design rules for these molecular-colloidal assemblies to become the energetic ground states. Much of prior work focused on exploration of nanocolloidal interactions & self-assembly, where multipole-like electrostatic, elastic & magnetic interactions play important roles. Understanding of these interactions now puts the PIs in a position to demonstrate LCs with different symmetries of order.

**Fig.3.6.** Molecular-colloidal nematic LCs. (a) Monoclinic nematic formed by thin discs dispersed in a nematic host with molecular ordering direction shown by magenta lines. The symmetry plane & axis are marked. Green regions next to particle edges are regions where order of the molecular host is perturbed by the colloidal surfaces. (b) Point group symmetries & transformations of orientational order that can emerge in mesostructured nematic LCs formed by a uniaxial  $D_{\infty h}$  molecular host doped with colloidal particles with various geometric shapes. Chiral & nonchiral phases are depicted with magenta & yellow colors, respectively.



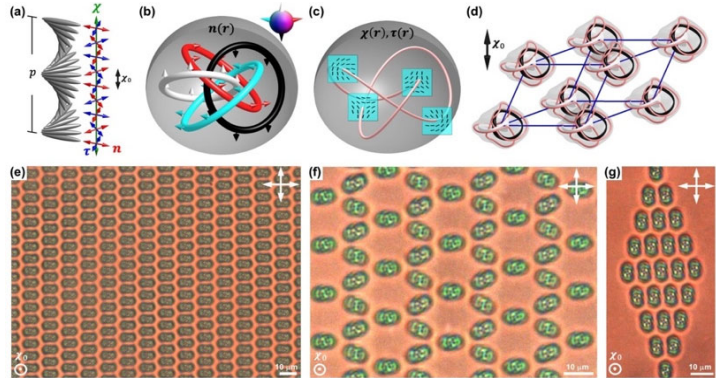
PIs Dijkstra, Smalyukh & co-PI Tasinkevych will design & demonstrate highly sought-after mesostructured composites with low-symmetry orientational order and fluidity, like triclinic nematics (having uninhibited fluidity combined with low-symmetry order that has no symmetry operations apart from trivial ones). In the preliminary work they obtained early evidence of this lowest symmetry triclinic nematic LC fluid by dispersing asymmetric bent-core silica nanoparticles in a molecular nematic host fluid. Once robustly demonstrated in experiments, the various low-symmetry nematic LCs will then serve as host fluids for new types of topological solitons, where symmetries are related to the order parameter spaces.

Unlike in solids, where symmetries of the crystal basis are required to be compatible with crystallographic lattices, no such constraints apply to nematic LC fluids that can adopt even a larger variety of symmetries yet to be discovered. However, the general design rules for obtaining molecular-colloidal hybrid LCs with various unusual symmetries of orientational order and fluidity, like the triclinic nematics, remain to be revealed, which will be a key part of the proposed research effort. The emergent orientational order with different symmetries will be designed to arise from a thermal self-reconfiguration of relative orientations of the molecular and colloidal subsystems supplemented with competing anisotropic elastic, steric and electrostatic colloidal interactions. Analytical modelling of electrostatics-modified & steric interactions between bent-core colloidal particles & the anisotropic molecular interactions at colloidal surfaces will be used to predict and explain the temperature-concentration phase diagram for different colloidal surface charge and the experimental orientational distributions in the triclinic hybrid molecular-colloidal LC, as done in Smalyukh's recent study of monoclinic nematics [*Nature* 2021]. In the preliminary studies, our colloidal silica nanoparticles with bent-core  $C_{2h}$ -symmetry indeed seem to form the triclinic  $C_{1h}$ -nematics under conditions when the surface-interaction-controlled ordering axes of the particles are different from the molecular nematic host's principal director. For large opening angles ( $\sim 150^\circ$ ) of the bent-core colloidal particles, three unique axes of orientational ordering are observed, all at oblique angles to each other, with one corresponding to the molecular & two to the colloidal building block subsystems. The researchers will tune the volume fraction (number density) of colloidal particles in the molecular host to explore how the elastic nature of nematic colloids can define the ensuing colloidal LC phases. Experimentally, colloidal interactions will be probed using a combination of laser tweezers, video microscopy, light scattering & nonlinear optical imaging capable of mapping different director fields of the triclinic and other mesophases. The PIs will pursue systematic studies of molecular-colloidal LCs to elucidate how formation of different mesophases & lyotropic-thermotropic phase diagrams depend on the particle's surface charging, geometric shapes (opening angle of the bent-core particles, etc.) & surface boundary conditions (perpendicular versus tangential versus conically degenerate), as well as the nature of the LC host fluid (e.g., chiral versus nonchiral). Senyuk & Smalyukh will collaborate with Mertelj to study magnetic switching of molecular & colloidal directors; Dijkstra & co-PI Tasinkevych will supplement experimental efforts by numerical modeling of the ensuing phase diagrams. Thermodynamically stable



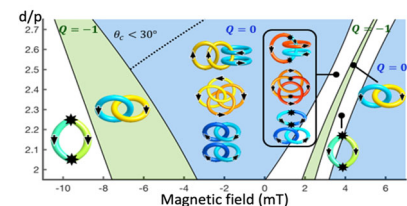
triclinic nematic LC phases will reveal how such low-symmetry orientational order & fluidity can co-exist.

**Fig. 3.7.** Topology & crystals of heliknotons. (a) Field comprising a triad of orthonormal  $\mathbf{n}(\mathbf{r})$ ,  $\mathbf{x}(\mathbf{r})$  &  $\mathbf{\tau}(\mathbf{r})$ . (b) Preimages in the smoothly vectorized  $\mathbf{n}(\mathbf{r})$  of a heliknoton coloured according to their orientations on  $S^2$  (inset). (c) Knotted skyrmion structure in  $\mathbf{n}(\mathbf{r})$  co-located with knots of vortex lines in  $\mathbf{x}(\mathbf{r})$  and  $\mathbf{\tau}(\mathbf{r})$ . Gray isosurfaces in (b,c) show regions of distorted helical state. (d) Primitive cell of a triclinic crystal; isosurfaces of distorted helical background are co-located with red vortex knots black/white & preimages of  $\mathbf{n}(\mathbf{r})$ . (e,g) closed & (f) open heliknoton crystal lattices.



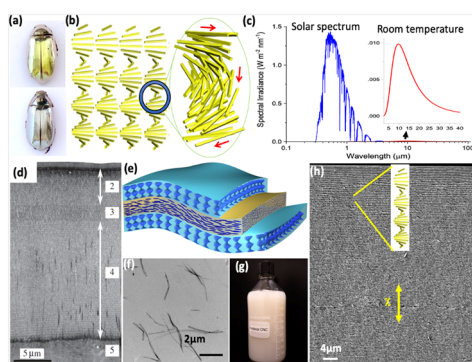
While topology recently plays important roles in phase discovery in hard condensed matter, phases with topologically nontrivial field configurations can also arise in soft matter, enriching behavior of chiral LCs. Some of the most exotic condensed matter phases, such as twist grain boundary & Abrikosov phases, also contain arrays of topological defects in their ground states. 3D particle-like topological solitons can be the building blocks of exotic phases too, especially when realized in low-symmetry nematic LCs. Smalyukh recently discovered so-called “heliknotons” (Fig. 3.7) [Tai & Smalyukh. *Science* **365**, 1449-1453 (2019)], a type of 3D topological solitons with a dual nature of being a non-singular Hopf soliton in the material director field  $\mathbf{n}(\mathbf{r})$  & a vortex (disclination) knot in the immaterial fields of helical axis  $\mathbf{x}(\mathbf{r})$  (Fig. 3.7b,c). Heliknotons form various crystalline lattices, open and closed, including triclinic crystals (Fig. 3.7d-g). An important question is what it would take for heliknotons to self-organize into solitonic LCs with only orientational ordering of the solitons? In Senyuk & Smalyukh’s recent studies, the interactions between heliknotons already could be controlled between few  $K_B T$  and hundreds of  $K_B T$ , as well as effective shapes could be controlled between nearly isotropic and highly elongated. Preliminary studies reveal that heliknotons emerging in chiral nematics with submicron pitch can also self-organize into a disordered amorphous phase, as well as into an orthorhombic nematic phase, where all building blocks are particle-like topological solitons (similar to the ones shown in Fig. 3.7d,e, but smaller and more elongated). This brings about hierarchical liquid crystallinity, where nanometer-long organic molecules form a chiral nematic LC host medium that hosts heliknotons and then these micrometer-long topological solitons form yet another, solitonic nematic LC on larger scales. What are the nematic mesophases that can emerge in such systems? Preliminary studies indicate richness of behavior in terms of multi-stable switching that involves soliton states with the same or different topological invariants, the Hopf indices, as well as what can be controlled by confining the host nematic fluids into thin layers (as in our prior results, Fig. 3.8). What types of new physical behavior and properties can arise because of these stable phases formed by topologically nontrivial solitonic field configurations? Technological needs & fundamental needs call for research to reveal LCs with different symmetries, topological diversity & varying combinations of order & fluidity.

**Fig. 3.8.** Phase diagrams of stability of solitons phases under confinement in a thin film of thickness  $d$  for a chiral colloidal LC with helical pitch  $p$ , explored via tuning magnetic field.



The particularly interesting high-dimensional order parameter spaces are  $SO(3) = S^3 / \mathbb{Z}_2$  of triclinic &  $SO(3) / D_2 = S^3 / Q_8$  of orthorhombic nematic LCs discussed above. The allowed topological solitons in these systems are understood based on homotopy theory, but little is known about their stability and interactions. What types of solitonic knotted field configurations can exist in these soft matter systems? For example,  $\pi_3(S^3 / Q_8) = \mathbb{Z}$  and  $\pi_3(S^3 / \mathbb{Z}_2) = \mathbb{Z}$  topological solitons would be rather interesting analogues of the  $\pi_3(S^3) = \mathbb{Z}$  Skyrme solitons in high energy physics, but can they emerge as global or local free energy minima in these systems & can they form space-filling crystalline states? Here, the two approaches for new nematic LC designs can hypothetically merge; even more colorful spectrum of hierarchical LCs will emerge if this happens. Smalyukh will collaborate with Leonov & search for this other layer of hierarchical nematic LC self-assembly in our exploration of both molecular-colloidal & solitonic nematic LCs, as well as will employ our discovery of light-powered colloidal spinning [*Nature* **570**, 214-218 (2019)] to develop active matter analogs of these systems. New symmetries of molecular-colloidal & solitonic LCs could impart material properties. They also may inspire the quest of low-symmetry condensed matter states in molecular, polymeric, micellar & other systems. The road of discovery ahead is promising entirely new worlds of these beautiful states of condensed matter & their technological utility.

**Emergent knots & chirality in bioderived systems.** Orientationally ordered photonic structures, often resembling the ones in LCs, are common to many forms of life, ranging from beetles to crabs, fish & birds, & are even found in fossils of dinosaurs. These mesoscale features evolved to become nature's all-in-one solutions for specific needs of survival or advantages, for example, enabling spectrally selective or broadband reflections of solar radiation and thermal energy management under harsh ambient conditions. Many photonic structures in nature reflect in the near infrared range (responsible for over 50% of energy due to solar radiation that tends to transform to heat), typically to enable thermal management. Certain ants, like *Cataglyphis bombycina*, survive under extreme temperature conditions not only using broadband visible and near-infrared reflection (responsible for their silvery appearance), but also by dissipating heat via radiative cooling and exhibiting porous structures to enable low thermal conductivity. While various photonic & metamaterial designs have been developed recently to both control selective or broadband reflectivity and for radiative cooling, nature keeps surprising us by revealing similar designs. Biological solutions for light and thermal regulation, many of which remain to be discovered and understood, are important for inspiring development of biomimetic and bioderived materials. For example, technological needs of thermal management in modern buildings (responsible for 40% of energy use) are largely reminiscent to those faced by diverse forms of life on Earth over the past hundreds of millions of years. Consequently, nature's light control and thermal management solutions can be adopted in developing more efficient building materials, smart clothing, and so on. Various photonic reflectors and thermal barriers found in nature can be mimicked to produce energy-efficient building materials for applications in windows, walls, roofs and other parts of building envelopes. Moreover, such materials can be made from the most abundant biopolymer, cellulose, derived from wood and even from dirty initial feedstocks like waste. Nature's particularly interesting approach for controlling light & heat involves helicoidal cholesteric structures, which in their simplest form can work as one-dimensional photonic crystals; more sophisticated forms of such nature's designs can allow for gold- or silver-like reflection-based appearance, narrow- or broad-band spectral reflectivity, various types of focusing & light/heat re-direction & so on. The diverse properties of such structures in various natural embodiments are achieved by varying the helical pitch, the distance over which the constituent building blocks rotate 360°, which determines the wavelength of reflected light, as well as by forming various spatial gradients of pitch, defects, multi-layer configurations, and so on. For example, Smalyukh and Vignolini recently developed solar-gain regulating smart window films that mimic multi-layer structures found in the cuticles of beetles (Fig. 3.9), where layers of helicoidal structure are inter-spaced by a nematic-like birefringent layer. While this may already sound like an exceptionally sophisticated design for a beetle to develop within evolution, they were surprised to find evidence for topological solitons dubbed "heliknotons" that Smalyukh discovered in synthetic LCs [*Science* 2019]. Although the concept of heliknotons has been around for only two years, it is likely that beetles and other forms of life invoked such topological solitons in optical and thermal management for over hundreds of millions of years (see the lower helicoid in Fig. 3.9d). This calls for fundamental exploration of solitonic topological structures in cuticles of beetles, as well as in cellulose-based LCs & templated by them solid films with imprinted LC order. The researchers will uncover physical principles behind energetic stability & potential technological utility of spatially localized solitons in such systems.



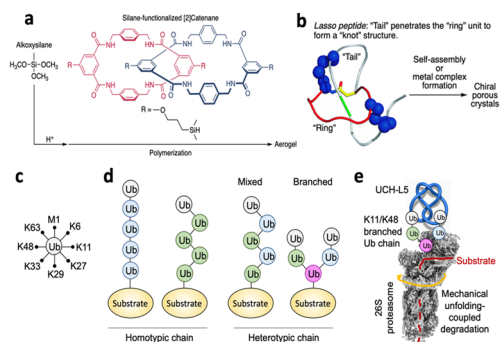
**Fig. 3.9.** Natural & bioinspired helicoidal structures & solitons. (a) Photos of *Chrysina resplendens*, the gold scarab beetle (top), and *Chrysina chrysargyrea*, the silver scarab beetle (bottom), both achieving broadband optical reflections by helical structures in their cuticles. (b) Schematic of a chiral structure formed by cellulose nanocrystals mimicking that in cuticles. (c) Solar spectrum at Earth's surface & (inset) thermal spectrum at room T. (d) A cross-section through the outer part of the cuticle of *Chrysina resplendens*, showing regions: epicuticle (1) & exocuticle comprising upper helicoid (2) nematic-like layer (3) & lower helicoid (4), & endocuticle (5). Image from [J. Roy. Soc. Interface 14, 20170129 (2017)]. (e) Schematic of assembly with near-100% reflectivity formed by 2 helical layers separated by a nematic retarder, found in the cuticle. (f,g) A TEM image (e) of nanocellulose & a photograph of an aqueous colloidal nanocellulose at ~10 wt.% (g). (h) SEM image of the helical structure of cellulose nanocrystals.

The advent of man-made photonic crystals allowed for deepening the understanding of how they interact with light, allowing for both optical and thermal management in different forms of life. However, little attention was paid to spatially localized configurations found in such systems, which are often embedded in a uniform far-field background like that of cholesteric helicoidal configurations and which resemble topological solitons like heliknotons and skyrmions recently extensively

studied in synthetic LC materials. This calls to understand and re-create them in nanocellulose-based chiral nematic LCs to demonstrate energetically stable topological solitons like skyrmions, hopfions and heliknotons in the nanocellulose-based LCs and to explore their potential relations to similar spatially localized structures found in nature (Fig. 3.9). Smalyukh, Vignolini & co-PI Matczyszyn will also uncover potential uses of solitonic structures in cellulose nanomaterials for visible light and thermal management and for controlling how such organizations can be explored for templating well-defined localized mesoscale structures. Topological solitons are marvels of mathematical/nonlinear physics, but the potential of finding them in nature and in biologically derived materials remains unexplored. We will address this need through a combination of experiments (Smalyukh, Vignolini & Lin) & numerical modeling (Tate); it is anticipated to be transformative because of enabling thermal & optical management applications, nanotemplating of localized structures, energy-efficient metamaterials and so on. We will focus on identifying the *organizing principles* behind topology-dictated self-organization, & on using the ensuing self-organized structures to, in return, control light & heat/energy transfer. The proposed research will also provide a fascinating platform for training of students and will be integrated with a large number of outreach activities.

**Crystals of knotted and linked molecules.** PI Sato has recently realized a porous crystal consisting of molecular knots, or catenanes, where [2]catenane was used as a structural component; the ensuing porous crystal exhibits an extremely small Young's modulus among all known crystalline materials and can flexibly change its macroscopic shape like gummi candy before and after the application of mechanical stress, despite being a crystal [Sato team. *Nature* **598**, 298-303 (2021)]. Within this WPI program, Sato will work on the development of such "knotted" materials with excellent mechanical and thermal properties consisting of various types of molecular knots, focusing on the following three efforts.

Chiral molecular knot-based crystals with superior mechanical & thermal properties will be developed in collaboration with Smalyukh & modeled by PIs Kalman & Kotorii & co-PI Shokef (Tel Aviv Univ., Israel). The previously reported porous crystal [Sato & team. *Nature* **598**, 298-303 (2021)] crystallizes in a chiral space group, and the [2]catenane components are helically arranged in the porous crystal. We will investigate the mechanical properties of these crystals and clarify the relationship between chirality, knot invariants and mechanical properties. For example, it may be possible to evaluate the shear modulus produced when torque is applied to the porous crystal and it is twisted, and investigate the relationship between the direction of torsion and the arrangement of the molecular knots ([2]catenane). Chirality and the mechanical properties of materials are issues that are also relevant to various structures produced by living organisms and are fundamental issues that will be addressed within this program.



**Fig. 3.10.** Chemical design strategies of knotted molecular crystals & gels based on (a) silane-functionalized catenanes & (b) proteins, & the naturally occurring (d-e) protein knotting in biological systems.

Molecular knot-based aerogels will be developed by Sato in collaboration with Smalyukh & Senyuk. They will investigate the thermal insulation properties of porous materials composed of molecular knots rather than strong bonds such as covalent or ionic bonds. They will investigate thermal conduction in materials with both porosity and molecular knots, attempting to develop materials that exhibit excellent thermal insulation

properties and high optical transparency at the same time. Specifically, they will synthesize new aerogels by polymerizing various alkoxy silanes and silane-functionalized molecular knots (silane-functionalized catenanes) (Fig. 3.10a) and then investigate their physical properties.

Another strategy of forming knotted soft matter is by using knotted protein-based porous materials. We will develop new materials by assembling knotted proteins and peptides. By combining the intrinsic chirality of the knotted protein/peptide and the meso-scale chirality generated by the self-assembly process, novel material properties will be realized. As an example of a knotted peptide, a lasso peptide structure formed from approximately 20 amino acid residues will be utilized as components for porous materials (Fig. 3.10.b).

**Ubiquitin chain branching & topologically knotted proteins.** Another example is related to protein ubiquitination, a post-translational modification by which a ubiquitin (Ub) protein is tagged on to the target protein substrate through a cascade of enzymatic reactions to signal cellular functions. Another Ub can be attached to the first Ub that is anchored onto the substrate protein via one of the eight connecting points

on the Ub, including seven lysine (K) residues and a methionine (N) residue at the beginning of the polypeptide chain (Fig. 10c). Different Ub linkage types encode for different biological signals. The prototypical ubiquitination function is used in the ubiquitin-proteasome system, which requires a linear chain of K48-linked Ubs to be recognized by the 26S proteasome for mechanical unfolding and processive protein degradation of the ubiquitinated substrate. In addition to the homotypic Ub chains that are formed by a single Ub linkage type, heterotypic Ub chains have been reported, including linear but mixed Ub linkage types or a branched chain of which a Ub molecule can be modified at multiple sites to form a more complex topology (Fig. 10d). Given the large number of branching options of Ub chains, understanding the mechanism by which the Ub branching is made with appropriate spatial and temporal resolutions calls for new experiments & theory to be pursued by Hsu and Tate. A K11/K48-branched Ub chain is involved in cell cycle regulation and protein misfolding implicated in Huntington's disease. K11/K48 chains are recognized by the proteasome for substrate degradation. Interestingly, K11/K48 chains are preferred substrates for a 5<sub>2</sub> knotted ubiquitin C-terminal hydrolase, UCH-L5, whose ubiquitin-removing activity is activated upon binding to the proteasome (Fig. 10d). PI Hsu recently found the unprecedented stability of UCH-L5 to withstand the mechanical unfolding of a bacterial proteasome, suggesting that the knotted topology confers the mechanostability required for UCH-L5 to function in a hostile environment in a tug of war against the mechanical unfolding and degradation of K11/K48 ubiquitinated substrates by the proteasome. Hsu will biochemically reconstitute a K11/K48 chain in complex with the human proteasome and UCH-L5 for cryo-EM study to glean atomic insights into the structural basis of K11/K48 chain recognition by both the proteasome and UCH-L5. The long-term goals of this thrust area of our WPI are: (i) develop new technologies to quantitatively describe the topologies of different branched Ub chains, (ii) explore the use of UCH-L5 as a sensor to detect branched Ub chains, and (iii) understand the dynamic interplay between the knotted UCH-L5 & the proteasome. **KCM<sup>2</sup>** enables interdisciplinary collaborations to solve complex biological problems, potentially helping to delineate the Ub branching problem. In the spirit of the **KCM<sup>2</sup>**, mechanical characteristics of UCH-L5 under tension will also be explored.

**Integration of interdisciplinary efforts.** The above plans are just examples of many **KCM<sup>2</sup>** activities that will be pursued, so diverse that some may say they are unrelated. However, they are all inter-knotted & inter-linked by the topology, chirality & knot theory foundations on which the progress will build. The cross-pollination between these different fields will be enabled by co-supervising each student/postdoc by 3 PIs with different disciplinary backgrounds & geographic locations, as well as through a series of hybrid weekly virtual/in-person seminars, schools, conferences, etc.

## 2) -3 System for advancing the research

\* Describe the center's research organization (including its research, support and administrative components) and your concept for building and staffing the organization. Regarding the composition of the center's personnel, describe measures to obtain diversity such as gender balance.

We will create a center of excellence with efficient and cost-effective functioning capable of supporting the most ambitious research and education goals of the WPI Center. The prospective director Smalyukh will oversee & direct the overall research operations & governance, societal dissemination & administrative efforts as suitable for a WPI center, including the new hires of top young researchers via open international searches, where 5-10 new PIs will join within the 10-year implementation period. To help implement ambitious WPI-enabled reforms within the entire HU, Abe will initially combine his current role of HU's Executive Vice President with the role of WPI's Administrative Director. Afterwards, Abe will devote himself to the role of the WPI's Administrative Director as soon as possible. Sasaki will build on her experience of having career positions in different countries to coordinate the engagement of international PIs & young researchers in institutions like MIT, Cambridge U. & others with ones at HU, including research exchanges, conferences & joint international grant applications. Our WPI will take advantage of the past successful Core-to-Core Program, "Consortium for Spin-Chirality-Based Advanced Materials", that PI Katsuya Inoue has been leading since 2015. Building on his experience, Inoue will serve as a Deputy Director for Education missions. He will also oversee smooth integration of the Hiroshima Synchrotron facility and other state-of-the-art user facilities at HU with the newly added facilities of our WPI. Prof. Aida will lead the young researcher fostering effort; with Kotorii, they will form a dream team aiming at empowering women in Japan/HU to take leadership positions in Academic environments. Working closely with President Ochi, Abe & Smalyukh, Ikegami will build WPI's relations with the local government of Prefecture & Higashi



Hiroshima city, as well as industry partners. Ikegami & Shimabara will lead our WPI's Grants/Fundraising Program aiming at supplementing the WPI Award by government and industrial grants secured by PIs through separate individual proposals, as well as taking full advantage of sources of funding from individual philanthropists & private foundations both in Japan & Globally. Deputy Director Kotorii will oversee the outreach & societal dissemination efforts, bringing knot chirality science in the forms of exhibits and demonstrations to schools and the general public at places like the Atomic Bombing Site in the Hiroshima downtown. Prof. Yabuta will be the Deputy Director for Science. In total 4 women will serve on the Management Board, as outlined in the Administrative Link Diagram (Fig. 3.11). Moreover, Yabuta & Sasaki will form a strategic planning group as well, together with Abe, to help the Prospective Director Smalyukh. Kotorii, Senyuk, Yabuta & Inoue (Fig. 3.3) will also lead the WPI's four research thrust areas. The overall functioning of the center is summarized with the "Management Link" schematic (Fig. 3.11), where attention is paid to achieve a balance of gender representation, experience, young energy & the need of both using the WPI to seed reforms & maintain its administrative autonomy, per the vision of MEXT. Our leadership will be helped by highly skilled, dedicated staff members hired by the WPI center. The WPI leadership will plan & implement education and system reforms at this WPI as a seed to then reform the entire HU, with strong support from President Ochi, as well as other universities within the Chugoku-Shikoku region & entire Japan. Director & Admin Director will meet with HU President on a monthly basis to secure the WPI's support needs & to discuss implementation of reforms. Annual business meetings of all WPI members at summer/winter schools & symposia & monthly meetings of all PIs will help develop a strategy of WPI's long-term development, including additional joint grant proposals, seminar series, course development planning, etc. A steering committee of WPI leadership & administrators will meet on a weekly basis to assure effective day-to-day operations. Director will seek periodic advise from ~5 External Advisors, prominent researchers & other Center directors to help guide & independently evaluate the WPI's operations from a broad perspective.



**Fig. 3.11.** Administrative & research operations of the Center will be masterfully inter-linked to maximize its output of research, education, outreach & benefits for the sustainable future.

\* Describe your concrete plan for achieving the center's final staffing goal, including steps and timetables.

Our expectation is that the **SKCM<sup>2</sup>** center will keep growing and flourishing, and that it one day will employ thousands of employees. However, the short-term staffing goal within the implementation period is that we have about 20-25 PIs and about 150-180 core researchers in our WPI after 5-7 years of the implementation period. Our WPI will strive to hire women scientists & administrators. Out of the 5-to-10 new WPI faculty hires, we will recruit 50:50 male/female, Japanese/International, thus boosting gender balance and creating a stimulating, highly diverse cross-disciplinary and multi-cultural environment, with a large number of young talented researchers.

\* If the center will form linkage with other institutions, domestic and/or foreign, *by establishing satellite functions*, provide the name(s) of the partner institution(s), and describe their roles, personnel composition and structure, and the collaborative framework with the center project (e.g., contracts to be concluded, schemes for resource transfer).

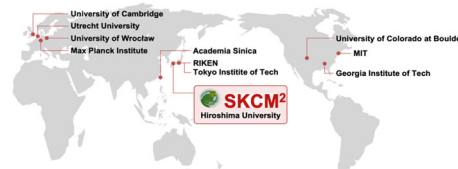
In ~2 years, we intend to hire a new PI with a possible cross-appointment at the Hiroshima branch of AIST, which is located right next to the HU campus; this potentially could lead to the establishment of a WPI satellite at AIST-Hiroshima, but this option will be considered later, jointly with the AIST and MEXT leadership. The vision here is that our WPI Director, Prof. Vignolini (PI from Cambridge U, UK) & the AIST-Hiroshima leadership will collaborate to consider the possibility of hiring a new, highly successful PI with a cross-appointment through an open international search. Very fruitful research partnerships between national laboratories & universities have led to many scientific breakthroughs & Nobel Prizes, like in the case of JILA (a joint institute of CU-Boulder & NIST). The AIST-WPI-HU collaboration could become an embodiment of such partnership between HU & AIST. By building on the pre-existing strength of AIST-Hiroshima in nanocellulose-related topology/chirality research, a collaborative effort on chiral topological nanocellulose systems will be established with a potential new joint appointment hire of a new PI. In this and other recruitment efforts, strong attention will be paid to achieving gender balance and attracting a diverse cohort of young talented researchers to HU.

\* If the center will form linkage with other institutions, domestic and/or foreign, *without establishing satellite functions*, provide the



names of the partner institutions and describe their roles and linkages within the center project.

Our current partnerships with the participating institutions (Fig. 3.12) do not involve formation of satellites. We currently have 2 WPI PIs at Japanese institutions beyond HU, Sato at RIKEN-UTokyo and Kalman at TokyoTech. Our partnerships and collaborations with Kalman and Sato are key to achieving the Center's missions from the standpoint of view of knot theory descriptions and chemical synthesis of materials with inter-knotted molecules, respectively. However, other scientific interactions of the **SKCM<sup>2</sup>** researchers in Japan and the ensuing joint publications will also involve researchers at about two dozen other institutions in Japan (as non-PI collaborators - they will secure their own funding for such collaborations). Our intention is to keep a flexible open-door policy and encourage mutually beneficial collaborations both within Japan & globally. Beyond research, our partnerships with the Tokyo-based PIs will also have outreach and education components; for example, Tokyo-based VR-based platforms will be used for outreach & education in North Japan (Tokyo Platform), where equipment will be available for mobile classrooms and will be used together with our collaborators in other Japanese institutions, which will differ from the separate platform intended for South Japan (HU platform).



**Fig. 3.12.** SKCM<sup>2</sup> as an international institute without walls.

The partner institutions outside Japan (Fig. 3.12) include 3 American Universities, the University of Colorado Boulder, MIT and Georgia Tech, the Academia Sinica in Taiwan, as well as 3 European institutions, the University of Cambridge in the United Kingdom, the Max Planck Institute in Germany and the University of Utrecht in the Netherlands. Beyond being the home institutions of the PIs, these institutions will host postdoctoral fellows and PhD students coming from Japan for collaborative visits and long-term stays. Beyond research and the use of various facilities, arrangements will be made to allow young Japanese scholars to take specialized courses while visiting these institutions, so that the breadth of interdisciplinary training of young researchers can be boosted. The PIs from these international institutions will co-mentor PhD students and will be the primary advisors for postdocs based in Japan, as well as will send their other students and postdocs to HU and other WPI nodes for collaborations. The international PIs will spend some time, typically 2-3 months per year, in Japan and will help co-organize various summer/winter schools, symposia, conferences and so on. The PIs will be compensated for their WPI-related efforts through a combination of salaries (e.g. summer salary when visiting Japan), consulting fees and bonuses, as described elsewhere in this document. Soon after the WPI grant is announced, the international PIs will visit Japan for extensive planning of joint research and education activities, as well as the Director and other representatives from HU will visit different nodes to efficiently integrate/interlink these partner institutions and research groups to pursue our Center's missions. The postdoctoral fellows and PhD students will be recruited internationally. The international PIs will help HU recruit talented women scientists in order to achieve better gender balance with our WPI center at all career levels. Young researchers will connect top global centers like MIT & Cambridge with HU & will erase disciplinary boundaries between the fields (by working with multiple co-mentors) ranging from math to physics, & planetary science. Empowered by partnerships with the top international research institutions, our WPI will seed university reforms & boost reputation, making HU like the Harvard of Japan, educating a new generation of researchers with a global perspective & contributions towards energy demand reduction, climate change mitigation, Japan's society 5.0 goals & economic growth.

- \* Appendix 5: "List of Principal Investigators" (attached)
- \* Appendix 6: "Biographical sketch of principal investigator" (attached)
- \* Appendix 7: "Composition of personnel in center" (attached)
- \* Appendix 8: "Letters from researchers invited from abroad or other Japanese institutions expressing their intent to participate in the center project" (attached)

a) Principal investigators (professors, associate professors, or other researchers of comparable standing)

\* Paste onto table a) in Appendix 7.

	At beginning of project	At end of FY 2022	Final goal (Date: April, 2027)
Researches from within the host institution	9	9	10
Foreign researchers invited from abroad	8	8	10
Researchers invited from other Japanese institutions	2	2	4
Total principal investigators	19	19	24

## b) Total number of members

\* Paste onto table b) in Appendix 7.

	At beginning of project		At end of FY 2022		Final goal (Date: April, 2027)	
	Number of persons	%	Number of persons	%	Number of persons	%
Researchers	39	/	78	/	156	/
Overseas researchers	17	43.6	35	44.9	79	50.6
Female researchers	14	35.9	32	41.0	79	50.6
Principal investigators	19	/	19	/	24	/
Overseas PIs	10	52.6	10	52.6	12	50.0
Female PIs	7	36.8	7	36.8	12	50.0
Other researchers	20	/	59	/	132	/
Overseas researchers	7	35.0	25	42.4	67	50.8
Female researchers	7	35.0	25	42.4	67	50.8
Research support staffs	2	/	4	/	4	/
Administrative staffs	7	/	13	/	13	/
Total number of people	48	/	95	/	173	/

	At beginning of project		At end of FY 2022		Final goal (Date: April, 2027)	
	Number of persons	%	Number of persons	%	Number of persons	%
Doctoral students	8	/	22	/	72	/
Expected employment	8	100.0	22	100.0	72	100.0

**2) -4 Securing research funding****Past record**

\* Give the total amount of research funding (e.g., competitive funding) secured by the principal investigators who will join the center project. Itemize by fiscal year (FY2017-2021).

The table summarizes funding of the current cohort of PIs. For example, Vignolini & Smalyukh have the level of funding from various government and private funding sources exceeding 2 million USD per year. Some of our PIs are young in their career, but very successful in attracting funding, able to do so even while still being postdocs & students, e.g. via competitive fellowships & grants.

FY	Total amount (yen)	
	All PIs	All personnel
2017	649,865,481	834,889,314
2018	658,549,889	864,233,723
2019	576,281,565	837,314,565
2020	571,884,136	882,617,136
2021	561,063,726	788,393,393
2017-2021	3,017,644,798	4,207,448,131
Average	603,528,960	841,489,626

**Funding prospects after the establishment of the center**

\* Based on the past record, describe your concrete prospects for securing resources that match or exceed WPI grant (FY2022-2026).

The international PIs currently secure 5-10 times more funding than HU PIs. Part of the reason is that the researchers at HU & in Japan generally rarely pursue sources of funding outside of Japan, but this will change once this WPI is funded. Coaching sessions on how to apply to international foundations will be introduced & HU PIs will gain access to funding from many private/philanthropic foundations around the World; the English-speaking personnel of our WPI will be able to support such grant applications. Furthermore, extensive collaborations of HU PIs with PIs at top research institutions globally will make their applications more competitive. We therefore expect that the grant totals per PI for HU researchers will increase 3X within the next 5 years and 5X by the end of the project implementation period. The research funding of international PIs is anticipated to double in 10 years. The above estimates account only for the external funding not including the WPI grant from MEXT that will be based on this proposal.

\* Calculate the total amount of research funding (e.g., competitive funding) based on the amount of funding that the researchers will allocate to the center project. Be sure that the funding prospects are realistically based on the past record.

Based on the past record, we expect that the total funding of individual international PIs will range between 1 and 3 million USD per PI within the project implementation period. For Japan-based PIs, the anticipated funding of the PIs and co-PIs with whom they collaborate will range within 0.2-1 million USD per PI. While the funding of additional grants secured by PIs will soon exceed that of the WPI grant from MEXT, all our WPI's PIs and co-PIs will jointly operate the annual considerably larger than that of the WPI award alone,

which will grow within the implementation period so that the formal end of the WPI project after 10 years will be inconsequential for the Center's operations. Overall, to help sustain the proposed Center after 10 years, we will pursue external funded projects, including by new WPI hires, will retain the University's commitment and will secure funding from international foundations (see section 4.3 below for details).

## **2) -5 Interdisciplinary research**

\* Describe the fused research domains, why interdisciplinary research is necessary and important in the target field(s), and what new field(s) can be expected to be created by way of this project. Describe your concrete strategy for fusing different research domains and creating new field(s) by the fusion.

Topology and chirality manifest themselves in phenomena on many length and time scales, across the natural hierarchy, from elementary particles to biological and cosmic systems, as well as in pure math, like in the knot theory, in planetary sciences and cosmology, and so on. Topology and chirality are both examples of a "poster child" for emergence, the notion of the sum of the parts being less than the whole, so that a reductionist goal of reassembling understanding from well-understood components is not possible. Promising significant new discovery, the emergent synergy of knot topology and chirality requires dealing with a hierarchy of length and time scales as well as with creation of entirely new concepts, laws and generalizations, which are only possible within an interdisciplinary international research network, like the one we propose to establish. For example, chirality of structure can enable spatial-time configurations with the chirality of motion and vice versa, but understanding these emergent phenomena is hindered by disciplinary boundaries. This motivates us to cross-pollinate and fuse the topology- and chirality-focused research domains, bringing together researchers that rarely meet. This philosophy provides the underlying motivation of our proposed institute. It will create a new interdisciplinary knotted chiral meta matter emergence-focused research domain that is not a branch of physics, chemistry, biology, or material science, nor that is a subfield of engineering, but rather is an intrinsically interdisciplinary mixture of these, a pursuit in which substantial progress is made simultaneously in the context of all these fields. Our Center will holistically explore the enabling role of chirality and knot topology at subatomic-to-cosmic scales, with a focus on the tabletop research and translation of fundamental knowledge into applications, leading to the new field of knotted chiral meta matter. Mathematical concepts, like the ones of knot and homotopy theories, will aid us with understanding, classification and generalization of findings. While the bulk of our research will focus on experimentally highly accessible systems, like liquid crystals, colloids, magnets and biopolymers, our findings will have immediate impacts for the studies of objects and phenomena on less accessible scales, like black holes and elementary particles. Conversely, theories of particle physics and cosmology will inspire us to develop deeper understanding and practical utility of related phenomena based on these accessible biological and condensed matter systems. The anticipated future technological applications enabled by the Center's fundamental research will range from sustainable energy-efficient building technologies to materials for extraterrestrial habitats to biomedical detection and treatment of diseases and to spintronics and data storage devices. Cumulatively, these future values of our research will help assure a sustainable future.

## **3) Global Research Environment and System Reform**

### **3) -1 System for advancing international research**

\* Describe your concrete plan for building an international research center including the makeup of its foreign researchers, establishment of oversea satellites, or similar functions. Include a time schedule for the plan.

\* Describe concretely your strategy for staffing foreign researchers (e.g., postdoc positions) through open international solicitations.

Describe the procedures you will use to do so.

\* Describe measures to help foreign researchers sustain & strengthen activities under conditions when international exchange is limited.

We intend to establish an institute without walls, a Center of research excellence with the prominent global presence and visibility. Therefore, we have attracted international PIs with highest research visibility and from top institutions globally to participate in our effort. While we plan to have no international satellites, we intend to strongly engage the international PIs and co-PIs, as well as the young researchers, as key contributors to all research and education missions of our WPI center. This will be done by inter-knitting our activities through joint advising/mentoring of young researchers who will mediate inter-PI interactions

and partnerships. The young researchers will be hired through international searches while making the selections/recruitments jointly with PIs at the international nodes, so that candidates for these positions will meet everyone's high expectations, as needed for fruitful international collaborations. The director will oversee all key decisions related to internationalization, including personnel, hiring, budget, etc. His leadership team, outlined in the "Administrative Knot" diagram, will assist with the implementation of vision and goals of the proposed project, so that we can hit the road running once the WPI award is announced. Once we hear about the WPI funding, we will work immediately (by starting with securing visa paperwork, if needed) to have international PIs & co-PIs come to visit HU. HU will buy out fractions of teaching/service effort time of foreign PIs from their institutions, to increase the time they can spend at HU, e.g. through long-term sabbatical & other stays, cross-appointment, consulting & other agreements. Foreign PIs will be the primary advisors for postdocs hired at HU, who will spend 50% time abroad in labs of these PIs. All Center-supported PhD candidates will have foreign PI co-mentors, spending 50% time abroad. Joining a research group is like becoming a family member for our Center's PIs, so that the foreign PIs will be all inter-knotted with family-like links & knots to their HU-employed group members. Welcoming new group members is what foreign PIs look forward to (see their commitment letters). These PIs will be great role models for HU young researchers to follow, giving them global research perspectives & collectively integrating knowledge of best practices in mentoring from ~100 top institutions globally. Young researchers will connect the top global research centers with HU & will erase disciplinary boundaries between the fields (by working with multiple co-mentors) ranging from math to physics & planetary science. The international scope of the proposed WPI will also benefit from Smalyukh's diverse international experiences, ranging from undergraduate education in Ukraine to PhD studies and faculty career in the USA, and to a series of extended stays and sabbatical visits in Germany, France, Israel, United Kingdom, the Netherlands and Japan. His experience will serve to help build success in interactions between HU and other PIs and co-PIs. Building on experiences (transferred via multiple past & future discussions) of three other WPI Directors of previously funded WPIS who are based in the US home institutions, Smalyukh will work to maximize his time available to be devoted to different missions of the WPI, including the time when he will be physically in Japan. He will also travel to different nodes of the WPI Center while leading administration, collaborative research efforts at HU, CU & globally, building the research community. His day-&-night, 24/7, year-round strong commitment, enthusiasm & dedication will be vital for inspiring & educating a new generation of researchers with a global perspective, as well as to building up the center's organization and putting its operation in order at HU, which will receive his very direct & full involvement. A regular in-person seminar series at HU will have a zoom component, allowing international researchers join, with timing chosen to make this comfortable for WPI members in different time zones. If the pandemic continues limiting international exchanges, we will mitigate its impact by using VR and teleconferencing platforms, remote experimental training with the help of GoogleGlass and similar tools.

### **3) -2 Establishment of international research environment**

\* Describe your concrete strategy for establishing an international research environment, administration system, and support system (e.g., appointment of staff who can facilitate the use of English in the work process and provision of startup funding) to accommodate researchers from overseas.

A robust and highly effective environment with optimal conditions for international collaborations and young researcher exchanges will be established (Fig. 3.13). PIs from international institutions will have their research group footprints at HU and will physically stay 2-3 months a year in Japan/Hiroshima to direct collaborative research, mentoring & co-mentoring postdocs & students at HU. There will be regular research seminars & other meetings every week online to share progress with other WPI members. WPI schools will be organized every year; all members will get together for a week or two to allow the extensive discussions to exchange the ideas. We recognize that the close communication among the members is the top priority in this WPI management. The frequent exchange of ideas at various organized occasions will ensure productive inter-disciplinary research in a cross-pollinating way. Some of key efforts will include:

- Reforming graduate education & cross-disciplinary training
- International research exchanges, schools, conferences & forums
- Public lectures by Peace Nobel Laureates complementing science at the HU-WPI winter schools
- Partnership and synergy with Hiroshima Peace Forum
- Development of synergies with Boulder TASI & Cond. Matter Schools
- A KITP Program at UC Santa Barbara in 2027, to be organized by Sasaki, Smalyukh & Mark Bowick

(Assoc. Director of KITP, UCSB) to bring together an even broader community for about 12 weeks  
 → We will hire at least 20% of staff from outside of Japan, will handle paperwork & all activities solely in English & will set a highly effective environment for international engagements as described below

\* Concretely describe how the center will provide an environment in which researchers can work comfortably on their research by being exempted from duties other than research and related educational activities (e.g., allocation of adequate staff support to handle paperwork and other administrative functions) including your procedure and time schedule.

To expeditiously achieve the center's goals and missions, various cumbersome procedures will be eliminated; the administrative staff will be granted extensive discretionary powers to be more effective and proactive. In addition, staff will be allocated to provide "one-stop support" for all procedures and paperwork related to employment and daily life (Fig. 3.13). The workload of HU PIs will be reviewed and tasks that do not have to be done by persons with a professor-level skillset will be delegated to the support personnel; in conjunction with this, to further enable the center director and PIs to focus on research, an adequate number of secretaries and other administrative assistants with appropriate skills will be hired by the center. These measures will be implemented by the end of FY2023, so that the WPI center can release its researchers from nonessential administrative duties as quickly as possible. The URA unit of the university will provide dedicated support in attaining international grants, in recruiting scientists and promoting relationships with other entities, such as local government and industry, as well as other institutions in this part of Japan. We will strive to keep the workload related to service and all administrative duties of WPI PIs/Director within 10-20%, so that most of their time can be dedicated to research and education/outreach efforts.

**Fig. 3.13.** The Center will establish the international research environment.

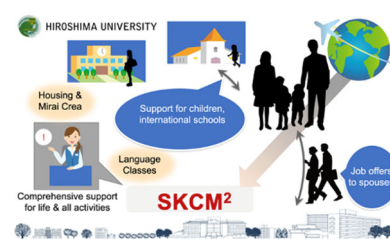
\* Describe your strategy, procedure and timing for periodically holding international research conferences or symposia (as a rule, at least once a year).

Smalyukh, Inoue and practically all PIs have extensive experiences (Fig. 3.14) in organizing international meetings like summer schools, symposia and conferences. For example, Smalyukh organized an annual series of summer schools, called Inter-continental Advanced Materials for Photonics (iCAMP summer schools, <https://www.colorado.edu/i-camp/>) that took place on all inhabited continents in countries such as USA, UK, Argentina, Uruguay, China, Australia and South Africa; their success was highlighted in multiple articles by researchers and editors, including in journals like Nature Photonics, Physics Today, Liquid Crystals Today and many others. Inoue organized a large number of international meetings as part of his Core-to-Core program at HU funded by the JSPS. Figure 3.14 shows photos with exciting thank you notes from students at the events organized by Smalyukh (top) and Inoue (bottom). Building on this experience, we will run a series of summer/winter schools and other meetings to deliver on education and international scientific exchange missions of the proposed WPI center. The major goal of the summer and winter schools of our WPI will be to combine advanced graduate-level education with learning about diverse cultures and the best practices of research/education around the World. While some of the schools will be held at HU, the others will be organized at our other WPI nodes, and also in other locations to be chosen; in all cases, the lectures will be webcast in real time and later archived. The WPI's symposia and workshops will complement the education missions of the extended schools (one-two weeks) by bringing the top international researchers to shorter meetings, in order to exchange the excitement about the most recent scientific developments in the field. We intend to organize at least one school and one symposium or workshop per year, though some years will see more meetings organized.

**Fig. 3.14.** Building on past successes, the Center will organize a series of summer/winter schools, symposia, workshops and other meetings.

### 3) -3 Center management and system reform

The proposed Center is envisaged as an independent research organization, acting as an autonomous unit within HU, envisaged as a test bed to reform HU & other universities.





\* Describe the role of the center director and the administrative director.

Our WPI nominates Professor Ivan Smalyukh as its Director. Ivan started his career as an undergraduate student and a research assistant in Lviv, Ukraine. He then did his PhD and postdoc in the USA, before starting his independent career at the University of Colorado Boulder in 2007. Dr. Smalyukh has experience running a large research group (30-40 people at a given time within the last 10 years, with the total number of group members within 2007-2022 now approaching 200). Ivan is well acquainted with the establishment and management of institutes as he is a founding fellow of the Renewable and Sustainable Energy Institute in Boulder, Colorado (a joint institute of the National Renewable Energy Laboratory, NREL and University of Colorado) as well as served on a Founding Task Force and Executive Committee of the Materials Science Engineering Program at the University of Colorado. His excellent achievements, broad perspectives and outstanding communication skills will help the newly formed WPI to attract top-quality researchers from around the world and organize them as effective research enterprises. As many of the attached letters confirm, he is the best candidate for the proposed Center's director post. He will spend maximum possible time at HU and more broadly in Japan on a regular basis, aiming to oversee the management of the entire center. While on a sabbatical leave from CU-Boulder, in addition to many other visits over last 7 years, Smalyukh cumulatively already spent nearly a year in Hiroshima. His collaborations with researchers at HU & in Tokyo flourish. Building on experiences of three other US-based WPI Directors at Harvard University, University of Illinois Urbana-Champaign and University of California at Berkeley, he will strive to maximize the time devoted to the WPI, including the time when he will be physically in Japan. Smalyukh will have daily zoom calls with staff when not in Japan & will be aided by the Yabuta-Kotorii committee in planning activities & running the Center. The HU president's office will work closely with Smalyukh to ensure that he has all the needed support to lead a very successful international institute. Soon after receiving a positive notification from MEXT, Smalyukh will work with HU president's office & CU-Boulder to sign memorandums of understanding (MOUs) specifying all relevant matters needed for the his effective leadership. Within the HU, our WPI will have a level of considerable autonomy envisaged by MEXT for WPIs. The Director will make all key decisions related to personnel, hiring, budget, etc. His leadership team (see the "Administrative Knot" diagram, Fig. 3.11) will assist with the implementation of vision and goals of the proposed project.

Prospective Administrative Director Abe will cooperate with the Director & coordinate the administrative support necessary for the execution of center's missions, including execution of plans designed by the Director and supervising administrative staff in the course of all administrative duties. Dr. Abe has been engaged in top-level chemical science research and fully understands the research missions of the center. As an Executive Vice President of the entire University, he also has an in-depth understanding of how to effectively use the WPI-based reforms as a testbed to reform the entire University system. His personal networks will help recruit talented administrators. His experience on the international stage and excellent language skills will also facilitate communication with foreign researchers and administrative staff. Abe will initially combine his current HU's Vice President role with the role of WPI's Administrative Director. Afterwards, Abe will devote himself to the role of the WPI's Administrative Director as soon as possible.

\* Concretely describe your concept for establishing the center's administrative organization, the center's decision-making system and how authority will be allocated between the center director and the host institution. (Describe concretely the mechanism for decision making when the person in charge of management and the person in charge of research and education in the center are different, and describe the responsibility relationship between the two.)

The center Director is given all the needed authority related to organization and management of the center, playing the following major roles in the institute's functioning:

1. The Director defines strategic missions and goals, including both long- and short-term missions and goals, as well as determines the plans and timetables that effectively lead to their implementation
2. The Director develops ideas, designs and plans that maximize the interactions and effective collaboration of researchers, strengthening the Center's organization as an entity within HU
3. The Director recruits & continuously updates the composition of a strong leadership/administrative team that can be effective in delivering on assigned tasks
4. The Director initiates and oversees the recruitment of promising young researchers & new PIs
5. With help of his leadership team, the Director oversees the dissemination of the Center's research outcomes to the scientific community & society, as well as oversees the investment/spending of various resources

The Administrative & Deputy Directors will communicate with other center members while the Director

is occupied with tasks, like international activities. Deputy Directors Kotorii, Yabuta & Inoue will bring to the table tremendous experiences in conducting outreach/dissemination activities, overseeing science missions & organizing international exchanges/collaborations & reforming graduate education.

\* Concretely describe how the center will adopt a rigorous system for evaluating research and will introduce a system for merit-based compensation (e.g., annual salary scheme). Describe your procedures and timing for operationalizing these systems.

The salary compensation for international scholars recruited by the WPI and collaborating with the WPI members on a part-time special appointment basis will be at a complete level, comparable to that of top US-based research institutions. Japan-based scholars traveling to other countries in which our WPI nodes are located will be compensated & supported at a level comparable to that of host institutions. This is important as, for example, the minimum salaries of postdoctoral fellows at MIT are ~\$60,000 or higher (depends on the number of years after PhD), where the University can issue necessary paperwork for the visiting postdoc scholar only if such minimum requirement is met. Therefore, our WPI will handle each exchange visit of young/senior researchers with thoughtful & generous considerations of all related aspects to assure that the researchers are comfortable & well supported while pursuing international collaborations. While the annual salary of the participating PIs will be set by their home institutions, including in cases of joint/cross appointments, our WPI will strive to reward exceptional productivity and contributions to our WPI's development by bonuses allocated based on merit-focused evaluations (the concept of meritocracy will be introduced by our Director). To implement this bonus-assigning procedure, the Institute will calculate the so-called "PI Performance Index of WPI" ( $\text{PIPI}_{\text{WPI}}$ , denoted as  $\Pi_{\text{WPI}}^2$ ) in the beginning of the performance period & then on an annual basis. In partnership with HU-based PIs, the Director derived the following expression for this index:

$$\Pi_{\text{WPI}}^2 = \sum_{i=0}^n \delta \eta_i + \pi \sum_{j=0}^m \chi_j / \delta + \pi^2 \sum_{k=0}^l \Omega_k + \pi^3 \Delta - \pi^4 Z,$$

Where,  $\pi \approx 3.14$  and the first term  $\sum_{i=0}^n \delta \eta_i$  intends to reward publications, with  $\delta$  being the number of PIs of the center involved as co-authors of a publication;  $\eta_i$  is the impact factor of a journal in which the article is published, summed over  $n$ , the number of articles published by a PI in a given year (only journals with  $\eta_i > 1$  count). This term encourages collaborative publications in high-impact journals. The second term rewards additional research grants that the PIs will secure to supplement the WPI grant from the MEXT, where  $\chi_j$  is the number of equivalents of 1 Million USD in a grant secured,  $m$  is the number of research grants received within a given year. The 3<sup>rd</sup> term rewards major national and international awards received by PIs in a given year, where  $\Omega_k$  counts major awards for research and education accomplishments, summed over the number of such awards in a given year, whereas the 4<sup>th</sup> and 5<sup>th</sup> terms reward and "punish" for other positive contributions  $\Delta$  and negative impacts  $Z$  on our WPI, respectively. Each year, a threshold value of the  $\Pi_{\text{WPI}}^2$  index will be determined and a "bonus bank" will be allocated to the PIs in proportion to their  $\text{PIPI}_{\text{WPI}}$  indices. This scheme for rewarding excellence in research & outstanding service to the WPI missions. It will be perfected based on experience and eventually considered for adaptation at entire HU. The  $\text{PIPI}$ -based meritocracy scheme was discussed extensively with the PIs and received their approval, though feedback on its further improvement is welcome and considered up until it will be implemented with the start of the project performance period.

### 3) -4 Research environment

\* Concretely describe how equipment and facilities, including laboratory space, will be provided in a manner appropriate for a "world premier international research center." Include your procedure and timing.

To provide a space and environment for productive research, HU will secure research space currently occupied by nine of the HU PIs, which will be available for our WPI from the time of adoption, along with the full access to user facilities at no cost (Fig. 3.15). The WPI Center will be initially housed in an HU research space (1,800 m<sup>2</sup>, owned by the PIs affiliated with the University) and the Venture Business Laboratory (VBL, 1,510 m<sup>2</sup>). In addition to these spaces, a new research building, which will be directly connected to the existing building, will be secured to enable the physical gathering of the WPI members under one roof. The new research building, which will serve as the core of the center, will have an open space, the Exchange Lounge, which will provide an environment for meetings & informal discussions to promote the fusion of different fields and brain circulation. In addition, HU has established a network that allows for a collaborative use of research facilities of five universities in the Chugoku region, with facilities including Hiroshima Synchrotron Radiation Center (HiSOR), an important national joint-use facility, as well

as RIKEN and AIST labs in the surrounding area. All of these shared-use facilities are well equipped. By FY2025, a new research building (5,000 m<sup>2</sup>) will be completed to provide a physical environment where approximately 150 people can conduct research under one roof. The new research building, which will serve as the core of the Center, will have a conference space and lounge to provide an environment for meetings and open discussion to promote interdisciplinary collaborations. The Phoenix Intl. Center MIRAI CREA at HU was recently built, equipped to house researchers with families, also having many conference rooms for meetings.

**Fig. 3.15.** Shared research facilities & capabilities at HU, to which the WPI members will have access at no cost.



\* Describe measures taken with regard to the research environment to sustain and strengthen research activities under conditions when international exchange is limited.

To maintain & strengthen research activities in situations where human exchange is restricted, like during pandemics, the following system for foreign scholars will be established:

- 1) develop & adopt remote training & communications that utilize modern platforms like GoogleGlass, distributing such tools among all international & domestic nodes of the WPI
- 2) digitization of communications about research ideas & outcomes with Slack & similar tools
- 3) enhancing support for remote & automated equipment operation
- 4) reforming educational activities with VR-based education & outreach platforms, aiming at seamless communication between HU & Tokyo platforms & also among collaborating researchers nationwide
- 5) support for families: employ foreign researchers' spouses in positions of their choice, such as researchers, URAs & administrative staff, through resource allocation at the President's discretion
- 6) in cooperation with local governments, such as Higashi-Hiroshima City, provide English-language support for the daily lives of researchers & accompanying persons, including schooling & housing
- 7) create an environment in which all administrative work can be completed solely in English, with staff who can handle it; to learn how to support overseas researchers, we will send administrative staff & URAs to international nodes for training to strengthen the support system & will recruit 20% staff from abroad.

\* Concretely describe how the center will consider arranging for its researchers to participate in the education of graduate students.

The Center will fully support the salary of students as Research Assistants when they are involved in WPI-related research. Each student will be co-mentored by 3 PIs with different backgrounds, with one PI being the primary mentor. The Center will oversee the creation of new graduate coursework & tutorials, which will be co-developed by PIs from different international nodes that constitute our WPI Institute.

\* Describe new measures to improve or abolish existing systems and practices in the host institution toward optimizing the center's research environment.

Streamlining the research- and education-related processes and boosting efficiency are among the key objectives of the proposed center. HU has created 24 unique incubation research centers & independent research centers, which represent the University's distinctive research efforts. When establishing our WPI, these existing centers will be reviewed, reorganized, integrated & restructured, forming five new interdisciplinary centers serving as permanent research institutions. This will help reduce the administrative burden, saving operational costs and overall boosting the output of our research/education enterprise. Our WPI will play the role of a key testbed for these centers. Therefore, as shown in the appropriation plan in this proposal, resources will be intensively allocated to support the WPI center over the long term, including budget, human resources, facilities and equipment. This means that the entire university will work together to promote the establishment of this WPI center.

\* Describe your measures other than those described above for ensuring that world's top researchers from around the world can comfortably devote themselves to their research within an international and competitive environment at the center.

Overseas members will stay at HU Phoenix Intl. Center MIRAI CREA (fully furnished) on campus for mid- to long-term stays/visits. MIRAI CREA has rooms & facilities for science meetings & needs of family members, so that visiting scholars can productively generate new ideas & focus on research at ease.

International Engagement Lead Sasaki will oversee &, with help of staff, coordinate the schedule of visits of foreign PIs with families for longer periods of time to assure that, in addition to productive research, their children can enroll in schools or daycare & the families receive all the needed support.

#### 4) Values for the Future

##### 4) -1 Generating and disseminating the societal value of basic research

\* Describe concretely and quantitatively the center's policy for widely disseminating the societal significance and value stemming from the results of its basic research to the general public.

The SKCM<sup>2</sup> Center intends to be the most productive WPI center out of all that were funded up to now, with hundreds of high-quality publications in top international high-impact journals published every year, hopefully attracting great interest of other researchers & the broader community to which these outcomes will be disseminated. In addition to researchers themselves, these efforts will be supported & managed by dedicated science communicators & illustrators; the overall outreach efforts of the SKCM<sup>2</sup> will be led by Dr. Kotorii, communicating the ability of our WPI's basic research to solve global problems (Fig. 3.16).



**Fig. 3.16.** Outreach demos in a high school in Ohio, USA conducted by Smalyukh (left) & in Hiroshima conducted by Kotorii & Smalyukh (2 middle images). Right: *KCM<sup>2</sup>* outreach with elementary schoolboys.

Through high-impact publications & outreach, we will convey to scientific communities & the general public how our fundamental research helps address many knotty problems that Japan & the entire World face, like the growing energy demand & its impact on climate change. For example, buildings consume 40% of all generated energy for cooling and heating; 20% out of it is lost through windows, the least efficient part of the building envelopes. Could one maintain the desired environment within a building interior without energy consumption, like in a thermos? Sato & Smalyukh collaborate to develop such transparent super-insulating materials by cost-effective fabrication of novel aerogels via knotting/linking molecules. Jointly with Vignolini, they will also develop materials for the building envelope inspired by gold & silver beetles that use porous chiral structures for thermal regulation (silver/gold reflections play a role like silver coatings in a thermos, though instead noble metals beetles use the emergent power of chiral self-assembly of chitin fibers). Learning from nature, we will develop low-cost energy-efficient materials from nanocellulose. The architectural appeal of golden- & silver-looking materials might help with future deployment of this technology. From yet another perspective, further developments of electronics require miniaturization, which is limited by quantum effects at small scales. These limits can be overcome by our chiral magnetic spin systems and topological insulators. For example, the superior racetrack memories can utilize topologically protected multi-dimensional solitons like hopfions as information carriers to design entirely new principles of future electronic devices, where topological objects like knots in fields can serve as information carriers. From the standpoint of biomedical applications, changes of knotting in proteins can cause protein metamorphosis diseases, such as Alzheimer's disease, so the ability to detect and control these processes may aid in developing biomedical treatments. Knots are also found in the viral RNA genome of coronavirus whereas the spike protein coat that changes with mutations of coronavirus may be responsible for vaccine inefficiency, as studied by our PI Hsu, showing how our research may help to address pressing problems that the World faces while achieving missions of Japan's Society 5.0. We will pursue a vast variety of outreach activities designed to elevate public awareness of our sustainability enabling *KCM<sup>2</sup>* research paradigm & to attract talented young people to science careers, under the oversight of Prof. Kotorii, Deputy director for outreach. WPI's summer schools will have public lectures & outreach activities designed to interest the public in Japan in science for sustainability. Mimicking the US NSF's guidance for dissemination of research outcomes to public, each PI will develop their own unique outreach component of the WPI-related activity to broadly share the excitement about the research. Public lectures by Peace Nobel Laureates will complement science programs of WPI schools, calling for important roles to be played by scientists to sustain global peace. Our WPI will seed reforms & boost reputation, making HU like the Harvard of Japan, educating a new generation of global researchers & contributing to energy demand reduction, climate change mitigation, Japan's society 5.0 goals & economic growth.

##### 4) -2 Fostering next-generation human resources linked with higher education

\* The center should be a platform for establishing a research system in which new interdisciplinary domains can be created within a rich

international environment. Describe concretely and quantitatively the initiatives to be taken to foster young researchers, including doctoral students, through participation in such a research system within the center.

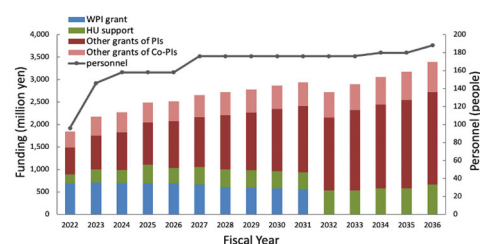
A key goal of our center is to develop the next generation of talented researchers and educators who have deep expertise in the interdisciplinary fields of knotted chiral meta matter. Our WPI will provide training and career development support at each stage, from graduate student to post-doctoral fellow to tenure-track or tenured faculty, where the support of young researchers will be our top priority. Over 50% of the WPI grant funds will be dedicated to supporting young scientists, including PhD students. To promote highly interdisciplinary research, we will introduce a system of co-mentoring young talented researchers, doctoral students & postdocs, who will have 3 co-advisors with different backgrounds. For example, a doctoral student in Physics at HU might be co-advised by HU PIs in chemistry or math & by another PI from an international node. Specialized graduate coursework will be co-designed & taught by our WPI PIs. Our strategy will take advantage of the top international research centers in this area, allowing students and postdocs from HU, TokyoTech and RIKEN-UTokyo to spend extended periods of time at the other WPI nodes, such as MIT, Cambridge & CU-Boulder. Conversely, Japanese institutions will host young researchers & PIs from the international nodes. Special arrangements will allow doctoral students to take specialized courses at the partner institutions. Furthermore, to help reform graduate education & cross-disciplinary training, we will introduce new coursework, along with the international research exchange, schools, conferences & forums to bring the broader interdisciplinary community together. Our WPI will pay PhD students' salary, like in the USA graduate programs, as well as will sponsor student/postdoc exchanges between Japanese & international nodes. Using matching funds, 5-10 new young PIs will be hired within the implementation period, striving to attract the most talented young researchers & achieve gender balance & diversity. Our WPI will seed reforms of education & research at HU & throughout Japan, will promote internationalization & gender balance in academia, will mobilize & reinforce global research efforts for a sustainable, peaceful future. The WPI will strive to hire women PIs, students, postdocs & administrators. We will collaborate with institutions corresponding to its nodes outside Japan & with EPSRC Centre on Topological Design at Univ. Birmingham to manage our newly formed Ph.D. program while adopting the best practices from around the World. Out of 5-10 faculty hires, we will recruit 50:50 male-female, Japanese/International, thus boosting gender balance & a stimulating multi-cultural environment. Young researchers will connect top global centers like MIT & Cambridge with HU & will erase disciplinary boundaries between the fields ranging from math to physics, chemistry, biology & planetary science.

#### 4) -3 Self-sufficient and sustainable center development

\* The center needs to become self-sufficient and sustainable after the funding period of 10 years ends. Describe the host institution's mid- to long-term plan and schedule for supporting the center's development, including the reform of the host institution's organization, the provision of personnel with priority allocation of tenured posts to the center, fundamental financial support, and material support including land and buildings.

Our center management will motivate (including through salary bonuses) the PIs to seek additional funding from both government & private/philanthropic organizations. Young researchers, postdocs & students, will be encouraged & aided to apply for various fellowships & scholarships. In addition to the MEXT WPI grant, PIs will pursue multiple individual applications in Japan & elsewhere (Fig. 3.17). Our ability to attract such funding will be enhanced further by the network of collaborations & visibility of research outcomes of the **SKCM<sup>2</sup>**. Besides these conventional funding sources, we will pay attention to private foundations (like the Simons, Templeton & Moore foundations in the USA) & will establish Endowed Chair positions & student-postdoc fellowships jointly with philanthropists & industry in Hiroshima/Japan/globally, as well as local governments of Hiroshima prefecture/city. While several young PIs will join HU-WPI with the start of WPI grant & will be initially supported by it, these WPI positions will be converted to tenured & tenure-track positions within the performance period & before the end of this project. While HU's support will be sustained after 10 years, the supplemental funding will grow with each success, making **SKCM<sup>2</sup>** a fully independent permanent center of excellence at HU, self-sustained after the implementation period. The newly constructed building will be WPI's headquarters both within & beyond the 10-year implementation period.

**Fig. 3.17.** Our research budget & personnel projections for achieving a successful, sustainable Center within & beyond the implementation period.





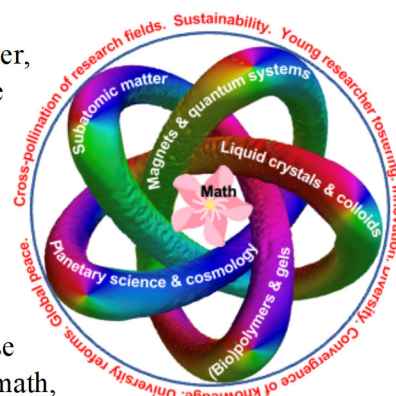
## Vision of the prospective director, Prof. Ivan Smalyukh

Everything, ourselves included, is made of molecules and atoms, which are made of electrons, protons & neutrons, which are made of quarks and leptons... Researchers revealed smaller and smaller building blocks of matter, classified them, & detected their “fingerprint” signals coming from far riches of the Universe and its history. With each breakthrough, we felt “touching the depths of nature with bare hands”, though we have been playing by nature’s rules all along, uncovering just tiny fragments of its vast unknown. Feynman’s words “What I cannot create, I do not understand” resonate with my vision to develop new building blocks of matter, analogs of nature’s quarks, protons, atoms & molecules, which would boost our understanding of nature’s inner workings and allow for making new forms of matter by design. I have been introducing such building blocks [*Nature* 2013, *Science* 2019, *Nature* 2019] & phases of matter [*Science* 2018, *Science* 2019, *Nature* 2021] that so far have no direct analogs in natural systems. I now seek to establish an entire research paradigm of **knotted chiral meta matter (KCM<sup>2</sup>)**, with knots in fields as building blocks, through cross-pollinating topology with chirality knowledge across disciplines & scales & through fostering technological innovation to solve the most challenging global problems. The WPI program of MEXT is the only one in the World uniquely adequate for these ambitious goals, with the excitement & support at Hiroshima University (HU) creating a fertile ground.

Each time I returned from my visits to Japan, I brought Mizuhiki presents for my family and friends. Within this artform, many beautiful things can be made from a humble building block, the rice paper cord. When giving public lectures, I explain my research motto by drawing parallels with this art. What nature did not give us, I want to make by knotting and knitting physical fields, molecules and colloids. I want to understand nature’s inner workings at the subatomic-to-cosmological scales by exploring the fabric of spacetime and recreating it in observable physical fields, by understanding & controlling tangles of biological molecules like proteins & RNA. A Mizuhiki artist’s hand can create almost anything. In our designs of building blocks of matter, “knot chirality” can play the role of the artist’s hand by enabling the stability of knots in physical fields and polymer strands. This may help understand how nature uses different types of broadly defined chirality within the entire hierarchy of length and time scales, like charge-parity (CP) violation to prevail existence of matter over anti-matter and molecular chirality to control conformations of biopolymer strands essential for life. Learning and mastering such nature-inspired skills can endow us with the abilities to create new materials, cure diseases, & understand nature’s inner workings.

The tradition of Mizuhiki is said to have brought people together throughout the millennia of history. The dream of establishing a new interdisciplinary field of science brings together my team of PIs. We will interknit together mathematical knot theory and subatomic and cosmological physics with creations of knotted fields in magnets, liquid crystals and colloids, and with observations of knotted strands of proteins, RNA of coronavirus genome, and so on. Our center will tie together basic science with reforming graduate-level education in Japan and globally, dedicated both to expanding the bulk of scientific knowledge & to enabling a sustainable future. We dream about a large international scientific network with a **central mission to identify the organizing principles for emergent KCM<sup>2</sup> phenomena**.

Our interest in chirality relates to its emergent co-creation power, stabilizing particle-like solitons and knots in phenomena across the entire hierarchy of length and time scales, from subatomic to biological and cosmic systems. Promising significant discovery & differing from simpler disciplinary definitions of chirality, like in chemistry, this knot chirality requires dealing with a hierarchy of length and time scales & creation of entirely new concepts, laws & generalizations, which is only possible within a research effort uninhibited by disciplinary boundaries. Our “knot chirality” is a “poster child” for emergence, motivating us to cross-pollinate and fuse diverse research fields, defining the **identity** of our WPI. Our **KCM<sup>2</sup>** is not a branch of math, physics, chemistry, biology, material science, or engineering, but rather is an intrinsically interdisciplinary mixture of these, a pursuit in which progress is made simultaneously in the context of all these fields. Our WPI will holistically explore the role of knot chirality at subatomic-to-cosmic scales, with a focus on tabletop fundamental research, leading to a new field of the **emergent KCM<sup>2</sup> science**.



Mathematical concepts, like the ones of knot and homotopy theories, will aid us with generalization of findings. While we will focus on systems like liquid crystals (LCs), colloids, magnets and (bio)polymers, our findings will provide insights into related phenomena in experimentally less accessible systems, like black holes, elementary particles & origins of life in the pre-biotic world. Conversely, theories of subatomic physics and cosmology will inspire us to deepen our understanding of related phenomena in these highly accessible condensed matter systems. For example, mathematical solitons can materialize in open crystal lattices of the heliknotons found in chiral LCs & in ones formed by bioderived cellulose nanocrystals & in configurations within cuticles of *Chrysina resplendens*, the gold scarab beetle. Porous thermally super-insulating materials with interknitted molecules & designable reflectivity can be used in building envelopes (cumulatively responsible for 40% of all generated energy) to reduce the energy demand. From the biomedical standpoint, mis-knotting in proteins can cause diseases, such as Alzheimer's, so the control of these processes may aid in treating diseases. Our fundamental science can aid in solving the most challenging problems by enabling technologies that reduce the energy demand to slow down climate change, a threat bigger than that of a nuclear war. Knowledge traditionally took decades to “diffuse” across disciplines. We will reduce this time 100-fold by removing disciplinary boundaries & building on Japan/HU's strengths while developing our new paradigm.

Our WPI will sponsor exchanges of students and postdocs between HU, Japanese institutions, and those of foreign PIs, circulating young talent between our global network's nodes. Combined with recruiting efforts, we will hold annual meetings with subsidized participation for young researchers, building on my experience of organizing annual inter-continental advanced materials for photonics schools (iCAMPs). PhD training will define a context for the formation of a community of graduate researchers, built around activities designed to broaden the education base, foster scientific growth and expand global perspectives. By team-teaching courses and drawing students from different preparation backgrounds, our WPI will become a focal point for interdisciplinary training, enabling students to learn by performing projects in a collaborative environment. We will partner with HU's existing programs to support young researchers ranging from students to professors. The new WPI will become a magnet attracting & a knot inter-connecting young talent globally. It will create a testbed for research-based education reforms within & beyond Japan. Young researchers face big challenges in the early stages of their careers, some of which are specific to Japan. There is a strong intention to introduce changes, but the process is slow. Our WPI will reform this system profoundly and expeditiously, not through “writing and reading the air”, adopting the best practices of US & UK PhD programs while “customizing” them to Japan and making them even better.

WPIs funded so far seem to strengthen elite Japanese institutions that are already well-funded research centers. For HU, the WPI would be a game-changer, a chance of attracting many outstanding international researchers while working hand-in-hand with top research centers in Japan and globally by fostering research exchanges. Strongly committed to gender diversity, our WPI would help HU with recruiting talented leading researchers with very high global recognition & visibility, as well as talented postdocs & students from other countries & premier research centers globally, whom HU cannot attract otherwise. For MEXT, this is an opportunity to truly co-create a center of research excellence. Our WPI would help foster research excellence by bringing together top international leaders in the emerging *KCM<sup>2</sup>* field/paradigm under one roof of the WPI building at HU for interdisciplinary collaborations, potentially enabling future Nobel Prizes & Fields Medals.

Meetings with other current US-based WPI directors convinced me that it will be possible for me to focus on science and the “big picture” while directing the WPI. I will approach this endeavor creatively, like research and everything I do, but I will need help in running the WPI. The support of President Ochi is amazing: he offered a new building & his administrative “right hand”, Administrative Director Abe, to help implement reforms. Also important will be the support of my scientific soulmates, with whom we share the vision to create our WPI dedicated not only to expanding the bulk of scientific knowledge but also to enabling a sustainable future. We will interknit natural & social sciences through science-based fostering of young researchers and engagement of female students to interest them in academic careers, as well as through university-public-industry-Government relations & outreach, strengthening the public support for science that promotes sustainability & peace. A beautiful chiral object, the Oleander flower is a symbol of the rebirth of Hiroshima, & a symbol of our passion to create the new WPI and the paradigm of *KCM<sup>2</sup>* – **IT WILL BLOSSOM!**

# World Premier International Research Center Initiative (WPI) FY2022 the Second Screening Proposal

## Host Institution's Commitment

June 1, 2022

To MEXT

Mitsuo Ochi  
President, Hiroshima University

I confirm that the measures listed below will be carried out faithfully and concretely as follows regarding "the I<sub>2</sub>SKCM<sup>2</sup> Center." if it is adopted under the World Premier International Research Center Initiative.

### Concrete Measures

· Describe the concrete measures that the host institution will take to satisfy the following requirements.

- 1) **For the center to become a truly "world premier international research center" and independent by the time WPI support ends, the host institution must clearly define the center's role within its own mid-to-long-term strategy and provide its comprehensive support from the time that the funded project starts, while showing that the center contributes to achieving the host institution's missions, etc.**

※ Describe how the center will contribute to achieving the host institution's missions, enhance the founding spirit/philosophy of the host institution, and contribute to realizing the objectives of its operation, etc.

※ Describe the center's role within host institution's own mid-to-long-term strategy.

Hiroshima University's mission is to contribute to the well-being of humankind by realizing a free and peaceful society based on the following five guiding principles: The Pursuit of Peace; The Creation of New Forms of Knowledge; The Nurturing of Well-Rounded Human Beings; Collaboration with the Local, Regional and International Community; and Continuous Self-Development. As specified in HU's fourth MEXT mid-term (2022-2028) goal, the university aims to become a world-class research institution with a concentration of intellectual assets, including cutting-edge education and research facilities, that serve as a hub for international academic achievement. The establishment of the SKCM<sup>2</sup> Center strongly aligns with the University's guiding principles and top-priority issues. **Therefore, the University will match or exceed the financial support from the WPI program in order to develop the center as an independent organization involving world-class researchers and students.**

- 2) **Provide a mid-to-long-term policy on the direction of the host institution's operating organization, one that includes the reform of the institution's existing organization in ways that will achieve the center's independence and create a permanent place for it within the organization. A concrete plan must be established and a schedule set for carrying out the restructuring of the host institution's organization.**

※ Describe your mid-to-long-term policy on the direction of the host institution's operating organization and provide a concrete plan and schedule.

### Basic policy

During the third MEXT mid-term period (2016-2022), the University created 24 incubation/independent research centers that have developed into distinctive research clusters. The University will restructure these research centers into five permanent interdisciplinary research organizations, with the SKCM<sup>2</sup> Center as a symbol of them. In this restructure, resources will be allocated to support the Center over the long term, including funds, human resources, and facilities and equipment. The entire University will work together to promote the establishment

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of this world-class research center.

## Plan and schedule

MEXT (FY2022) funded a new HU administrative division, established under the HU president, to be responsible for the strategy and promotion of the University's research capabilities. This division, the Headquarters for Research in Collaborative Sciences Enabling the Future, has the mission to create a center for interdisciplinary research by consolidating and reorganizing the research centers that the University has created on its own during the third MEXT mid-term period. **This center is truly a symbol of the university's centers for interdisciplinary research. The consolidation and reallocation of existing centers will be discussed by the headquarters, and resources, including budget, human resources, and facilities and equipment, will be allocated to this center over a long period of time.** The SKCM<sup>2</sup> Center will be the core institution, and HU will revise its university regulations to make the Center a permanent educational and research organization by the end of FY2022, thereby demonstrating university-wide support. In FY2022, HU will start the necessary procedures for the reform of the University's graduate school education and research program, as well as prepare laboratories and a research support system to accept PIs from outside for the full-scale operation of the Center, starting in 2023. Also, we will start preparing for the construction of the new facility with HU funds and will also submit a budget request to MEXT. The facility will be completed by FY2025.

### 3) Describe the host institution's concept for allocating its basic and other budgets and provide sufficient support for carrying out the center's operation and research activities, including necessary human, financial, and system support. In addition, when utilizing external funds other than the WPI grant for the center's operation and research activities toward realizing the missions of the host organization, show the relationship between the center and the other external funds.

\* If a prospect exists for utilizing external funds other than the WPI grant for the center's operation and research activities, indicate the application/acquisition status of the relevant external funds and the relationship between them and the center. (If the following programs are included, be sure to describe them. Their relationship to the center can be illustrated if appropriate.)

- WISE Program (Doctoral Program for World-leading Innovative & Smart Education),
- Supereminent Program for Activating Regional Collaboration (SPARC),
- Open Innovation Platform for Industry-Academia Co-creation (COI-NEXT),
- Center of Innovation (COI) Program,
- Program for Promoting Regional Revitalization by universities as Center of Community (COC+ Program)

## Resource allocation and other support

In order to maintain the center, priority personnel allocation to this center has been determined by the University-wide Personnel Committee using the long-term personnel allocation plan formulated in the 4th MEXT mid-term goals. From the start of this project, about five English-speaking administrative staff will be assigned to support the operation of the Center. In the sixth and later years of the Center's activities, the personnel expenses contributed by HU will be increased to secure employment expenses for about five new PIs. **Funds for researchers and support staff after the sixth year will come from HU's 75th anniversary campaign (2024), "Fund to Revitalize Hiroshima through the Dynamism of the University," seeking donations of 10 billion yen from within and outside of the University. A specially appointed fund manager will be hired to conduct a variety of fundraising activities to ensure the sustainable operation of this center.**

**In addition to the amount of support provided by the Program, the University will allocate the same or greater amount of resources to the following measures.** These measures will continue after the end of WPI program.

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- (1) In addition to the space used by PIs affiliated with HU (approximately 1,800 m<sup>2</sup>), the VBL building (1,510 m<sup>2</sup>) will be renovated, and a new research building of approximately 5,000 m<sup>2</sup> will be constructed to provide research space, offices, and space for collaboration and communication. A conference room with a web conferencing system will be installed to accelerate the fusion of new fields and brain circulation.
- (2) To attract excellent researchers from all over the world, the Center will allocate 100 million yen per year in discretionary funds to the director to ensure independence in the management of the Center and to acknowledge researchers' achievements.
- (3) 200 million yen in personnel expenses and 100 million yen in facility maintenance expenses (building maintenance, utilities, etc.) will be allocated annually.
- (4) Research administrators dedicated to the Center will be assigned to provide full support for the acquisition of large-scale research grants. In addition, support staff with excellent English language skills will be assigned to ensure smooth and productive interactions and collaboration among the very diverse personnel at the Center.
- (5) HU will establish flexible personnel systems such as cross-appointment to recruit excellent researchers from Japan and overseas.
- (6) Faculty members employed by the Center will be recognized as professors or young faculty members who are conducting particularly outstanding research and will be exempted from teaching, academic affairs, and administrative duties during the WPI project period if they so desire, providing an environment in which they can devote themselves to research. During this period, the educational and research programs concerned will be supplemented with additional personnel.
- (7) A web-based authentication system that allows for decision-making and payment even from overseas will be introduced.

### **External Funding Plan**

The university's president has taken the lead in promoting collaboration with companies and local governments, and has constructed a hall for international conferences and an international exchange center with donations of over 2 billion yen from Satake Corporation and 500 million yen from Higashi-Hiroshima City. In the current fiscal year, Hiroshima City has donated 1 billion yen and Satake Corporation has donated 500 million yen, and the center will further strengthen its education and research capabilities. After the establishment of this center, the entire university will continue to actively work on obtaining external funding. The university has already introduced a naming rights system for on-campus facilities and a system that increases the indirect cost of joint research with companies to 30%. The increased amount of external funds obtained through these efforts will be replenished to this center in order to build a foundation for permanent activities. Each PI will contribute to the new academic research area of *KCM<sup>2</sup>* and actively apply for large domestic research funds. In terms of overseas funds, we will strive to jointly apply for funds from Horizon Europe, NIH, NSF, NASA, etc. in the U.S. with international PIs. In addition to conventional funds from government agencies, we will establish endowed courses and fellowship programs in collaboration with private foundations (e.g., Simons Foundation, Templeton Foundation, Moore Foundation, etc. in the U.S.). We will work diligently to obtain these additional funds and make the center self-supporting in 10 years.

For local funding, Research Administrators Ikegami and Shimabara will help maintain close relationships with Hiroshima Prefecture, Higashi-Hiroshima City, and key industrial partners, with the cooperation of the President and Administrative Director Abe. The University's Open Innovation Platform will provide support for intellectual property management and joint research with companies.

- 4) Provide for the independent operation of the center including after the WPI grant period ends. Provide necessary support to include the long-term provision of human and financial resources, facilities, equipment and other elements needed to retain the center as a "World**



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**Premier International Research Center.” Also, secure and provide from an early stage of the center’s establishment the infrastructure needed for it to carry out its activities (e.g. land, research facilities and equipment, research space), and do so with a commitment to continually maintaining this infrastructure after the WPI grant period ends.**

### **Facilities and equipment**

From FY2022, The Center will be located in an HU research space (1,800 m<sup>2</sup>, owned by 9 PIs affiliated with the University) and the Venture Business Laboratory (VBL, 1,510 m<sup>2</sup>). Addition to VBL, by FY2025, a new research building (5,000 m<sup>2</sup>) will be completed to provide a physical environment where approximately 150 people can conduct research under one roof. **The new research building, which will serve as the core of the Center, will have a conference space and lounge to provide an environment for meetings and open discussion to promote interdisciplinary work and collaboration.** These facilities and equipment environment will be available after the end of WPI program.

In addition, the University has established a rich network of shared-use facilities with five universities in the Chugoku region, as well as with Hiroshima Synchrotron Radiation Center, which is a national joint-use facility, RIKEN, the National Institute of Advanced Industrial Science and Technology (AIST), and National Research Institute of Brewing.

Overseas members, including Prof. Smalyukh, will stay at the Phoenix International Center MIRAI CREA at HU. MIRAI CREA was recently built and is fully furnished and equipped with appliances using a donation of 500 million yen from the city of Higashi-Hiroshima. The facility is also equipped with space for researchers with families and conference rooms for discussions. To facilitate the long-term stays of foreign PIs & their families, HU will work with the WPI director to make arrangements for local transportation means available for the researchers during their extended stays at HU.

**5) Provide a system that will in practice allow the center director to make decisions in implementing the center project, including personnel and budgets, and that will secure the autonomy of the center’s operation.**

### **Decision-making structure**

**Since the Center will be established as an independent education and research organization in accordance with the university regulations, a system in which the center director makes the final judgment and decision on education and research activities and budget execution is ensured.** Regarding personnel affairs, the 4th MEXT mid-term plan allows for flexible personnel planning such that **personnel assignments can be made based on plans determined by the director.**

The director will be informed on the research progress, funding, and personnel status in order to decide on the allocation of expenses for equipment and personnel and to give timely advice to each team member. The director will receive such information through periodic interviews with PIs and through a project management web tool, thus introducing a system to continuously enhance the research capabilities of the entire center. Effective measures found in the Center’s improved research capabilities will be relayed back to the graduate schools, leading to organizational reforms to improve the research capability of the university as a whole.

Prof. Abe currently holds the positions of Executive Vice President for Academic and Social Cooperation and Professor at the Graduate School of Advanced Science and Engineering. After the adoption of this WPI, to help implement ambitious WPI-enabled reforms within the entire HU, Abe will initially combine his current HU’s Executive Vice President role with the role of WPI’s Administrative Director. HU plans to replace Abe with a new

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Executive Vice President as soon as possible so that he can start devoting himself to the role of WPI's Administrative Director throughout the rest of the implementation period.

In addition, a "Knot-Chiral Steering Committee" will be established to help with the Center's management, facilitated by the administrative director (Figure 5.1 and 5.2) and deputy directors. In particular, the committee will assist the Director in assuring the effective administrative and technical support of not just research and education but also other operations, including aspects related to extended stays of the foreign PIs & co-PIs at HU, exchange research visits of HU & foreign young researchers, enrolment of foreign PI's children into English-speaking schools in Hiroshima, as well as related housing & local transportation matters. With the help of Admin. And 3 Deputy Directors (Fig. 5.1), the Director will use the steering committee to initiate and implement key initiatives related to Science, Education, Outreach & Dissemination of WPI accomplishments, Administration of Center's resources and support of grant applications, recruitment of PIs & young researchers, and so on. For example, the HR/Diversity Lead Aida will help director with recruiting new PIs and young researchers while paying attention to gender balance and internationalization needs. Deputy Director Yabuta will help the Director with overseeing and encouraging interdisciplinary collaborations whereas Deputy Director Inoue will work with the Director to Develop new team taught courses and establish a system of co-mentoring of students by HU & foreign PIs. Deputy Director Kotorii will, on the other hand, work with the Director and staff to plan and implement various outreach forums and public lectures, as well making the general public in Japan and beyond aware of our WPI's research and other activities that aim contributing to the sustainable future via highly fundamental research. Led by the Admin Director Abe, the Administrators will assist the Director with managing resources, preparing various reports and overseeing staff supporting the WPI researchers. For example, the committee and staff members will assist the foreign PIs in purchasing equipment for the shared experimental research facilities, planning renovations of these facilities, planning/designing collaborative research space for the new building that is planned to be built. Along with the science writer/illustrator and other staff members, the steering committee and designated staff will assist Kotorii, the Deputy Director for outreach and dissemination, in organizing outreach activities and public lectures, as well as in acquisition of the needed VR equipment. As described in the project description document, the work of steering committee will interknit the efforts of Director, Deputy/Administrative Directors and the administrative leads, so that cost-effective and efficient operation of the WPI can be assured, including its research, education & other missions. The four research thrust leads, on the other hand, will help implementing research collaborations among PIs, including the implementation of co-mentoring and research exchange functions, also with the help of the WPI Center's staff (Fig. 5.1). External scientific experts and advisors with administrative experiences of running large centers, departments and other institutions will consult the Director and the entire steering committee on the best practices of managing large research operations. Gender balance will be assured when forming and updating the structure of the committee (Fig. 5.2).

The Center will be managed with independent personnel and funding, parallel to the overall university operation, and research administrators will be assigned within the Center's support group to assist in obtaining grants and domestic and international donations to supplement WPI operating expenses.

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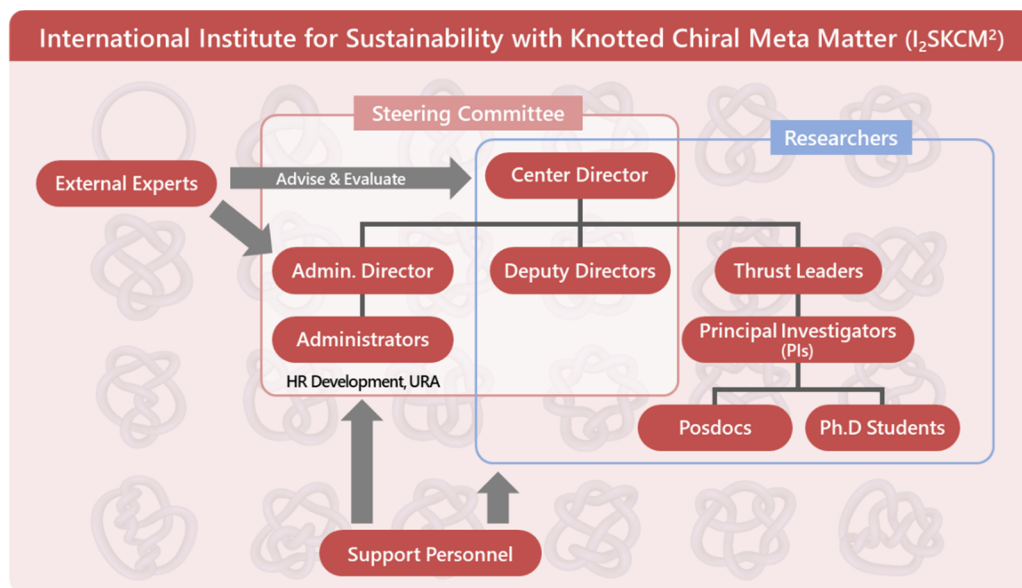


Fig. 5.1



Fig. 5.2

- 6) Provide support to the center director by coordinating with other departments regarding assigning researchers to the center and creating an effective environment for the center within the host institution. Needed adjustments to do so should be made proactively while giving consideration to their effect on the educational and research activities of those departments.

### Graduate school reforms

HU will reorganize the graduate school structure to promote the fusion of research fields and the internationalization of graduate education. The Center will establish HU's first interdisciplinary "International Program for Collaborative Sciences Enabling the Future" and accept doctoral students from any of the current four graduate schools (Figure 5.3). Specifically, graduate school programs are currently established by field, such as mathematics, physics, chemistry, biology, etc., and education and research are conducted in each field, but we will break down the barriers between these fields and implement reforms in graduate school education that squarely face the development of human resources to lead a sustainable society.

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In addition to the reorganization of the graduate school structure that has been implemented by the university, new partnerships with global centers such as MIT and Cambridge University will be utilized to promote the internationalization of graduate education and the fusion of disciplines.

Under the strong leadership of the Center's Director, the Center will promote educational reforms for doctoral students, fusion research in mathematics, physics, chemistry, and biology, and international joint research. HU promotes education to foster scientists who will lead a

sustainable society through science and technology emerging from the fusion of disciplines. This will provide strong support for the creation of new scientific fields pioneered by the Center Director.

In order to effectively support young researchers and international exchanges and collaborations, more than 50% of the Center's budget will be used to support young researchers. The director will determine the required financial support, such as accommodation expenses at collaborative research sites. These efforts will be planned and implemented with the strong support of the center director, the Center executives (Drs. Abe, Inoue, Kotorii, Yabuta, and Senyuk), and President Ochi. The center director will regularly exchange opinions with the university president, once a month or more frequently, in order to discuss the current status and resources necessary for the operation of the center.

The Director, Deputy & Administrative Directors will also periodically meet with leaders and Administrators of different Departments at HU, assuring effective and productive cooperation. Under the leadership of the Center Director, the meetings of Steering Committee of WPI & HU leaders and administrators will be held regularly, with the Center Director, Deputy Directors, Administrative Director, and PI representatives joining to discuss important matters related to personnel, budget and policies. Furthermore, Director will seek periodic advise and suggestions from ~5 External Advisors, prominent researchers & other Center directors to help guide & independently evaluate the WPI's operations from a broad perspective.

**7) Offer cooperation in flexibly applying, revising, or supplementing the host institution's internal systems as needed for the center to effectively implement new management methods unfettered by conventional modes of operation (e.g. English-language environment, merit-based pay, top-down decision making, linkage to graduate school education).**

### Improvement of existing systems and elimination of customs

In 2016, HU established its own key performance indicators (KPIs) and launched the "University-wide Personnel Committee," which allows the president to make all decisions from personnel assignment to selection. A rigorous personnel evaluation system based on research achievements is in place to centralize the evaluation criteria for

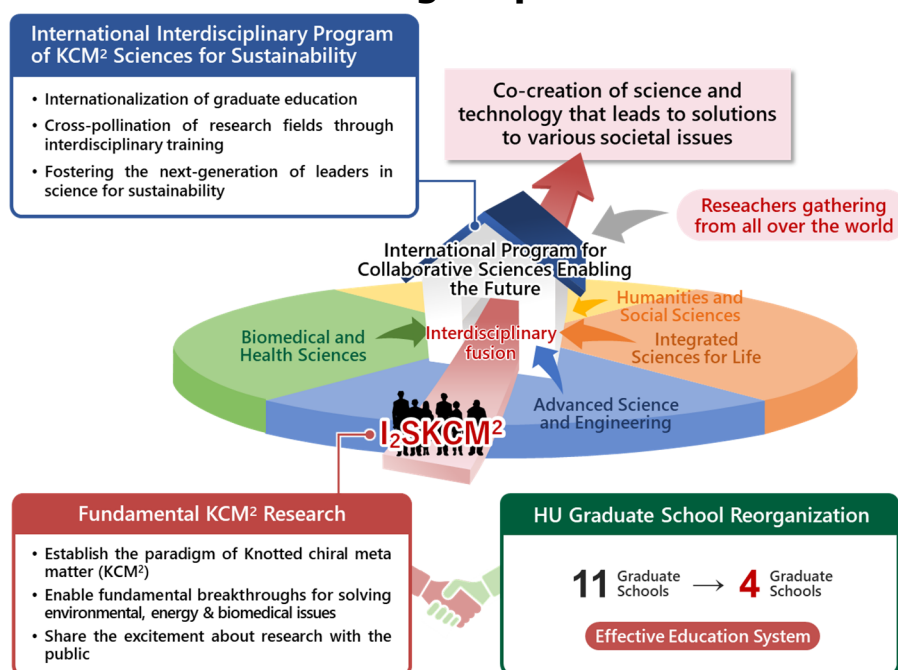


Fig. 5.3

## **World Premier International Research Center Initiative (WPI) FY2022 the Second Screening Proposal**

researchers under the originally developed KPIs and reflect performance in annual salary. Once the Center is established, research and educational activities will be evaluated within the Center, **and the concept of "meritocracy" will be introduced under the leadership of the director.** In order to promote groundbreaking research that will be published in top international journals, the annual cumulative number of citations of each PIs' papers will be calculated and used to help decide the allocation of resources and salary (taking into account differences between disciplines, such as materials science and pure mathematics). In a similar way, to facilitate international research grant applications of HU PIs along with the international PIs, including to private foundations, the successes in bringing additional grants will be also rewarded through the meritocracy-based evaluations by the director. International awards, outstanding service to the WPI missions & various other outstanding accomplishments of HU and international PIs will be also rewarded via the meritocracy-based evaluations led by the director, with the corresponding salary bonuses.

At the early stages of the WPI project's implementation period, we will introduce a new system of meritocracy for the evaluation of PIs, administrators and staff members, which will be reflected as a bonus from the director's discretionary budget (100 million yen). The support of international PIs during their stays at HU will be comparable to that of outstanding researchers in Europe and the U.S. The newly recruited PIs and postdoctoral fellows will be offered competitive salaries, equipment and facility allocations and startups. This system will be a demonstration of potential new initiatives for faculty recruitment and improvement of the academic environment. Both the institutional and operational aspects of the system will be developed to eventually be expanded to the entire university. In addition, we will improve the administrative system at HU by collecting best administration practices from the institutions of our foreign collaborators.

### **8) Provide other types of assistance to give the center maximum support in achieving its project and in becoming a world premier international research center in both name and deed.**

Many HU administrative departments will contribute to the Center so that it can implement its vision and become an independent world-class research center: the Organization for the Promotion of Academic and Social Collaboration, which is directly under the president, will provide the university-wide organizational structure; the Industry-University Collaboration Division will obtain research funds from companies; the Intellectual Property Division will provide support related to intellectual property; the Research Strategy and Promotion Division will provide researcher support and competitive funding acquisition; the Technology Center will provide research equipment support; and the Fund Office, International Affairs Division, Human Resources Division, Public Relations Division, and each department of the Corporate Headquarters, such as the Endowment Office, International Affairs Department, Human Resources Department, and Public Relations Department, will provide any additional required support.

Since the startups for new faculty hires are often not competitive with the international counterparts, say in the USA, the International Researchers newly joining the WPI at the beginning or during the project implementation period will be prioritized in terms of allocation of equipment and facility support, in order to allow the start new research groups expeditiously and effectively. Skilled staff will assist the foreign PIs with expeditious purchasing of equipment items and organizing both their research efforts and their daily life in Japan. HU and the WPI will assure the availability of English-language schooling, daycare, local transportation and other needs of families of the foreign PIs and young researchers who come to work at HU permanently (like the new PIs being recruited) or for extended visits like 2 months to one-year periods expected for the foreign PIs and co-PIs. Funds and other resources will be set aside to organize English-language schools and daycare and/or to pay the fees for accommodating needs of children of PIs in existing private schools/daycares in the Hiroshima city and vicinity. Efforts will be made to assist spouses of the visiting PIs and foreign PIs being recruited to HU by providing jobs or helping them find jobs in the Hiroshima area. Streamlined procedures will be used to



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expeditiously meet the needs of international scholars in terms of applying for visas, establishing bank accounts in Japan, reimbursing for the travel and other expenses. Various picnics, receptions and even hiking activities will be organized to bring together the WPI leadership and the leadership of HU and Hiroshima city/prefecture, as well as local industry leaders. These meetings could be used to discuss the possibilities of donations for the sustainability-focused research within the WPI, forming endowed chair positions for the outstanding WPI PIs, creating scholarships and awards for young researchers.

To help with outreach and dissemination of results, HU lecture rooms and other facilities will be provided for the needs of organizing public lectures, outreach forums WPI's open-door days for the visits of public and so on. HU will also assist the WPI center with the Information Technology (IT) and other needs. To assist the WPI with its research and education missions, and, conversely, help with the adoption of the WPI's best practices and reforms within the entire HU's system, Director and Admin Director will meet with the University President and his leadership team on a monthly basis.

**9) The host institution is to self-evaluate the results of the system reforms achieved by the center and distribute the results that it evaluates highly to all of the departments throughout its organization.**

The current HU PIs represent many different departments within HU, which they will continue being affiliated with during and after the WPI implementation period. Furthermore, the PIs hired by the WPI will choose or be assigned additional departmental/academy affiliations depending on their background. Additionally, during or immediately after the project implementation period, the newly hired PIs of the WPI for whom HU is the primary affiliations will be given tenured or tenure track positions associated with these department.

The Center will establish an education and research support system in English to **provide an environment in which researchers and students from overseas can concentrate on their research.** This initiative will be expanded to HU more widely. Additionally, I<sub>2</sub>SKCM<sup>2</sup> establishes other new initiatives related to meritocracy, improvement of gender balance and diversity, and enhancement of outreach, which will be used to guide similar initiatives for the University. Together, these will improve the research environment, promote internationalization at HU, and generally contribute to Japan's international competitiveness.

**10) (For host institutions that already have an existing WPI center and/or Academy center) Fully support and sustain the existing WPI and/or Academy center and advance its development as a world premier international research center, while being capable of fully supporting the new center at the same time.**

N/A

**11) (For host institutions that already have an existing WPI center and/or Academy center) Take the initiative to spread the existing centers' good system reform results to other departments throughout the host institution and apply them to implementing the host institution's own reforms.**

N/A

## World Premier International Research Center Initiative (WPI)

### List of Principal Investigators

- If the number of principal investigators exceeds 10, add columns as appropriate.
- Place an asterisk(\*) by the name of the investigators who are considered to be ranked among the world's top researchers.
- Give age as of 1 April 2022.
- For investigators who cannot participate in the center project from its beginning, indicate the time that their participation will start in the "Notes" column.
- If there are changes from the PI list in the first screening application documents, describe the points changed and reasons in the "Notes" column.
- Include principal investigators affiliated with satellite institutions. Give the name of their satellite institutions in the "Notes" column.
- Fill in the achievements of each PI in the "Biographical Sketch of Principal Investigators."

	Name	Age	Current affiliation (Department/ School/Institution) · Title	Specialization	Effort (%)	Notes
1	Ivan I. Smalyukh*	49	Basic Chemistry Program, Academy of Hiroshima University (Graduate School of Advanced Science and Engineering), Specially Appointed Professor / Dept. of Physics & Renewable Sustainable Energy Institute, University of Colorado, Boulder, Professor	Topological solitons, knotted matter, pre-designed building blocks of matter	80%	Center director
2	Yuka Kotorii	37	(1) Associate Professor/Academy of Hiroshima University, Graduate School of Advanced Science and Engineering, Mathematics/Hiroshima University (2) Visiting Scientist/Interdisciplinary Theoretical and Mathematical Sciences Program (ITHEMS)/RIKEN	Mathematics (topology, knot theory)	70%	Deputy center director (Outreach & Dissemination)
3	Katsuya Inoue*	57	Professor/Academy of Hiroshima University, Graduate School of Advanced Science and Engineering, Chemistry/Hiroshima University	Experimental material sciences, chemistry	70%	Deputy center director (Education)
4	Hikaru Yabuta*	47	Professor/Academy of Hiroshima University, Graduate School of Advanced Science and Engineering, Earth and Planetary System Science/Hiroshima University	Cosmochemistry, geochemistry	70%	Deputy center director (science)
5	Claire Donnelly*	30	Lise Meitner Group Leader/Max Planck Institute for Physical Chemistry of Solids	3D topology in magnets, nanoscale imaging	30%	
6	Kenta Kuroda*	35	Associate Professor/Academy of Hiroshima University, Graduate School of Advanced Science and Engineering, Physical Science/Hiroshima University	Solid state physics, momentum-space topology in quantum matter	70%	
7	Elisabetta Matsumoto	36	Assistant Professor/School of Physics/Georgia Institute of Technology	Geometry and topology of soft matter	25%	
8	Hiroshi Sato*	41	Unit Leader/Emergent Molecular Assembly Research Unit, Cross-Divisional Materials Research Program/RIKEN Center for Emergent Matter Science	Chemistry, material science	50%	
9	Silvia Vignolini*	41	Professor/Department of Chemistry/University of Cambridge	Chiral bio-materials, self-assembly	30%	
10	Andrey Leonov	42	Associate Professor/Academy of Hiroshima University, Graduate School of Advanced Science and Engineering, Chemistry/Hiroshima University	Condensed matter theory, focusing on chiral magnets	70%	
11	Chihiro Sasaki*	44	Professor/Institute of Theoretical Physics/University of Wroclaw	High-energy particle and nuclear physics (theory)	70%	
12	Jörn Dunkel*	45	Associate Professor/Department of Mathematics/Massachusetts Institute of Technology	Applied math, topology	25%	
13	Shang-Te Danny Hsu*	46	Research Fellow/Institute of Biological Chemistry/Academia Sinica	Biophysical chemistry, structural biology, knotted proteins, COVID-19	30%	
14	Tamás Kálmán	47	Associate Professor/Department of Mathematics/Tokyo Institute of Technology	Low-dimensional topology, combinatorics	40%	
15	Bohdan Senyuk*	50	Senior Research Associate/Department of Physics/University of Colorado Boulder	Chemical physics, soft matter, liquid crystals physics	70%	
16	Kenta Shigaki*	54	Professor/Academy of Hiroshima University, Graduate School of Advanced Science and Engineering, Physics/Hiroshima University	High energy nuclear physics (Experiment)	70%	
17	Marjolein Dijkstra*	54	Professor/Faculty of Science, Debye Institute for Nanomaterials Science/Utrecht University	Condensed matter theory, topology	30%	
18	Takeharu Haino*	57	Professor/Academy of Hiroshima University, Graduate School of Advanced Science and Engineering, Chemistry/Hiroshima University	Chiral supramolecular chemistry	70%	
19	Shin-ichi Tate*	60	Professor/Academy of Hiroshima University, Graduate School of Integrated Sciences for Life, Mathematical and Life Sciences/Hiroshima University	Biophysics math, applied math	70%	

\* Percentage of time that the principal investigator will devote to working for the center vis-à-vis his/her total working hours. (Activities carried out using competitive funding can be included as effort as long as they correspond to the purpose of the WPI center and are conducted for the center.)