Annex - **Case Studies**

Science Case 1: **Advanced materials for energy and environmental sustainability.**

Challenge: *Energy storage* (Advanced materials for energy and environmental sustainability; Critical raw materials; Circular economy; Climate change).

Abstract: The goal of reaching net zero emissions within 2050 demands the development of sustainable and resilient energy solutions. Novel materials with enhanced properties and functionalities, that can be viable alternatives to critical raw materials (CRMs), can promote the rapid improvement of energy storage devices and conversion systems.

Nanomaterials offer unique physical and chemical attributes that can be tailored to meet specific requirements in energy applications. However, their implementation in electrochemical devices requires a clear understanding and tracking of the degradation mechanisms and dopant dynamics from the microstructural to the cell level. This can be effectively performed by combining complementary state-of-the-art experimental techniques, such as X-ray fluorescence, X-ray/neutron diffraction and imaging, photon-neutron spectroscopy, and fast-neutron irradiation.

This science case aims at setting up a collaborative platform where IM@IT researchers will cooperate to synergistically implement a diverse array of tools and methodologies. The focus is the development of novel materials and electrochemical devices for energy applications, as well as related non-destructive analytical methods. The involved facilities will share a suite of expertise, advanced preparation, and characterization techniques, from materials science, polymer and formulation chemistry, photon and neutron probes, radiation physics and metrology.

Key capabilities span from the preparation and integration of nanomaterials, and the transformation of biomass-based waste into environmentally friendly electrodes, to the combination of elemental and morphological analysis of samples and/or structured devices. With this science case IM@IT will provide facilities able to fabricate novel sustainable solutions for energy storage systems, together with non-destructive, rapid, multi-element analysis with both quantitative and qualitative insights, invaluable methods and tools for research and industrial applications.

Science Case 2: **Safeguarding water: Tracing novel entities by advanced analytical tools.**

***Challenge**: Environment and Climate* (environmental observation; safeguarding water; neutron science with aerosols: from fundamental water research to clouds and extra-terrestrial ice geysers; atmospheric studies).

Abstract: The qualitative and quantitative safeguarding of water resources is stated as a priority for the environmental policies in the EU. To identify these chemicals and safeguard water it is fundamental to consider the interconnection between human activities and water in all its states and the complexity of the environment. IM@IT aims at developing new methods enabled by advanced analytical techniques that may help in the monitoring of the water cycle in all its complexity and highlight anthropic impacts.

Among the novel entities that require to be traced and can be the object of the development of new methods with the advanced analytical instrumentation available within IM@IT we identified microplastics and nano plastics, plastic-associated contaminants, organic emerging contaminants, heavy metals, and radionuclides.

Advanced spectroscopy techniques such as Raman spectroscopy and Fourier Transformed Infrared Spectroscopy are nowadays the golden standard for microplastic identification, while techniques based on mass spectrometry may help in the recognition of both the polymeric fraction and the plastic-associated contaminants and plastic accumulated pollutants.

IM@IT will concern the study and detection in different water bodies, snow, ice, and moisture/aerosol of micro and nano plastic, plastic-associated contaminants, emerging micro-organic contaminants, and heavy metal.

Specifically, ICPMS, Raman, and FTIR will be used to study the occurrence of micro, Nano plastic, and plastic-associated contaminants in freshwater, seawater, ice, and aerosol. LC-MS and GC-MS will be used to discover and trace water emerging contaminants. ICPMS and PGNAA will be also used for elemental analysis.

Science Case 3: **Neutron science with aerosols: from fundamental water research to clouds and extra-terrestrial ice geysers.**

Challenge: *Environment and Climate* (environmental observation; safeguarding water; neutron science with aerosols: from fundamental water research to clouds and extra-terrestrial ice geysers; atmospheric studies).

Abstract: Paracelsus considered water to be one of four elements and wrote that it is the matrix of the world and of all its creatures. Centuries later, water is a vital component for a

wide range of processes in biology, chemistry, geology, materials science as well as atmospheric and space research. Yet, many of water's famous anomalies are still poorly understood. Recent research suggests that the key to understanding liquid water may be hidden at low temperatures in the deeply supercooled regime where a second critical point may exist.

At temperatures below this critical point, low- and high-density liquids may form, yet this scenario has very recently been further complicated by our discovery of medium-density amorphous ice. Despite recent progress using mainly advanced X-ray techniques and other optical probes there is still no complete understanding of supercooled water. Our own research suggests that the low-temperature glass transitions of the amorphous ices correspond to the unfreezing of reorientation dynamics and that the unfreezing of translational motion should take place at higher temperatures in deeply supercooled water corresponding to the famous fragile to strong transition. Evidently, further studies of deeply supercooled water are urgently needed. The freezing of supercooled water is also still poorly understood including the structure of ice immediately after crystallisation and secondary processes such as the ejection of supercooled liquid jets, cracking of frozen droplets and strain-effects in the resulting ice crystals. In addition to substantial gaps in our knowledge of pure supercooled water, the situation becomes even more complex for real-world scenarios such as in clouds, where dust particles mix with supercooled water droplets, and extra-terrestrial ice geysers, such as on Enceladus, where complex salt mixtures are dissolved in the liquid ejecta.

Neutrons are in principle fantastic probes for studying supercooled water across wide ranges of length and energy scales. Yet, so far, there is a clear lack of neutron studies in this area which is mainly due to the experimental problems of preventing and controlling crystallisation during the typically quite long neutron measurements.

IM@IT aims at building a new sample environment for creating deeply supercooled aerosols under dynamic flow conditions. This will enable characterising constantly replenishing supercooled water droplets with a wide range of neutron techniques including standard and small-angle diffraction as well as deep-inelastic, quasi-elastic and inelastic neutron scattering. To complement these analyses, users may benefit from advanced tools of the IM@ITs' suite of MRF.

***Science Case 4:* Neutron Space Weather and its impact on the ageing human body, biological systems, and terrestrial electronic systems.**

Challenges: *Health, Digital, Security (improving and protecting health and well-being; health technologies and tools; technologies and digital solutions for health and care; Health Space, materials, coatings, and electronic components qualification; Development and verification of a new class of neutron detectors)*

Abstract: Extreme Neutron space weather conditions have a crucial impact on humans and ageing, on biomedical and electronic devices, as well as give rise to a high neutron dose to humans. A network of ground-based neutron monitors is key to the understanding of the nature of extreme neutron space weather events that give rise to strong enhancements of the fast-neutron intensity at ground and aerospace level. The combination of better understanding of the nature (neutron Ground Level Enhancements) and effect (through irradiation studies) of extreme space-weather on electronic systems at the ground will enable our society to be more resilient to the potential large-scale disruptions from such neutron space weather events. An extreme solar storm would give rise to a substantial power outages and damage to the power grid, severe disruption of communications, aviation, and satellites, and, concurrently, altering space weather anomalies modifying the degree of radiation exposure such as radioactive-, ultraviolet-, or geomagnetic radiation can have either direct or indirect adverse effects on human health and physiology.

The two standard designs of neutron monitors date back to 1957 and 1964 and do not allow an immediate detailed understanding and prediction (size and energy-spectrum) of these so-called Ground Level Enhancements (GLEs). Advanced neutron monitors are more compact in size and can potentially allow some energy discrimination of the spectrum of incoming neutrons. These monitor together with neutron irradiation facilities based at MRF and LSF will be used to better understand the nature and effect of GLEs and how they disrupt severely many aspects of modern life such as electronic systems for our safety (e.g., aerospace, autonomous automotive systems) and the economic activity (e.g., autonomous production, internet infrastructure, transport systems, banking systems, data centres, cloud, IOT etc.).

Ageing effects on humans and on specific biomedical electronic devices and biophysical systems can be affected at different levels depending on the type and intensity of environmental radiation. At ground level, the induced radiation dose by neutrons, as both primary and secondary particles, can change depending on the latitude and altitude, as well as function of the materials in the proximity of a given place of interest, such as rivers, lakes, snow, or mountains.

The final aim of the IM@IT will be to deploy a new generation of compact neutron monitors (CNMs) at different latitudes and altitudes to study the relation between neutron irradiation at the condition detected by such CNMs and the ageing effect on humans, electronic and biological systems, and biomedical devices. Such approach needs to be highly interdisciplinary, as mixes together know-how from hard sciences, related to the physics of neutron detection and interpretation of space weather conditions, as well as the latest technologies on which are based electronic devices and engineering, together with life sciences expertise to guide the exploitation of studies on the ageing effects of biological systems.

Science Case 5: **The new frontier for Medical Application: cross-scale, multi-modal disease trans-phenotyping.**

Challenge: Health *(Radiopharmaceuticals, Drug design, Biomaterial characterization, Personalised medicine, Biomarkers, Cross-scale and multimodal trans-phenotyping and data integration, Molecular-based disease phenotyping, Theranostics)*

Abstract: A crucial issue in biology remains the knowledge of how atoms and molecules organise themselves and move to accomplish a biological function. The long-term "dream" is to observe macromolecules at work in vivo and to describe not only the positions of atoms but also the atomic motions and conformational changes that occur. However, this is no longer sufficient. Once such a phenomenon has been properly assessed it's necessary to understand the larger picture, the multiscale pathological changes - be it at the level of cell, tissue or of the whole organism - by putting its pieces together. This is possible by integrating data from nanoscopic-microscopic to meso-macroscopic techniques.

Today, neutron scattering is still "underused" in biology, where it occupies a kind of "niche". Such a situation reduces its potential importance and impact in the medical field. We envisions the following area will significant benefit from the application of neutron technique in the biological-medical area: i) assessment of new materials for biomedical applications with particular reference to the analysis of natural biomaterials, biocompatible, bioelectronic materials and bio inks which are used for 3D printing of organs and transplant development, ii) study of protein structure and function, atoms and molecules organisation and movement to accomplish a biological function; iii) analysis of the composition of human body samples in the healthy population and disease to bridge the multiscale pathological changes by integrating data from nanoscopic-microscopic to meso-macroscopic techniques. Another important aspect of this research area will be expanding the use of neutron scattering methods in medical research to contribute to the design of new chemicals including drugs and polymers and the study of material. The neutron community significantly contributed to cyclotron-based neutron sources to produce radionuclides such as Molybdenum-99 and Lutetium-177, are used for diagnostic imaging and molecular radiotherapy of cancer patients.

The final aim of the research will be to bridge basic scientific research to clinical medicine. With the development of genomics, proteomics, and metabolomics, the organic combination of macro and micro imaging technology, and the progress in information and AI technology, clinical pathology will be promoted towards the pattern of cross-scale, multi-mode “disease phenotyping.” Such a comprehensive multiscale system combined with clinical information will provide timely and accurate disease models facilitating diagnosis for patients, and guide clinicians to make optimal and individualised therapeutic regimes. The establishment of the integrated model would help to conduct neutron research beyond the current scope, further driving current medicine to precision medicine in the future. Furthermore, this innovative model would target the hallmarks of ageing, even at clinical, subclinical than molecular levels, like oxidative stress at mitochondrial level and/or organs’ sub-chronic inflammation. The resulting goal would be to prevent markers of chronic diseases, especially in subjects with not phenotypic symptoms, to anticipate the pathologies and to reach a physiological and healthy ageing.

Science Case 6 - New Materials and methodology for restoration of art.

Challenge: *Cultural and Education (safeguarding cultural heritage, promoting training and higher education, improving and protecting health and well-being)*

This case Study proposes a holistic approach (investigation and remedial conservation of CH) on several representative types of artefacts, using advanced materials and methodologies. The main approach is to develop innovative multifunctional and sustainable materials, by exploiting the concept of nanostructure both as fillers or water/solvent droplets dispersed in a polymeric matrix, enhancing the conservator capabilities in the cleaning, consolidation and protection of artworks. The cooperation with renowned museums and conservation centres to restore iconic historical and artistic items grants high visibility to the RI.