Strategy to be implemented in the use of national funding in CERIC-ERIC

Executive summary

The CERIC-ERIC consortium was set-up 10 years ago (July 2014), upon the initiative of the participating Governments in Centre East Europe, with the scope of strengthening their research capabilities in Research and Innovation of Materials and Biomaterials.

Its innovative approach, fully implemented in the first 10 years, has been based on the availability of research infrastructures (Partner Facilities) by the participating Countries with their open access as an inkind contribution and a financial support provided only by the Hosting Country, allowing CERIC to support the outreach to selected international researchers and the opening to industrial access for all the Partner Facilities (PF). The international access, adding to the national access, has helped the national infrastructures to evolve in quality by building synergies based on their complementary use and by targeted additional investments, allowing for a multi-technique approach, unique at the global level, as required in Materials Analytical Sciences.

The quality and the impact have been monitored in detail by independent international peer review and has been evaluated as very successful, and presented in the annual reports and in specific national assessments. Furthermore, the success of the integration and its potential is evidenced by several key indicators: the increasing number of proposals received each year over the years, with 333 proposals in 2023¹; the active participation of CERIC-ERIC in Horizon Europe Projects¹; and the high-ranking publications in the consortium's strategic priority areas, such as battery research, as detailed in the last three annual reports^{1,2,3}.

To further expand and implement this approach and its impact, the management of CERIC has proposed, and its General Assembly has approved, to integrate the in-kind contribution with a limited financial contribution by each participating Country, marginal as compared to the value of the research infrastructures already provided and their operation costs. This would allow for focused and coherent CERIC reinvestments in each Country, enabling further increase of the synergies and the multiplying effect of the national activities coordinated in an international environment by the Consortium.

The strategy which has been discussed and is herewith proposed is to use this additional funding for two main activities:

- Strengthen the capability in each Country to outreach and support the international impact of the national scientific community in using the full potential by investing in training and involving additional personnel specially trained in the scientific and managerial requirements to operate in an international environment.
- Strengthen the national research capability and its complementarity with that available in the other partner Countries to allow for an increased capability to attract international talents, ideas and financial opportunities, including for industry development.

¹ CERIC Report 2023

² CERIC Report 2022

³ CERIC Report 2021



Strategy for the allocation of CERIC's membership fees in support of the integration of CERIC capabilities

Austrian Partner Facility

Introduction

In its resolution 8th May 2023, the General Assembly (GA) agreed that as long as the contribution by the Host Member State of CERIC-ERIC allows covering the statutory operations fully, 90% of the Member's annual contributions are dedicated to supporting actions integrating the capabilities of the Member's Partner Facilities, **such as PhDs, post-docs, joint research projects, infrastructure investments and promotion of CERIC-ERIC Partner Facilities research offer.** These will be agreed upon by the GA, assuring that, over a 5-year average, this support to each Partner Facility will equal at least 90% of the cash contribution provided by the relevant Member during this period.

To enable the decision of the GA, the **Directors of the PFs should define the strategy and an annual program with a five-year outlook** for their own Facility within the CERIC collaboration framework and discuss it in the BoD for submittal to the GA through the ED, with the opinion of the ISTAC.

In the following, the PFs are requested to submit their proposal, possibly coordinated and agreed upon with other Partner Facilities, to allow for a discussion and development of a joint strategy at the October BoD meeting.

Proposing CERIC Partner Facility: Graz University of Technology (TU Graz)

Proposal summary (up to 200 words)

In the period 2024- 2028 the outstation of the Austrian partner facility at ELETTRA will undergo a fundamental reconstruction of the key instruments - the High Flux SAXS beamline (HF-SAXS) and the Deep X-ray Lithography beamline (DXRL), which is caused by the refurbishment of the storage ring ELETTRA to transit from ELETTRA to ELETTRA 2.0. Due to the performance parameters of the new ring the current optics of the HF-SAXS beamline will be obsolete and will be decommissioned, while the Deep X-ray Lithography beamline will need to be partially refurbished and repositioned at the same beam exit. Additionally the TU Graz will be partner of the new High Brilliance SAXS beamline at ELETTRA 2.0, which will require further investments from the TU Graz's side.

First, the investments for the HF-SAXS are secured by internal budget shifts of the TU Graz (1.2 M \in) and by the internal **CERIC-ERIC project HF-SAXS** (0.48 M \in). However, to further improve the offer and efficiency of CERIC-ERIC user access a further automatization of the beamline with a sample handling robot and accessories is required. We ask CERIC-ERIC to support this proposal with 100 k \in .

Second, to expand the capabilities of the **Deep X-ray lithography beamline**, the energy range needs to be extended to the soft X -rays (1-3KeV). For the required installation of a mirror chamber with two movable plane mirrors at the beamline we ask CERIC-ERIC for 200 k \in .

Third, for the **CERIC-ERIC life science initiative** we ask 135 k€ for the financing of a PhD working at the partner facility. **Project costs: 435.000 Euro.**

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Section a: Current Status and future evolution of the PF

The Austrian Partner Facility operates in the framework of the Institute of Inorganic Chemistry belonging to the Faculty of Technical Chemistry, Chemical and Process Engineering and Biotechnology and is located partly on the premises of the Austrian Representing Entity, the Graz University of Technology, and partly on the premises of the Italian Representing Entity, Elettra Sincrotrone Trieste.

It consists of several different instruments:

- The AustroSAXS beamline at the Elettra Storage Ring in Trieste (SAXS), opened to users in 1996
- The Deep X-ray Lithography beamline at the Elettra Storage Ring in Trieste (DELI), opened to user in 2002; co-operation with ELETTRA and the Austrian partner facility since 2012
- Three different Dynamic Light Scattering instrument with different wavelengths in Graz and one Static Light Scattering instrument (LSLTUG), opened to users in 2014
- Anton Paar SAXSess mc2 Laboratory SAXS instrument in Graz (SXFTUG) and, on an informal basis, access to the "SAXSpoint 2.0 The Laboratory SAXS/WAXS/GISAXS Beamline" of the SoftMatterLab is used frequently for CERIC applications due to its better data quality, opened to users 2014

With this portfolio of techniques offered to CERIC, the TU GRAZ opens access to top instrumentation for conducting cutting edge basic and applied research on nano-scale materials in a broad range of fields, such as life science, pharmacy, till chemistry and material science

The partner facility operates in the framework of the. Lately the focus was increasingly targeted towards the focused research topics of CERIC-ERIC: batteries, fuel cells and life sciences.

The partner facility has a publication record of more than 1000 papers since the opening of the HF-SAXS beamline. In the period 2019-2023 the partner facility has published 240 papers in peer reviewed journals (SAXS: 224, TUG SAXS: 8, Light Scattering: 0, DXRL: 12). A list of the publications is given in Appendix A.

The team of the Austrian partner facility currently includes: on the TU GRAZ side, 8 persons (director, 3 senior scientists, one technician, 2 PHD students – 1 CERIC PhD Battery research), and part time administrative staff; on the ELETTRA side, 4 persons (2 beamline scientists, retired collaborating scientist and one part time technician); on the side of CERIC-ERIC, 2 postdocs (Infrastructure project & Ukrainian Postdoc). At present several positions (senior and PhD level) are open.

The financing of the beamline activities as well as of the CERIC activities of the TU Graz is part of the 3years performance agreement (Leistungsvereinbarung) between the Austrian Federal Ministry of Education, Science and Research and the university.¹ For the period from 2022 to 2024 in average 806 k€/year are given to salaries and 150 k€ for investments as well as consumables. Additionally, 51.5 k€ are given directly to ELETTRA for beamline fees and extra room rentals. Note, project funds and on-time investments, e.g. the implementation of the SOMAPP Lab (Soft Matter Application Lab) in Graz also supporting the partner facility for serving CERIC users, are not included in the sums.

Additionally the partner facility is involved in several projects (external and CERIC-ERIC). Below there is a list of external projects, which are integral part of the activities of the partner facility.

A.) External Projects

¹ Originally separately funded as part of the integration of research units of a former institute belonging to the Austrian Academy of Science (ÖAW), the financing is now a full part of the general budget of the TU Graz via performance agreement with a funding distribution: 80% for beamline and CERIC activities and 20% personal costs integrated from the ÖAW.

| Title | Applicants | Source | Start | Budget (€) |
|---|--------------------------|-------------------------|-----------|---------------|
| Technology development for a microfluidic sensor platform based on cellulose materials and mesoporous hybrids | H.Amenitsch (Partner) | TU GRAZ Lead project | 2018-2021 | 135.000 |
| NEP-NFFA | H.Amenitsch (Partner) | H2020 | 2021-2026 | 210.000 |
| New routes towards hierarchically porous metal sulfide films for catalysis | H.Amenitsch (Partner) | TU GRAZ Lead project | 2022-2025 | 135.000 |
| IMPRESS | B.Marmiroli (Partner) | Horizon-Europe | 2022-2025 | 65.000 |

The partner facility is deeply involved in the activities of CERIC-ERIC, which were fostering the integration within the consortium. During the CEROP project a collaboration was initiated with the Czech and ELETTRA Partner facility, which continues very successfully up to date. RENEWALS project triggered the extended use of the μ -fabrication facility and DXRL. The participation within NEP-NFFA and IMPRESS (Horizon EU) is a consequence of the strengthening of the μ -fabrication. The INTEGRA project supported strongly the life-science part of the Austrian SAXS beamine, which resulted in ongoing collaborations with SloNMR, SYRMEP beamline, the structural biology and nano-laboratory@ELETTRA.

B.) CERIC-ERIC Projects

1) Research projects

INTEGRA project (PI): 150.000 euro (mainly equipment)

CEROP project: 114.000 euro (1 Phd student for 3 years)

RENEWALS project: about 26.290 Euro (for instrumentation: Plasma system, rolling mill for film lamination Keithley 2420 sourcemeter and others, consumables, open access publications) **HF-SAXS 2.0 project**: 480.000 Euro

2) Human Resources

a) PhD program

PHDs funded by CERIC: 2 position (MOF and Battery research) for 3 years: 265.000 euro **b) Post Doc for 2 years:** INCITE 157.000 euro (MOF, in collaboration with ELETTRA)

c) Post Doc positions for Ukrainian citizens: 1 post doc position out of 4 offers in collaboration with BNC and Czech Partner facility is filled.

Section b: Five-year development plan of the PF

The proposers should describe (1 page maximum):

- 5-year objectives of the PF (what it wants to achieve in 5 years in collaboration with the other CERIC PFs) and an outline of a program to reach the objectives.

- key needs of the PF within the next five years (where possible, refer to the ISTAC recommendations) and how the proposal fits within this five-year program and with a joint program with the other CERIC PF's

In the period 2024 – 2028 the partner facility is devoted to improve the offer to the CERIC user community based on the pillars instrumentation and research:

(i) Modernization and expanding the capabilities of the HF-SAXS for the preparation of ELETTRA 2.0
(ii) Development of a microfabrication laboratory in connection with expanding capabilities of the DXRL beamline

(iii) Development and installation of a new SAXS beamline on an in-vacuum undulator - "High Brilliance SAXS beamline" (HB-SAXS beamline), which installation should start in 2026.

(iv) Strengthening the ties between the different partner facilities in life science – a research field currently underrepresented in CERIC. The scope of the proposal is aligned to the target topic in life science proposed by Slo-NMR: osteoporosis.

In July 2025, ELETTRA will upgrade its facilities by implementing a new storage ring with a symmetric six bend achromat magnetic lattice (ELETTRA 2.0) and refurbishing its beamlines. The upgrade will improve beam quality in terms of reduced dimensions, higher current, and 60-80 times better emittance. The new source quality will enable the utilization of very small X-ray beam and coherent properties of the light produced, opening the door to completely new classes of experiments.

To exploit the new capabilities, a new HF beamline replacing the current Austrian SAXS beamline will be installed at an exisiting port of the superconducting wiggler and optimized for more standard experiments, which will allow for efficient use and remote access of users. This is in line with the ISTAC recommendation of 2021 for a ramp of "automation and remote access services, especially for the new beamlines on the future ELETTRA 2.0 ring".

The ELETTRA upgrade allows a redesign of the DXRL beamline, in the framework of a gradual transformation of the existing DXRL support lab to a microfabrication laboratory. Here the incorporation of soft-X-ray energies into the existing DXRL will provide unique opportunity for enhancing the access of CERIC users to such Lithographic techniques.

In parallel, the development of a second "High Brilliance SAXS beamline" (HB-SAXS beamline) is planned, with its installation in the early 2026. It will feature a tunable energy between 4 - 16 keV and an up to 10000 times higher flux density at the sample position. The HB-SAXS should complement the portfolio of the available SAXS techniques with cutting edge applications like coherent imaging, photo correlation spectroscopy, ps-pump probe experiments or SAXS tensor tomography.

The current strength of the partner facility is mainly in the field of material science. In the five years program the initiated activities/investments in the field of life science should be reinforced and consolidated by targeted collaborative research between the partner facilities. Here the proposal of SloNMR to investigate the structure of genes related to bone diseases (more specifically osteoporosis) and the overall structure of their interaction with proteins is an opportunity to reach this goal.

Section c: Rationale and Scientific and technical description of the proposal

The Proposal should concisely describe its rationale and, how it fits in the five-year outlook, how the scientific and technical quality will be assured. For proposed PhD students, list also the University(ies) awarding the degree and the name of the proposed supervisor (s) (maximum 1 page).

The existing Austrian SAXS beamline will be transferred to an existing, currently free branch of the superconducting wiggler. The new optical layout will allow for smaller spot sizes with >10 times higher flux density at the sample position with a fixed X-ray energy of 11.4 keV. Simultaneously, the estimated SAXS resolution will be in the order of 500 nm, i.e., 3 times improvement. The overall performance of the instrument will make it competitive at the world level. The experimental stage will be converted into a highly specialized "High Flux SAXS beamline" (HF-SAXS beamline) dedicated to standard experiments in transmission and grazing incidence SAXS with a time resolution from milliseconds to minutes. The focus will be on standardized high throughput bioSAXS measurements in batch or in combination with size exclusion chromatography (investments of CERIC-ERIC project INTEGRA) and on the in-operando experiments regarding energy storage materials with applications in batteries, super capacitors, or fuel cells. To increase efficiency, an **automatic sample robot** will be employed for exchanging standardized

sample compartments for liquids, powders, and thin films, allowing for efficient use and remote access of users.

The development and installation of the automatic sample robot and the required sample environment for the various sample types is part of this proposal.

For the DXRL and microfabrication laboratory an increase of fast track/regular proposals is observable (2021: 8, 2022: 7, 2023: 6), indicating that this facility is of increasing interest to the CERIC community. At the same time the access request from the ELETTRA partner facility and neighboring institutes to single instruments in the microfabrication lab is going from 2021: 12, 2022: 25 to 2023: 78. Moreover the model of combining a microfabrication laboratory with characterization techniques was implemented in various European and national projects: NFFA (Horizon-Europe), NEP-NFFA (Horizon), IMPRESS (Horizon), NanoRegion (Interreg Slo-Italy) and RIANA (Horizon).

In order to consolidate the current investments and shape the future perspectives of the laboratory, the installation of **Soft-X-ray Lithography option** will boost the capabilities of the DXRL beamline in terms of resolution, thin film exposure and mask-development. This must be seen also in view of the decommissioning of the current Soft X-ray lithography beamline at ELETTRA (owner: CNR-IOM). In this project the installation of **a mirror chamber with two retractable mirrors** will be foreseen, which will allow the shift of the peak of incoming X-ray radiation in the energy range between 1 - 3 keV.

The Slovenian partner facility proposed research on **Osteoporosis** having a severe health impact on the aging society in Europe with enormous associated costs. The experimental work on protein-nucleic acid interactions will pose challenges that will require the advanced use of the research infrastructure already available within CERIC, such as the coupling of NMR spectroscopy with SAXS and Cryo-EM will lay the groundwork for future projects dealing with protein-DNA/RNA complexes, establishing CERIC as a consortium that can routinely offer such services to internal and external users. The related work at the Austrian partner facility will be performed by **a PhD student**. The student will be enrolled in a study program at the Graz University of Technology with Assoc. Prof. Heinz Amenitsch as the proposed supervisor.

Section d: Impact

(i) The part of the project regarding the sample robot is in line with the developments on other synchrotron facilities will strongly support the current scientific focus of CERIC-ERIC in structural biology, material science and energy research. Here the automatization with the robot and accessories will be optimally used as dedicated set-up which will lead in combination with the improved performance of the HF-SAXS beamline to an efficient use of the beamtime and at the end to a higher number of accepted CERIC proposals. The remote access will contribute to the green transformation of Europe and to reach the target of 50% CO₂ reduction till 2030.

(ii) The support of a microfabrication laboratory that can give access to standard UV, soft-lithography, and X-ray lithography would be advantageous for all of the consortium. In particular the large scale infrastructures will benefit for the development of advanced sample environments, which is currently taking place locally at ELETTRA but also at the international level as seen by the funded research projects. Therefore having both energies, soft and hard, in a single access point, would increase the potential number of users. Miniaturization of components, such as in microfluidic devices and lab-on-chips, is becoming fundamental for applications in energy and life science. Moreover, the controlled irradiation of novel materials in order to exploit and tailor their functionalization, as well as the possibilities for the fabrication of chips for (bio) sensing and catalysis. The proposed upgrades therefore strongly support CERIC core topics of research.

(iii) In combination with the studies of the participating partner facilities, the SAXS studies of the structures and conformations of osteoporosis-related genes and their interaction with proteins will provide a

knowledge base for developing new therapeutic strategies in combat of the disease. This exercise for a collaboration between the partner facilities on a thematic topic in structural biology will strengthen the experimental portfolio of CERIC in life science.

Section e: Description of the implementation

(i) The design and installation of the robotic sample changing system will be conducted together with the project of the new HF-beamline. The optimization and testing of the robotic arm will be performed during the dark period of the ELETTRA up-grade. The know-how and experience of existing systems (local: e.g. XRD II and remote: e.g. Diamond) will be used to adapt the system for the specific sample environments, such as multi-sample holders for powders, paste holder, capillary holders, multi sample holders for GISAXS samples etc. In the project also the inserts for the various holders into the sample position at the beamline as well as the off-line storage will be designed and implemented, which should allow for an easy preparation of the remote experiments with mailed in samples.

(ii) DXRL mirror chamber: The up-grade of the DXRL beamline will be performed in the periode 2027-2028. The front end will be supplied by Elettra-Sincrotrone Trieste, refurbishing the present one. The 4 slits after the front end will be provided by TUG for a total expected cost of 25.000 €.

The selection of the photon energy level will be carried out through the insertion on the photon path of a High Harmonic Rejector (HHR), an optical system which is a low-pass photon energy filter. The HHR will consist of two parallel plane silicon mirrors whose angle of incidence is adjustable. The appropriate choice of the incidence angle will allow to obtain a photon energy in the requested 1-3 keV range.

Preliminary calculations have shown that with the current beryllium windows, 50% of the low energy photons will reach the sample, which is sufficient for the requested application. We plan to buy 100 mm wide x 400 mm long mirrors. They will cost about 40000 euros each. A rough estimation of the cost of the whole chamber fabrication including mirrors, water cooling system and motors both for mirror alignment and for mirror removal in case high energy beam usage is 200.000 Euros. In hard X-ray operation mode the functionality of the currently installed filter chamber will be maintained: the use of filters allows the selection of higher irradiation energies useful in thick materials exposures to obtain a more uniform energy deposition. The calculation of the optics and the design of the chamber will be performed in kind by TU Graz and Elettra-Sincrotrone Trieste personnel.

(iii) Life science project on Osteoporosis: In collaboration with SloNMR and other CERIC PFs we will study interactions between suitable initial RNA targets, their modified counterparts and related protein partners in the system: promoter and 5'-UTR/3'-UTR regions. Here the structural results of SloNMR and the other partner facilities will be complemented by the SAXS measurements (batch or SEC-mode) and the subsequent determination of low resolution models of the overall structure at various conditions. The work will be conducted by the PhD student to be hired under the supervision of the members of the partner facility. If it is required, during the shutdown of ELETTRA for the ELETTRA 2.0 upgrade the required experiments will be conducted with beamtime applications at other synchrotrons.

The time evolution of the tasks are shown in the Gant Chart below.

| Activity | Plan Duration | | | | | |
|---------------------------------------|------------------|------|------|------|------|------|
| | (months) | 2024 | 2025 | 2026 | 2027 | 2028 |
| Robot System Specification | 3 | Х | | | | |
| Robot System Procurement | 6 | Х | Х | | | |
| Robot System Installation and Testing | 12 | | Х | Х | | |

| Mirror Chamber Design | 3 | | Х | | |
|-----------------------------|----|---|---|---|---|
| Procurement Front End Slits | 6 | | | Х | |
| Mirror Chamber Procurement | 12 | | | Х | |
| Mirror chamber test | 3 | | | | Х |
| PhD for Life Science | 36 | Х | Х | Х | |

Annex 1 – Human Resources: Resources connected to the activity of the required staff (total cost including overall estimated costs and use of the CERIC funding)

The personnel will be composed of Elettra-Sincrotrone Trieste people from optics group, of the current DXRL staff (Alessio Turchet and Benedetta Marmiroli) in the first year, and of Elettra-Sincrotrone Trieste people of alignment group and of the current DXRL staff in the second year.

| CERTC | | Total in Euro | | | | | | |
|---|--------|---------------|--------|--------|--------|--|--|--|
| CERIC | Year 1 | Year 2 | Year 3 | Year 4 | Year 5 | | | |
| Consumables | | | | | | | | |
| Personnel cost (PhD, researcher or technical staff) | | 40000 | 40000 | 40000 | | | | |
| Travel costs | | | 1000 | 1000 | | | | |
| Other costs (conferences fees, publications, training, etc) | | | | 3000 | | | | |
| TOTAL | | 40000 | 41000 | 44000 | | | | |

Annex 2 – Infrastructure Development: Resources (including overall estimated costs and use of the required CERIC funding)

The front end will be inserted in 2027/2028 therefore first the 25000 euros from TUG will be required in the first year to add the slits. Also the mirror chamber of 200000 euros is required the first year, 100% financed by CERIC.

| CERIC | Total in Euro | | | | | | |
|----------------|---------------|--------|--------|--------|--------|--|--|
| CERIC | Year 1 | Year 2 | Year 3 | Year 4 | Year 5 | | |
| Equipment | 40000 | 60000 | | 100000 | 100000 | | |
| Consumables | | | | | | | |
| Personnel cost | | | | | | | |
| Travel cost | | | | | | | |
| TOTAL | 40000 | 60000 | | 100000 | 100000 | | |

Annex 3 –SAXS publications, 2023 – 2019 (BLs and labs, incl. CERIC funded publications)

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Strategy for the allocation of CERIC's membership fees in support of the integration of CERIC capabilities

Croatian Partner Facility

Introduction

In its resolution 8th May 2023, the General Assembly (GA) agreed that as long as the contribution by the Host Member State of CERIC-ERIC allows covering the statutory operations fully, 90% of the Member's annual contributions are dedicated to supporting actions integrating the capabilities of the Member's Partner Facilities, **such as PhDs, post-docs, joint research projects, infrastructure investments and promotion of CERIC-ERIC Partner Facilities research offer.** These will be agreed upon by the GA, assuring that, over a 5-year average, this support to each Partner Facility will equal at least 90% of the cash contribution provided by the relevant Member during this period.

To enable the decision of the GA, the **Directors of the PFs should define the strategy and an annual program with a five-year outlook** for their own Facility within the CERIC collaboration framework and discuss it in the BoD for submittal to the GA through the ED, with the opinion of the ISTAC.

In the following, the PFs are requested to submit their proposal, possibly coordinated and agreed upon with other Partner Facilities, to allow for a discussion and development of a joint strategy at the October BoD meeting.

Proposing CERIC Partner Facility: Croatian PF@RBI

Proposal summary (up to 200 words)

The abstract (summary) should, at a glance, provide the reader with a clear understanding of the proposal, covering the main elements of the project, its implementation and cost.

During the years 2024 and 2025, a major upgrade of the RBI accelerator facility will be performed. Upgrade consists of building the new accelerator hall, relocation of the existing 1.0 MV Tandetron accelerator and all the existing beam lines and ion sources, as well as replacement of the old EN tandem van de Graaff with a new 5.0 MV Tandetron accelerator. Majority of funding is covered by the EU structural funds project O-ZIP. It is expected however that additional funding will be needed. In order to accomplish this, we presume that approximately 50% of available funds that will be available from the CERIC-ERIC membership fee (2024/25) will be used for procurement of equipment that could not be supplied through the O-ZIP project. The second half of funds is planned to be used for the better integration of Croatian partner facility into the CERIC-ERIC consortium network. After screening the research subjects that are of high interest to both the RBI laboratory and other partner facilities, while taking into account research priorities of consortium, it is planned to identify specific activities that have the highest synergistic effect. This will be done in years 2025/27 by the employment of young researcher that will represent RBI in those new collaborative activities.

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Section a: Current Status and future evolution of the PF

Provide (1-2 page):

- a brief summary of the present status of the PF, listing

- all its present research activities and programmes, including those not reported within CERIC (but a part of the PF);

- resources (main instruments, collaborating staff and all funding sources).

- list of the publications in the last two years.

- an outline on how the PF intends to evolve, particularly in collaboration/integration with the rest of CERIC. Briefly list the already ongoing activities with other CERIC Partner facilities. This should help to define the ongoing and future strategy.

- the possible need for new resources to make the PF more effective and visible, including administrative support to provide annual accounts. Please also explicitly refer to organisational needs within your hosting institution, allowing for a better definition and identity of the PF and its operation, its reporting and integration within CERIC...etc.

Research activities of the Laboratory for ion beam interactions are structured around the following directions:

- Basic research of interaction processes between the fast ions and matter.
- Development of ion beam analysis and ion beam modification techniques.
- Applications of these techniques in different areas among which are the most important:
 - Semiconductor radiation detectors their electronic transport properties.
 - Irradiation and analysis of materials of interest for fusion.

- Other applications in materials science, forensics, cultural heritage and environment. Also, first steps towards analysis of energy related materials have been done.

Research activities are funded presently by EU projects (EuroLabs, ReMadeArie, Eurofusion), project that funds Laboratory membership in Centre of excellence (CEMS), project of the national science foundation (HiRexs) and 2 IAEA research projects. The main funding source of the accelerator facility are funds available through the CEMS project and EU projects that funded Transnational access: RADIATE (until 2023), EuroLabs and Remade ARIE. Finally, here is a contribution of Ministry of science of Croatia for CERIC-ERIC experiments in the amount of 38000 Eur/year. In last several years about 200 kEur was allocated for operation and maintenance of the facility.

The accelerator facility is located on the premises of the Croatian Representing Entity, the Ruđer Bošković Institute. It is operated within the Experimental physics division and more specifically in the Laboratory for ion beam interactions (in further text mentioned either as Laboratory or RBI). Instrumentation of the facility is based entirely on the experimental beam lines and corresponding end stations, that utilize ion beams delivered by two electrostatic tandem accelerators. Both accelerators are of a tandem type, namely the 1.0 MV Tandetron and the 6.0 MV Tandem Van de Graaff. Each accelerator is equipped with two negative ion sources, one of which is dedicated to helium (3He and 4He) beams, and the sputtering ion source that provides majority of other ion species, starting with hydrogen. There are total 9 end stations, while 5 are offered to users' access through CERIC. The RBI accelerator facility is the largest research infrastructure in Croatia and the only one that regularly provides access to foreign researchers.

Concerning the human resources, Laboratory has 8 research scientists, 3 technical associates and 2 technicians on permanent contracts. On temporary contracts Laboratory has 4 PhD students and 3 postdocs.

Full list of publications for years 2022. and 2021. is attached in a separate file. There were total of 42 papers published in this period. The high impact papers (IF>5) in this period include Nature Physics, Environ. Sci. Pollut., Ceramics International, Appl. Surf. Sci., Surfaces and Interfaces.

Concerning the future of the PF within CERIC, the most important issue that must be noted here is the planned upgrade of the facility. Two weakest points of the facility now are: a) old buildings with inadequate conditions (temperature, humidity, electromagnetic fields, mechanical stability, etc.) and b) obsolete Tandem Van de Graaff (built in 1961) that can hardly be maintained in the future. Through the EU structural fund project O-ZIP, a new accelerator hall is now being built and a new 5.0 MV tandem accelerator will replace the present Tandem Van de Graaff. Commissioning of the new setup is expected by the end of 2025. Upgrades will affect experiments and CERIC obligations only for 3 months during 2024, when relocation of existing facility will take place, but also in 2025, when new 5.0 MV accelerator will be delivered and installed. Activities in the period 2024/25 will be very demanding to technical staff of the Laboratory. Since two technicians are about to be retired in 2025, it will be crucial to hire replacement technicians to acquire experience before retirements. Part of these funds are expected to be funded through CERIC (total 1 year)

Taking above into account it is hard to expect that in the next 2 years laboratory will be able to increase experimental work dedicated to joint projects with other CERIC partner facilities. However, this slowing down of experimental activities may be beneficial in bilateral contacts with perspective partners. Some of these are already planned through the CERIC human resources projects, jointly with Elettra and BNC. Specifically, these are: 1) DiMiNe project (Response of diamond radiation detectors in the mixed field of neutrons and gammas studied by ion microbeam induced sources of neutrons) to be accomplished with Budapest Neutron Centre. 2) LEMIS project (Analysis and imaging of Light Elements in Materials of Importance to energy Storage using ion beams) to be accomplished with Elettra. Experimental activities will be planned to complement possible difficulties expected in RBI during 2024/25. The DiMiNe project is important as it is the first CERIC activity in the research field that belongs to one of the 'core' activities of Croatian partner facility. Earlier, most of the joint activities were performed on topics outside of the main laboratory activities. We also expect that the LEMIS project will enhance plans to increase CERIC activities related to batteries.

Once the whole investment will be completed, we believe that stronger links with other CERIC partner facilities will be possible. However, it will be needed to hire researcher(s), probably at postdoc level, that will be dedicated entirely to these contacts, as most of the other staff have a lot of other obligations. It has to be noted that from the 1st October 2023, a new postdoc (Sabrina Gouasmia) is employed dedicated entirely to the performance of CERIC-ERIC activities. This position is funded by Ministry of science of Croatia. Concerning the administrative activities, RBI has good support including its project office, but it has to be mentioned that it deals with a whole Institute issues and it is overloaded. In terms of organization, all CERIC related activities are done within the Laboratory for ion beam interactions. It has to be mentioned that the current director of partner facility (Milko Jakšić) is in retiring phase, as after 31.12.2023. he can be employed only on contracts, as after the age of 65, Ministry does not fund research positions. The future head of Laboratory for ion beam interactions (Zdravko Siketić) will replace him in future as the Partner facility director.

Section b: Five-year development plan of the PF

The proposers should describe (1 page maximum):

- 5-year objectives of the PF (what it wants to achieve in 5 years in collaboration with the other CERIC PFs) and an outline of a program to reach the objectives.

- key needs of the PF within the next five years (where possible, refer to the ISTAC recommendations) and how the proposal fits within this five-year program and with a joint program with the other CERIC PF's

In the next 5 years period, the primary goal of development, will be the upgrade of the laboratory through renovation of existing building and construction of the new accelerator hall that will also host all the beam lines of the accelerator complex. Procurement of the new 5.0 MV Tandetron accelerator is now in contracting phase with expected delivery in summer 2025. Existing 1.0 MV accelerator will be

transferred to new hall already in 2024. The funding of this investment should be entirely covered by EU project O-ZIP. Unfortunately, due to the increase of prices of building and accelerator too, already now it is apparent that funding will be insufficient. It concerns mostly auxiliaries such as: gas handling system, electrostatic lenses (Q-snout) low energy side of accelerator, SF6 gas (2 tons are needed with expected value of 100 kEur) and expenses related to dismantling, transport and installation of beam lines. At this stage about 500 kEur are missing. Part of these funds could be allocated from the laboratory savings, but we believe that it will be also essential that CERIC-ERIC contributes in this major RBI investment. Specifically, costs that O-ZIP project allocated for the procurement of accelerator is 2.7 Meur, while additional 3 Meur are allocated for building a new accelerator hall. Therefore, we propose to use part of the funds available from membership fee CERIC for the procurement of one of the missing auxiliary equipment for the accelerator, most likely that will be the Q-snout lens.

With a new accelerator site being built, and all equipment being commissioned, we plan that from the beginning of 2026, Croatian partner facility will be fully operable with much more reliable operation and also a wider range of techniques available. This will be primarily due to the higher range of available ions and their respective energies. At that time (in 2026), a 3rd accelerator, namely a 200 kV ion implanter, is planned to be completed through the CERIC infrastructure project (Triple I). Also, through the second infrastructure project (EXIT), development of the new in air microbeam line will be also commissioned. In that respect, we are confident that the role of RBI in CERIC will be significantly increased in all respects.

Concerning the research areas and their harmonization with CERIC, it has to be noted that until today, the main activity of the Laboratory for ion beam interactions within CERIC was providing the beam time and assistance to external users. All other CERIC activities (meetings, training, contacts with other PFs, etc.) were much smaller in terms of staff involvement. Therefore, the Laboratory research program and strategy of development was not much altered yet by CERIC membership, mostly because of the project-oriented funding, which in the last ten years was coming primarily through the EU and national core research projects. However, with recently approved CERIC human resources projects, as well as through a possibility to reinvest a part of the membership fees, it is expected that the role of CERIC in further development of accelerator facility and research activities of Laboratory for ion beam interactions would be much stronger. This is also in a line of the ISTAC recommendation from 2023.:

The CoE encourages the PF to actively seek areas of common interest with other PFs, particularly where the Croatian PF might introduce new scientific opportunities. Such collaborations can enhance the facility's integration within CERIC and foster mutually beneficial partnerships.

This recommendation has been already partly accepted by the Laboratory, as two projects for PhD researchers will be done in collaboration with Elettra and BNC. Furthermore a postdoc dedicated to CERIC has been hired using funds of Ministry of science as of 1st October 2023. We also expect that from 2026 funding of the second researcher at the postdoc level, which is proposed here, will be in line of better integration of RBI in CERIC-ERIC. Specific research areas will be defined after planned scientific visits to other partner facilities that may offer the best synergistic effects.

Section c: Rationale and Scientific and technical description of the proposal

The Proposal should concisely describe its rationale and, how it fits in the five-year outlook, how the scientific and technical quality will be assured. For proposed PhD students, list also the University(ies) awarding the degree and the name of the proposed supervisor (s) (maximum 1 page).

The first two years of the 5-year period will be predominantly dedicated to successful accomplishment of the accelerator facility upgrade. If this activity will be successful and on time, it will have large impact to all research activities including those of CERIC from the year 2026 and beyond. Although financial strategy is not completely defined yet, we believe that with this proposal and others that are being prepared now, the whole investment cycle will be done.

The second pillar of this proposal is human resources development. Currently, involvement of RBI in CERIC internal research projects (e.g. fuel cells and batteries) is still in its starting phase (concerning batteries), mostly due to relatively small experience in these subjects that laboratory staff acquired in past. Concerning the possible joint research subjects that may be identified with other CERIC partners, activities are still in their initial phase.

Therefore, with this proposal we plan to enhance activities that will screen possible areas of collaboration, without stating yet here, which fields will be those with highest chances of success – for RBI, for other partner facility(ies) and CERIC as a whole.

When considering CERIC priorities it has been stated that (from the web page): *CERIC is providing open access to some of the most advanced analytical facilities in Europe to help science and industry advance in all fields of materials, biomaterials and nanotechnology, with a focus on energy materials and life sciences.*

By taking into account that mission, we can conclude that the strongest contribution to the excellence of RBI Laboratory and CERIC could be accomplished in the fields where the strongest expertise of staff already exists and/or where this expertise could be applied to topics of interest of other partners.

Therefore it is planned that mentioned screening phase will be performed during 2024, when relocation activities will reduce experimental work at RBI. Senior researchers of RBI, involved in different research areas will organize bilateral or multilateral meetings (at RBI or at other partners), dedicated to specific research areas which are currently in primary focus of the RBI Laboratory for ion beam interactions. These include the following subjects where RBI is currently very active and that could be attractive to other partners:

a) Investigation of wide band-gap semiconductors and their application to radiation detection and sensing technologies. Some of these materials can be used as photovoltaics and therefore contribute to the *'CERIC focus to energy materials'*

b) Development of MeV SIMS and PIXE techniques to the molecular and elemental analysis of biological samples including single cells, that can contribute to the *'CERIC focus on life sciences'*

c) Investigation of materials capable to withstand of large radiation fluxes important to nuclear energy materials including fusion, that can contribute to the `*CERIC focus to energy materials'*

Listed areas are given here only as an example, and do not exclude any other subjects that can be identified during the proposed screening phase.

We believe that only collaboration subjects where both (or more) of partners are strongly motivated, where exist worldwide recognised expertise of partners, and where the subject has high priority in terms of funding science (e.g. by EU and national), will create recognized and important outcomes.

In terms of staff involved, RBI Laboratory for ion beam interactions have currently 8 research positions, all of these can superwise postdocs that will be involved in these activities.

Section d: Impact

The Proposal should describe (0,5 page maximum) its expected impacts on the overall scientific and technical quality and capability of CERIC. How the proposal complements and fits in common developments with other activities both at the PF and in other PFs, aimed at integrating the facilities and overall strengthening of CERIC.

Again, we must consider first the impact of the accelerator facility upgrade at RBI. This upgrade will increase the range of available ion energies and ion beam currents and subsequently the reliability of the facility. This will be beneficial to all users including those that will use facility through CERIC. Also, indirectly, new and upgraded techniques will increase attractiveness of this facility and CERIC-ERIC as a whole.

Concerning the proposed human resources investments, we have to state that until today, involvement of the RBI staff was only a 'part time'. This means that all the staff involved in CERIC-ERIC activities has primary obligation to work on funded projects of laboratory and could allocate only limited time for CERIC related activities. For example, most of the PhD students and postdocs were assisting in past to 1 or maximum 2 user-access experiments per year.

But starting from this October, RBI has hired a postdoc that will entirely dedicated to the CERIC-ERIC activities. This will already increase integration of Croatian partner facility into consortium. With additionally planned 2 PhD students that will be hired through CERIC human resources projects (with Elettra and BNC), these links will be further enhanced. Final action, proposed here, that CERIC assists in employment of the additional postdoc and also to bridge a gap during 2025 by temporary employment of technician or engineer, will certainly by beneficial to strengthen the position of RBI in CERIC and also to overall strengthening of the consortium.

Specifically, newly hired postdocs will be able to dedicate themselves to: a) dedicate themselves to research subjects that will be selected in next 2 years as those off higher added value for CERIC and RBI, b) to increase visibility and attractiveness of techniques offered to consortium by RBI and c) to take over part of administration duties that current staff of the Laboratory and RBI administration is doing.

Section e: Description of the implementation

This section should describe (1 page maximum) in a clear way the maturity and implementation of the project and its timeframe. Please also describe a possible time-line of the proposed investment e.g. how the investment will accumulate over the 5 years after the contributions commence (2024). For proposals, including the hiring of personnel, outline the research/technical program.

There are 2 main pillars (tasks) of this ambitious plan.

The first task is the infrastructure development part, which will enable contribution of CERIC-ERIC to the current accelerator facility upgrade, to be accomplished in the period 2024/25. We propose a procurement of one of the crucial parts of the 5.0 MV accelerator, specifically the Q-snout lens, which could not be ordered through O-ZIP structural project, due to lack of funds. Unfortunately, about 0.5 MEur funds are missing due to the significant raise of prices, and in order to keep procurement of the main instrument (accelerator), some of its main parts and consumables (Q-snout lens, gas handling system, SF6 gas, radiation monitoring system, etc.) could not be added in the accelerator procurement. We believe that Q-snout procurement (82000 Eur) through CERIC-ERIC will be excellent sign of CEROC-ERIC commitment to actively contribute to the facility upgrade which will certainly increase reliability of experiments that will be perfomed in CERIC funded open access.

As a part of the infrastructure development investment plan, we also envisage assistance of CERIC-ERIC in hiring a technical staff (one technician), to bridge a gap in a period of retirement of one of the crucial accelerator operators that will happen in 2025. Since it is possible to get permission of Ministry of science to employ new technician only 6 months after the retirement of the former technician, hiring replacement person 6 months before the retirement will help enormously and it will also enable knowledge and expertise transfer from the experienced technician to a new, younger one. This is even more important as it will happen during the year of commissioning of the new accelerator.

The second pillar is the investment in human resources aiming for better integration of the Croatian partner facility into the CERIC-ERIC consortium. During the 2024., a series of travels of senior staff to other CERIC-ERIC partners is planned. These visits are aiming to review and identify research areas that have strong overlap between Croatian and other partner facilities. Since there are already established several contacts (e.g with Elettra, BNC and CEDAD-Lecce) we believe that such contacts will enable better integration of RBI into the CERIC. After the most important synergies will be identified, a young researcher (at the postdoc level) will be dedicated to projects identified in 2024. Three year salary of postdoc researcher is planned for this task.

Annex 1 – Human Resources: Resources connected to the activity of the required staff (total cost including overall estimated costs and use of the CERIC funding)

| CERTC | Total in Euro | | | | | | |
|---|---------------|--------|--------|--------|--------|--|--|
| CERIC | Year 1 | Year 2 | Year 3 | Year 4 | Year 5 | | |
| Consumables | | | | | | | |
| Personnel cost (PhD, researcher or technical staff) | | | 20000 | 20000 | 20000 | | |
| Travel costs | 6000 | | | | | | |
| Other costs (conferences fees, publications, training, etc) | | | | | | | |
| TOTAL | 6000 | | 20000 | 20000 | 20000 | | |

Annex 2 – Infrastructure Development: Resources (including overall estimated costs and use of the required CERIC funding)

| CERTC | Total in Euro | | | | | | |
|----------------|---------------|--------|--------|--------|--------|--|--|
| | Year 1 | Year 2 | Year 3 | Year 4 | Year 5 | | |
| Equipment | 82000 | | | | | | |
| Consumables | 10000 | 7000 | | | | | |
| Personnel cost | | 20000 | | | | | |
| Travel cost | | | | | | | |
| TOTAL | 92000 | 27000 | | | | | |


Strategy for the allocation of CERIC's membership fees in support of the integration of CERIC capabilities

Czech Partner facility

Introduction

In its resolution 8th May 2023, the General Assembly (GA) agreed that as long as the contribution by the Host Member State of CERIC-ERIC allows covering the statutory operations fully, 90% of the Member's annual contributions are dedicated to supporting actions integrating the capabilities of the Member's Partner Facilities, **such as PhDs, post-docs, joint research projects, infrastructure investments and promotion of CERIC-ERIC Partner Facilities research offer.** These will be agreed upon by the GA, assuring that, over a 5-year average, this support to each Partner Facility will equal at least 90% of the cash contribution provided by the relevant Member during this period.

To enable the decision of the GA, the **Directors of the PFs should define the strategy and an annual program with a five-year outlook** for their own Facility within the CERIC collaboration framework and discuss it in the BoD for submittal to the GA through the ED, with the opinion of the ISTAC.

In the following, the PFs are requested to submit their proposal, possibly coordinated and agreed upon with other Partner Facilities, to allow for a discussion and development of a joint strategy at the October BoD meeting.

Proposing CERIC Partner Facility: Czech PF@CUP: Surface Physics Laboratory - Hydrogen Technology Center (SPL-HTC) of the Charles University (CU) in Prague

Proposal summary (up to 200 words)

The SPL-HTC plans to focus in the following years 2024-2028 on the fundamental reconstruction of one of its key facilities - the Materials Science Beamline (MSB) at the Elettra synchrotron in Trieste, which is conditioned by the modernization of the synchrotron itself and its upgrade from Elettra 1.0 to Elettra 2.0. According to the synchrotron work plan, the existing MSB will be decommissioned in mid-2025 and, due to its layout and parameters, it will not be possible to reuse it once Elettra 2.0 is fully operational. We therefore propose to upgrade the existing MSB into an optical beamline called CUBES (Charles University Beamline for Electron Spectroscopy), based on a new concept, fully adapted and using the radiation characteristics that will be provided by the new Elettra 2.0 storage ring. The financial requirements for the construction of the CUBES have been estimated at 5.25 M€ (NET). The MSB is a strategic facility of the CU, therefore the CU will apply for national or EU funding for a significant part of the costs (4.5 M€ including VAT costs). To cover a part of the remaining costs we will apply for the Elettra synchrotron (about 0.5 M€) in accordance with the Cooperation Agreement between CU and the synchrotron on the operation of the Czech optical beamline. And within this proposal we ask CERIC-ERIC to support the project costs with 1,000,000 EUR, in agreement with the Ministry of Education, Youth and Sports (MEYS) of the Czech Republic. With the implementation of the CUBES project, the Czech PF will acquire a synchrotron radiation light source for the existing end station to carry out cutting-edge research in materials and chemical engineering and biophysics with a focus on the structure of materials, their composition and interaction with molecules in the field of soft X-rays.

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Section a: Current Status and future evolution of the PF

The Large Research Infrastructure (LRI) **SPL-HTC** (http://spl-htc.cz/, called SPL-MSB until the end of 2022) operated by Charles University (CU) has been the Czech partner facility (PF) of the CERIC-ERIC since 2014. It **consists of three laboratories** - the **Materials Science Beamline** (MSB) at the Elettra synchrotron in Trieste and the **Surface Physics Laboratory** (SPL) in Prague, newly extended (2023) by the **Hydrogen Technology Center** (HTC). The renaming of the LRI from the original SPL-MSB to SPL-HTC is linked to its extension to SPL-MSB-HTC.

The main strategy of the SPL-HTC is to provide users with open access to world-class and unique facilities for conducting excellent **basic and applied materials research**, **focusing on specific areas of surface physics and chemistry - catalysts**, **sensors**, **surface electrochemistry and operando research**.

Within the SPL and MSB laboratories, the LRI currently offers the scientific community access to 6 unique facilities:

1) Materials Science Beamline (MSB) at the Elettra synchrotron (opened to users in 2003).

2) Angle-resolved photoelectron spectrometer (XPS-XPD, opened to users in 2014).

3) High-pressure photoelectron spectrometer (NAP-XPS, opened to users in 2015).

4) High-pressure photoelectron spectrometer (EnviroESCA) for chemical analyzes of samples of all types including liquids, tissues, plastics, etc. (open access from 2022).

5) High Resolution Scanning Electron Microscope (FESEM, open access from 2014).

6) Focused Ion Beam Scanning Electron Microscope (SEM-FIB LYRA, open access from the second half of 2022).

As more and more users became interested in the CERIC-ERIC research topics: batteries and fuel cells, the HTC was opened under the Czech PF. From the second half of 2023, it will provide users with open access to advanced experimental systems to enable their research **in the field of hydrogen technology**, in particular **the testing of** electrocatalytically active materials in half cells, single cells and stacks of **water electrolyzers and hydrogen fuel cells**, including the possibility of self-production of samples of catalytic layers/inks in the applications laboratory.

Up to now, about 50 experiments per year have been carried out on the 4 SPL-HTC instruments made available to users (MSB, NAP-XPS, XPS-XPD, FESEM. As an illustration, in the years 2019-2022, 179 experiments were performed at the Czech PF and 140 scientific papers were **published** in international peer-reviewed journals, for a total of **about 375 publications so far during the period of the Czech PF operation within CERIC-ERIC**. The publications published in 2022 and 2023 are listed in **Annex 3**.

The SPL-HTC team currently comprises **17 members**, including the director, one administrative worker and a technician. Users are also supported by PhD students **of the Nanomaterials Group** (currently 12), which operates the LRI as part of its activities **at the Faculty of Mathematics and Physics, CU**. In addition, **the Nanomaterials Group carries out its own basic and applied research in all the above-mentioned fields and specializations**, which guarantees a high level of expertise of its members for the support of users of the SPL-HTC equipment offered by the Czech partner facility SPL-HTC.

The operation of the SPL-HTC PF is financed by the special-purpose support (2.7 M \in for 2023-2026) from the MEYS, the operation of the Nanomaterials Group by the institutional funding (100 k \in per year) from the CU. However, these sources do not provide investment funds. The own research of Nanomaterials group is financed from national and EU funds (MEYS, the Czech Science Foundation, the Technology Agency of the Czech Republic, the Ministry of Industry and Trade) through research grants (380 k \in per year for projects in progress, 1.04 M \in per year for accepted projects with 2024-2027 timelines). Within these scientific projects, if there are any investment funds at all, they are very limited, typically up to 30 k \in .

As a member of the CERIC consortium, the Czech PF participates in various joint projects, activities and events organized by CERIC. The Czech PF was a co-solver of the CERIC research grant RENEWALS (PI Dr. M. Kiskinova) and a solver of the CEROP project (PI Dr. J. Mysliveček). It is worth highlighting the fruitful collaborations established within these projects with the NIMP and with Dr Heinz Amenitsch's group at the TU Graz, which has successfully continued the joint work on catalysts for fuel cells and the design and implementation of the operando cell of a hydrogen fuel cell for the study of catalysts at the Austrian SAXS beamline at the Elettra synchrotron (the cell was successfully tested and the first measurements with our developed catalysts are currently underway). Next, we participate in the **PaNOSC** project, **Hercules School** etc.

The Czech PF was supported by the Battery Plan programme with an investment of almost 63 k \in . Furthermore, in the call for the development of CERIC-ERIC research infrastructure based on **Expressions of Interest** (EoI), CERIC has granted the APEMWE project of the SPL-HTC (204 k \in). Furthermore, the Czech PF received **3 PhD scholarships** within the CERIC-ERIC PhD PROGRAMME ACTIVITY (2 PhD students are studying, the third topic supported in the EoI 2022 call is currently vacant). As part of this activity, PhD student exchanges have taken place with Austrian and Romanian partner institutions.

Currently, the SPL-HTC PF is involved in the **CERIC programmes Battery Research**, **Fuel Cells Research** and the **Circular Economy Programme ReMade@AR**I. We are also participating in the Call for post-doctoral projects for Ukrainian citizens and residents affected by the war, where we are offering 3 post-doctoral positions.

The main strategy of the Czech PF in the coming years is to improve the international quality of research and results of the Czech PF in the field of materials research, through modernizing its key devices, in particular the MSB, expanding the portfolio of techniques offered, especially with the infrared spectroscopy technique integrated into the unique NAP-XPS device, and creating sufficient capacity for advanced research, in accordance with users' needs.

The Czech PF continues to plan active participation in joint activities and cooperation with CERIC PFs, namely in the field of energy materials, μ -fabrication and operando techniques together with Elettra, TU Graz, SOLARIS and NIMP.

Section b: Five-year development plan of the PF

In connection with the main strategy of the LRI SPL-HTC to create a capacity for advanced research and innovation in the field of materials science in state-of-the-art and unique facilities that will provide a deeper understanding of the functional properties of (nano)materials, and with the aim of supporting the international competitiveness of the CERIC-ERIC consortium, we assume the modernisation/upgrading of the Czech PF in the period 2024-2028 as follows:

Within the newly opened Hydrogen Technology Center, basic equipment is available to users, but it is necessary to supplement it so that it covers the basic range of systems both in the field of testing water electrolyzers and hydrogen fuel cells for the study of electrocatalytic materials, primarily from a scientific point of view. i.e. in areas of relatively low power (up to a few kW), and in sufficient capacity, which is currently one of the problems. The reason lies in the very different activity of the materials for the reactions running in these cells, and it is necessary for the HTC to be equipped with suitable equipment for their characterization and testing in optimal conditions. In the near future, the existing equipment will be expanded by two CERIC-funded electrolyser test stations as part of the APEMWE project (the contract is already ready for signing). We plan to purchase additional equipment (1kW fuel cell testing station, 3 potentiostats SP150e with 20A boosters) as part of the OP JAK RI I project (already submitted, total investment requested 1,350 M€ for 2024-2026). Next, we plan to solve the extension of the basic equipment of the HTC, depending on the demand of the users (however, their needs are difficult to estimate at the moment when the HTC has just been opened) and the availability of funds from national and European subsidy projects. From a national, European and global point of view,

hydrogen technologies are a priority interest and therefore we expect great interest in the devices/equipment made available to users within the framework of the HTC.

Within the SPL, our aim in the area of operando methods is to maximise the capabilities of the two state-of-the-art high-pressure photoelectron spectrometers - NAP-XPS and the newly acquired EnviroESCA environmental spectrometer - and to further develop the operando techniques, as understanding the properties and behaviour of functional materials in their working conditions is a very topical area of research. As part of the OP JAK RI I project, we plan to upgrade the above-mentioned spectrometers and to significantly extend the NAP-XPS system with an infrared spectrometer, which will be of great benefit to CERIC users. In addition, in the next few years we plan to present and make available to users 3 specially designed mini cells: a water electrolyser, a fuel cell and an electrochemical cell for cyclic voltammetry, which can be installed and operated in the EnviroESCA system for short periods of time, thus responding flexibly to user needs. A miniature water electrolyser cell, designed and built by us for this purpose, is currently being tested in this facility. Its installation will allow users to study changes in the chemical properties and behaviour of electrocatalytically active materials directly during electrolyzer operation. The tested cell represents a way to understand the mechanisms of electrochemical reactions and will provide important knowledge for the research and development of materials (not only) for hydrogen technologies.

The strategic priority of the SPL-HTC is currently the modernization of the key, so far the most requested and productive device by CERIC users – the MSB optical beamline operating at the Elettra synchrotron. The necessary reconstruction is linked to the upgrade of the synchrotron itself in 2025 and 2026. This unique, prestigious and very successful SPI-HTC experiment is a priority of the UK, which is looking for sources for its financing. Therefore, **part of the cost is** also **the subject of the present project**. It should be noted that due to a significant reduction in the MEYS funds allocated for the development of the LRI SPL-HTC within the call of OP JAK RI I, the reconstruction of the MSB is therefore is not included in the submitted project.

Section c: Rationale and Scientific and technical description of the proposal

The Elettra synchrotron facility has been in operation since 1993. In 1997, a project to build a Czech Materials Science Beamline (MSB) of the SX700 concept was launched as a collaboration between Elettra, the Czech Academy of Sciences and Delong Instruments Brno, providing high-resolution, linearly polarized, monochromatized radiation from the bending magnet for the Elettra end station and an electron energy analyser from Karl Franzens University in Graz. This end station was replaced in 2002 by a new one with a new analyser operated by the CU. After commissioning, the MSB was made available to external users through public tenders in 2003. Over the next 20 years, the end station was progressively upgraded to improve performance, expand the range of sample preparation and analysis methods, and simplify operation. Thanks to this process and the high quality of our user community, the MSB produces 20-30 scientific articles per year in peer-reviewed journals with high impact factors (>7), a total of 370 articles to date. In contrast to the end station, the beamline that determines the properties of the monochromized radiation has only been upgraded once - in 2008 the grating chamber of the monochromator was replaced by a new one that allows a wider photon energy range (20-1000 eV instead of 40-800 eV) with high reproducibility and reliability.

After more than 30 years of operation, the current version of the Elettra storage ring of 12-fold symmetry is going to be shut down in July 2025. In the following 15 months it is going to be replaced by a new one called Elettra 2.0 of a different geometry (symmetric 6 bend achromat) which will allow to reduce the beam size by a factor of 30 and to increase the brilliance and coherence by 1-2 orders of magnitude. The 2.5 times higher electron current should also result in correspondingly higher photon beam intensities.

However, the upgrade of the Elettra storage ring will have many consequences for the MSB. As mentioned above, the end station equipment is state of the art and will not require major investment. The situation is quite different for the optical part of the beamline. Most of the parts are more than 25 years old, with the exception of the mechanics of the monochromator, which was replaced 15 years ago. Due to the

different geometry of the new storage ring and beam parameters, they cannot be reused in the new configuration. The SX700 concept suffers from high aberrations of the toroidal mirrors in the case of the wide incoming beam from the bending magnet source, forcing us to work with slits that are too narrow, resulting in a very low utilisation of the original radiation. In addition, the optical components of the existing MSB do not have sufficient water cooling for the heavily X-ray illuminated.

In the context mentioned above, the old MSB will be decommissioned in 2025 and cannot be reused once Elettra 2.0 is fully operational. Therefore, **we propose** to dismantle the existing MSB and **to design and build a new beamline called CUBES as a light source for the existing end station for the implementation of top research in the field of material and chemical engineering and biophysics** with a focus on the structure of materials, their composition and interaction with molecules **in the field of soft X radiation**.

The necessary parts of the CUBES project are following:

1. Front end: This part is the first ultra-high vacuum (UHV) system between the light source (bending magnet) and the radiation shielding wall. It is a set of UHV chambers, valves, beam stoppers and shutters, water cooling of the highly irradiated components, pumps and gauges.

2. Optical concept: From the experience and preliminary calculations of the Elettra Optical Engineering Group, we know that the current SX700 concept is outdated and would not allow us to fully exploit the parameters of the new light source. A much better design may be the combination of cylindrical mirrors and variable line spacing grating (VLS-PGM), which has been successfully used in a recent BL02D bending magnet beamline at the Shanghai Synchrotron Research Facility (SSRF). Detailed calculations will therefore be carried out to confirm the VLS-PGM optical concept or to suggest a better one for the design of a beamline.

3. Beamline: Irrespective of the final optical concept resulting from the calculations, the typical soft Xray beamline consists of about **six optical elements** (X-ray mirrors for deflection and focusing, gratings for monochromatisation) and **two slits** (defining the resolving power), some of which have to be cooled by water circuits and/or moved by stepper motors, then **UHV chambers** with manipulators for all these elements, connecting UHV tubes, electrically controlled **valves**, **UHV pumps** and **gauges**.

4. Control System: Valves, motors, pumps and gauges need appropriate power supplies/controllers connected to a synchrotron control system that constantly reports correct operation to avoid risks.

5. Hutch: All parts located in areas with dangerous X-rays above the permitted limit must be enclosed in a radiation-shielding enclosure with lead walls, access to which must be controlled by an access control system.

6. Plants: Certified installations for electricity, cooling water, compressed air, gas nitrogen lines.

7. Network: The computer network must be designed and built.

8. Platform: The end station will be positioned on an elevated platform custom-made to fit in the available space at the Elettra.

In summary, the complete solution of the new CUBES beamline will provide:

- a wider energy range up to 1500 eV, allowing the study of elemental core levels currently inaccessible;
- higher beam intensity by up to an order of magnitude, allowing shorter data acquisition times and detection of lower concentration species;
- variable spot size that can be adapted to sample shape/form;
- improved reliability by replacing old parts.

As part of this proposal, we would like to ask CERIC for **support to cover parts of the CUBES project Nos. 4-7**. The reason for this is that the rules of the OP JAK programme, within which we plan to implement the CUBES project, do not allow us to cover the costs of anything permanently connected to the buildings where the PF equipment is operated.

Section d: Impact



The implementation of the CUBES project, partially within this proposal, will contribute to the overall improvement of the quality of the research environment and the services provided by the LRI SPL-HTC to the research community. The new CUBES will enable researchers to carry out more sophisticated experiments/studies in previously inaccessible areas, leading to a deeper understanding of the phenomena under investigation. It will help to meet the demands and needs of more users, thus supporting the growth of the regular user base. Advanced technologies and equipment will also increase the efficiency and productivity of researchers' work, which will support collaboration and knowledge exchange between different institutions at an international level, the development of innovative ideas and the solution of complex societal problems.

This project has the potential to play a key role in strengthening the position of the LRI SPL-HTC as a partner facility of the CERIC-ERIC consortium and of CERIC-ERIC itself, strengthening its international cooperation, involvement in international projects and competitiveness on the international research market. In addition, the high quality scientific user support provided by the members of the Nanomaterials Group operating the MSB - with over 20 years of experience at the MSB trained experts in the field of synchrotron radiation - increases the visibility and prestige not only of the LRI itself, but also of CERIC-ERIC at the international level.

Section e: Description of the implementation

We are planning **the implementation of the CUBES project** over the next five years in the following way, **according to the time schedule** shown below:

As a first step, we need optical calculations. These calculations are currently being entered and work is in progress. They should be ready by the end of this year.

In the meantime, the preparation of the OP JAK ERDF project will take place, including obtaining bids for the construction of a new optical beamline. It will be submitted to the competition at the beginning of 2024 and we expect the results at the end of it.

Tenders for individual parts of the new CUBES should be launched in early 2025. The period of their production varies from one to two years, according to market research and preliminary offers obtained. The construction of the optical beamline and its commissioning are expected in 2027.

| year | 2023 | | 2024 | ł | | | 2 | 2025 2026 | | | | | 20 | 27 | | | 2 |)28 | | | |
|--------------------|-------------------------------|------------------|------|------|-----|-----|-----------------------|---------------|-----|--------------------------------|-----|---------|-----------|--------------------------|------|------|---|-----|-----|-------|--|
| trimester | 3 4 | 1 | 2 | 3 | 4 | 1 | 2 | 3 4 1 2 3 | | | | 4 | 4 1 2 3 4 | | | 4 | 1 | 2 | 3 | 4 | |
| synchrotron | Elettra 1.0 operate | | | | | | Elettra 2.0 construct | | | Elettra 2.0 partial operate | | | ial | Elettra 2.0 full operate | | | | | | | |
| MSB | | | ope | rate | | | | dism antle | | | | | | | | | | | | | |
| 1. front end | order manufacture | | | | ire | | install | | | | op | operate | | | | | | | | | |
| 2. calculations | Optics and heat load | final project | | | | | | | | | | | | | | | | | | | |
| 3. beamline | | | | | | orc | ler | | man | ufactı | ure | | | | inst | tall | | | ope | erate | |
| 4. control system | | | | | | orc | ler | | man | ufacti | ure | | | | ins | tall | | | оре | erate | |
| 5. hutch | | | | | | orc | ler | | man | ufactı | Jre | | | | inst | tall | | | ope | erate | |
| 6. plants | | | | | | orc | ler | | man | ufactı | ure | | | | inst | tall | | | ope | erate | |
| 7. network | | | | | | orc | ler | | man | ufactı | ure | | | | inst | tall | | | ope | erate | |
| 8. platform | | | | | | orc | ler | | man | ufactı | ure | | | | inst | tall | | | ope | erate | |

Proposed time schedule:

The CUBES project is financially very demanding. The financial requirements for the construction of CUBES have been provisionally estimated by the Elettra Industrial Liaison Office (ILO) at 5.25 M€ (NET, see Annex 4). Therefore, we would like to finance it from **three sources**:

1. From **Czech national and/or EU sources**, namely own calculations (item 2), beamline (item 3) and platform (item 8). The estimated cost is 4.5 M€ including VAT costs.

2. We will request funds from **the Elettra** to pay for the front end (item 1). The front end is a part firmly connected to the storage ring and must be designed and assembled directly by Elettra staff. In addition, Elettra has agreed to provide the light as part of the Co-operation Agreement with Charles University. The estimated cost is $0.5 \text{ M} \in$.

3. As part of this proposal, we are asking **CERIC** for **support** and allocation of the Member's annual contributions to support CUBES investments in the form of items 4-7 with the estimated cost 1.0 M \in . According to the schedule, we expect the financial costs to be spread between 2025 and 2027. In 2025, there will be prepayments.

Annex 1 – Human Resources: Resources connected to the activity of the required staff (total cost including overall estimated costs and use of the CERIC funding)

| CEDIC | Total in Euro | | | | | | | | |
|---|---------------|--------|--------|--------|--------|--|--|--|--|
| CERIC | Year 1 | Year 2 | Year 3 | Year 4 | Year 5 | | | | |
| Consumables | | | | | | | | | |
| Personnel cost (PhD, researcher or technical staff) | | | | | | | | | |
| Travel costs | | | | | | | | | |
| Other costs (conferences fees, publications, training, etc) | | | | | | | | | |
| TOTAL | 0 | 0 | 0 | 0 | 0 | | | | |

Annex 2 – Infrastructure Development: Resources (including overall estimated costs and use of the required CERIC funding)

| CERTC | Total in Euro | | | | | | | | | |
|----------------|---------------|---------|---------|---------|--------|--|--|--|--|--|
| CERIC | Year 1 | Year 2 | Year 3 | Year 4 | Year 5 | | | | | |
| Equipment | 0 | 200,000 | 400,000 | 400,000 | 0 | | | | | |
| Consumables | 0 | 0 | 0 | 0 | 0 | | | | | |
| Personnel cost | 0 | 0 | 0 | 0 | 0 | | | | | |
| Travel cost | 0 | 0 | 0 | 0 | 0 | | | | | |
| TOTAL | 0 | 200,000 | 400,000 | 400,000 | 0 | | | | | |



Annex 3 – SPL-HTC: List of publication in the last two years

2023

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Antony, A; Hejduk, M; Hrbek, T; Kúš, P; Bičišťová, R; Hauschwitz, P; Cvrček, L **Laser-assisted two-step glass wafer metallization: An experimental procedure to improve compatibility between glass and metallic films** *Appl. Surf. Sci.*, **627**: Art. No. 157276 (7 pages), 2023. doi:10.1016/j.apsusc.2023.157276

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Hrbek, T; Kúš, P; Kosto, Y; Gamón Rodríguez, M; Matolínová, I Magnetron-sputtered thin-film catalyst with low-Ir-Ru content for water electrolysis: Long-term stability and degradation analysis

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Annex 4 - Offer for the construction of the CUBES beamline from the Elettra Industrial Liaison Office (ILO)

| | | | MANAGEMENT SYSTEM |
|--|------------------------------------|------|----------------------|
| Elettra Sincrotrone Trieste | Trieste, 08-06-2023 | (| COY |
| Elottra Sincrotrono Triosto S.C.n.A | То: | | CERTIQUALITY |
| Società di interesse nazionale ai sensi della Legge n. 370/99 | CHARLES UNIVERSITY | | UNI EN ISO 9001:2015 |
| Strada Stalale 14 km 163.5 in Area Science Park 34149 Basovizza, Trieste - ITALY - Tel. +39 040 37581 - Fax +39 040 9380906 | FACULTY OF MATHEMATICS AND PHYSICS | | 04130430012018 |
| VAT. N. IT00697920320 Capital€ 47.632.663,00 | Ke Karlovu 3 | | |
| No binding budgeton, quetation N_0/2022/RO | CZ-12116 Prague | | |
| No-binding budgetary quotation N. 9/2023/BG | CECA | | |
| | | Page | 1 of 2 |

Atn.

Dr. Tomaš Skala

| | Description | M.U. | Q.ty | Unit price | Dis. % | Amount |
|---|--|------|------|--------------|---------|--------------|
| | CUBES Beamline: | | | | | |
| 2 | Design and Project Management | · | 1,00 | 23.000,00 | | 23.000,00 |
| 3 | Front End | | 1,00 | 513.000,00 | | 513.000,00 |
| 4 | Beamline | | 1,00 | 3.701.000,00 | • | 3.701.000,00 |
| 5 | Hutch | | 1,00 | 649.000,00 | | 649.000,00 |
| 6 | Control System | | 1,00 | 65.000,00 | | 65.000,00 |
| 7 | Network | • | 1,00 | 52.000,00 | | 52.000,00 |
| 8 | Plants | • | 1,00 | 227.000,00 | | 227.000,00 |
| 9 | Platform | | 1,00 | 20.000,00 | | 20.000,00 |
| | Additional specifications are described in attached file: | | | | | |
| | "09_2023_QI_ILO_SpectTec.pdf" | | | | | |
| | Delivery Terms: | | | | | |
| | Shipment: EXW Elettra Sincrotrone Trieste (Incoterms 2020). Delivery: 24 months after receipt of the order. | | | | | |
| | Validity: | | | | | |
| | This non bibding quotation is valid for 90 days from the date hereof. | · | • | | | |
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No-binding budgetary quotation N. 9/2023/BQ/ILO



Page 2 of 2

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| For any inquiry please contact: | | | Industrial Liais | on Office | | | | |
| | Email: II0@elettra.eu Eax: +39.040.3758623 | | | | | | | |

Apro Frences



Strategy for the allocation of CERIC's membership fees in support of the integration of CERIC capabilities

Hungarian Partner Facility

Introduction

In its resolution 8th May 2023, the General Assembly (GA) agreed that as long as the contribution by the Host Member State of CERIC-ERIC allows covering the statutory operations fully, 90% of the Member's annual contributions are dedicated to supporting actions integrating the capabilities of the Member's Partner Facilities, **such as PhDs, post-docs, joint research projects, infrastructure investments and promotion of CERIC-ERIC Partner Facilities research offer.** These will be agreed upon by the GA, assuring that, over a 5-year average, this support to each Partner Facility will equal at least 90% of the cash contribution provided by the relevant Member during this period.

To enable the decision of the GA, the **Directors of the PFs should define the strategy and an annual program with a five-year outlook** for their own Facility within the CERIC collaboration framework and discuss it in the BoD for submittal to the GA through the ED, with the opinion of the ISTAC.

In the following, the PFs are requested to submit their proposal, possibly coordinated and agreed upon with other Partner Facilities, to allow for a discussion and development of a joint strategy at the October BoD meeting.

Proposing CERIC Partner Facility: BNC

The abstract (summary) should, at a glance, provide the reader with a clear understanding of the proposal, covering the main elements of the project, its implementation and cost.

BNC proposes to allocate the budget to establishing two dedicated positions for young scientists, who can carry out a collaborative research program based at BNC but taking advantage of various CERIC partner facilities. One position is devoted to studying the material analysis challenges of the circular economy. Waste electronic equipment (WEEE) is a secondary raw material source and can be a complement to direct mining or import. The reliable quantification of valuable components in waste electronics, the toxic ones listed in the Restriction of Hazardous Substances (RoHS), and the raw materials with high supply risk as defined in the Critical Raw Materials Act. The neutron, ion-beam and synchrotron-based composition and structure analysis techniques offered by the CERIC consortium are adequate methods to study the uncommon components non-destructively, as well as to assess reprocessing strategies and recovery yields. The other position aims to develop novel silica xerogel or aerogel-like nanomaterials and their composites as high-capacity selective adsorbents for the recovery of precious heavy metals / rare earth elements. Because of their non-toxicity and biocompatibility, these nanomaterials can easily find applications in medical and pharmaceutical fields. The surface chemistry, textural- and morphological properties of these materials impact their application properties. The complete characterization of these functional silica materials will be characterized using complementary techniques offered by BNC and CERIC facilities. The neutron techniques available at BNC will be completed by the ²⁸Si solid-state NMR spectroscopy (SloNMR) and SAXS (TUG) measurements offered by CERIC facilities. Together it will offer detailed information about the synthesized materials and guide the PF to establish a relation with their application-related performances and their structural properties from the molecular to macromolecular level. Using this opportunity, we strengthen the close collaboration, in which we had agreed, with the mentioned CERIC partners and develop new research areas interesting for all the partners.

T +39 040 375 8953 E info@ceric-eric.eu W www.ceric-eric.eu

Section a: Current Status and future evolution of the PF *Provide (1-2 page):*

- a summary of the present status of the PF, listing

- all its present research activities and programmes, including those not reported within CERIC (but a part of the PF);

- resources (main instruments, collaborating staff and all funding sources).

- list of the publications in the last two years.

- an outline on how the PF intends to evolve, particularly in collaboration/integration with the rest of CERIC. Briefly list the already ongoing activities with other CERIC Partner facilities. This should help to define the ongoing and future strategy.

- the possible need for new resources to make the PF more effective and visible, including administrative support to provide annual accounts. Please also explicitly refer to organisational needs within your hosting institution, allowing for a better definition and identity of the PF and its operation, its reporting and integration within CERIC...etc.

EU projects:

| Acronym | Project Number | Title | Start date | Duration month | Run from Oct2023 | # of Particant |
|-------------|-------------------|--|------------|-------------------|------------------------|-------------------|
| ARIEL | 847594 | Accelerator and Research reactor Infrastructures for Education and Learning | 01-Sep-19 | 54 | 5 | 25 |
| IPERION HS | 871034 | Integrating Platforms for the European Research Infrastructure ON Heritage Science | 01-Apr-20 | 48 | 7 | 24 |
| EURIZON | 871072 | European network for developing new horizons for RIs | 01-Feb-20 | 48 | 4 | 37 |
| TOURR | 945269 | Towards Optimized Use of Research Reactors in Europe | 01-Oct-20 | 36 | 1 | 9 |
| EASI-STRESS | 953219 | European Activity for Standardization of Industrial residual STRESS characterization | 01-Jan-21 | 36 | 3 | 15 |
| SECURE | 101061230 | Strengthening the European Chain of sUpply for next generation medical RadionuclidEs | 01-Oct-22 | 36 | 24 | 17 |
| ReMade@ARI | 101058414 | RECYCLABLE MATERIALS DEVELOPMENT at ANALYTICAL RESEARCH INFRASTRUCTURES | 01-Sep-22 | 48 | 36 | 37 |

National projects:

| Acronym | Project Number | Title | Start date | Duration month | Run from Oct2023 | # of Particant |
|-------------|---------------------------------|---|-----------------|-------------------|------------------------|-------------------|
| POC-KRY-MOD | ELKH-POC- 2021-024 | Development of a cryogenic moderator for a new type of high- brightness neutron sources | 01-Feb- 2022 | 24 | 3 | N/A |
| | ELKH-POC- 2022-029 | Developing non-destructive X-ray and neutron analytical techniques for the investigation of ancient pottery-forming techniques | 1-Nov- 2022 | 18 | 7 | N/A |
| MENL | RRF-2.3.1- 21-2022- 00009 | National Renewable Energy Laboratory (MENL) | 1-Jan-2022 | 45 | 24 | 10 |
| | OTKA 131814 KFF- | Large-scale examination of polished stone tools and toolstone | 01-12-2019 | 60 | 27 | 2 |

| | | 5970- 2/PALY | raw materials for the mapping of prehistoric long-distance and regional trade networks of the Carpathian Basin and its | | | | |
|--|--|-----------------|---|--|--|--|--|
|--|--|-----------------|---|--|--|--|--|

Resources:

The Budapest 10 MW Research Reactor (BRR) provides neutrons for research activities at the Budapest Neutron Centre (BNC) https://www.bnc.hu/. The operator of the BRR is the Centre for Energy Research (EK) https://www.ek.hun-ren.hu/en/ and is managed by the Reactor Department. It has 8 radial- and 2 tangential-, horizontal channels. In the reactor hall, there are six beam facilities (RAD, new instrumentation testing beamline, BIO, MTEST, TAS, PSD). One of the tangential channels is equipped with a liquid hydrogen-based cold-neutron moderator, which serves three neutron guide systems that deliver the coldneutron beams to the neutron guide hall. In this experimental hall, the ATHOS, REFL, PGAA, NIPS-NORMA, SANS, GINA, and FSANS instruments are installed on the three neutron beam guides. In addition, a TOF thermal neutron guide serves the TOF-diffraction instrument that is located in a dedicated building. The BRR has 40 vertical irradiation channels in its core which are utilized for industrial and radio-pharmaceutical irradiations, and material composition analysis by NAA. One of them hosts the BAGIRA instrument, a temperature-controlled instrument to study irradiation damage of materials. The research instruments are operated by the staff of two departments. These are the Nuclear Analysis and Radiography and the Neutron Spectroscopy departments. Altogether it means 25 researchers, 5 engineers, 5 technicians, and 2 administrators. Regarding financial resources, most of the budget is provided by the Hungarian Research Network (HUN-REN) (former name: Eötvös Loránd Research Network, ELKH) Secretariat. It is an independent public budgetary institution, see https://hun-ren.hu/en/about-hun-ren/about-us.

List of publications:

(134 items) in 2021-22 is in BNC_pubi2021-2022.xlsx EXCEL file.

Section b: Five-year development plan of the PF

The proposers should describe (1 page maximum):

- 5-year objectives of the PF (what it wants to achieve in 5 years in collaboration with the other CERIC PFs) and an outline of a program to reach the objectives.

- key needs of the PF within the next five years (where possible, refer to the ISTAC recommendations) and how the proposal fits within this five-year program and with a joint program with the other CERIC PF's

The Budapest Neutron Centre (BNC) operates a 10 MW research reactor, it is the main knowledge hub for nuclear/neutron research in Hungary. Although BNC has been an established organization for nearly 30 years and has reasonably good records in science and technology, this research infrastructure is embedded in a relatively poor R&I performing environment, resulting in significantly lower outcomes than that of similar facilities.

The main objectives of the near future are as follows

- Secure funding for stable operation. The reactor has been in operation for over 60 years and its license prolongation until 2033 is in progress. This is in line with recent government support (11 M€) that enabled the purchase of reactor fuel for the 5-6 years to come.
- Modernize the reactor and the neutron instruments. The refurbishment of obsolete components
 will ensure the safe and reliable operation of the reactor, while the modernization of the neutron
 instrumentation (cold source, neutron beam optics and end stations) may provide by several factors
 higher intensity and substantially improved measurement capabilities, i.e. better service in open
 access of the scientific community. The addition of new instruments, such as the NEAT inelastic
 scattering spectrometer, is also foreseen. The full cost for the total modernization has recently been

estimated to be around 12-14 M€.

- Maintain the medium/long-term sustainability of nuclear competence in the country, a project to consider a new neutron source technology is to be launched. The main objective is to undertake the necessary planning and designing for the brown-field transition of the current reactor site into a high-current compact accelerator-based neutron source (HiCANS).
- An important measure is to implement a robust human resource strategy. Assuming competitive salaries, and enhancing international scale recruitment, BNC staff shall be completed to achieve the critical mass. Maintaining nuclear competence is a top priority, with enhancing R&I capacities in this domain.

The support of CERIC and other international bodies is indispensable to acquiring domestic and EU funding and having access to top-level collaborators in emerging research fields.

Section c: Rationale and Scientific and technical description of the proposal

The Proposal should concisely describe its rationale and, how it fits in the five-year outlook, how the scientific and technical quality will be assured. For proposed PhD students, list also the University(ies) awarding the degree and the name of the proposed supervisor (s) (maximum 1 page).

The proposed topics are in line with the main research directions of CERIC, i.e., material science and the recent EU initiatives. During the proposed timeframe of 5 years, a young scientist can elaborate on the topic, establish partnerships within CERIC, as well as with the industry, and disseminate the results in the form of publications, and conference presentations, while also reaching out to policymakers and the general public.

We'd prefer a postdoctoral scientist for these positions. In the case of a PhD student stage, he/she can enrol in the Chemistry PhD program at ELTE University, Budapest, or Debrecen University, where many BNC scientists are registered as supervisors or consultants.

Section d: Impact

The Proposal should describe (0,5 page maximum) its expected impact on the overall scientific and technical quality and capability of CERIC. How the proposal complements and fits in common developments with other activities both at the PF and in other PFs, aimed at integrating the facilities and overall strengthening of CERIC.

The security of the supply chain for several critical materials has recently become equally important as the environmental and energy-efficiency aspects of the circular economy. Therefore, we believe this topic will be interesting to many CERIC PFs and complementary experiments can be done collaboratively.

The functionalization of silica gel for pharmaceutical purposes is in line with health as a priority topic of CERIC while the adsorption of heavy elements for the mitigation or cleaning of contaminated areas is part of environmental protection.

In general, this initiative will also advance measurement technology, metrology, validation of in-field measurement tools, development of materials, and help identify synergies of PFs.

Section e: Description of the implementation

This section should describe (1 page maximum) in a clear way the maturity and implementation of the project and its timeframe. Please also describe a possible timeline of the proposed investment e.g. how the investment will accumulate over the 5 years after the contributions commence (2024). For proposals, including the hiring of personnel, outline the research/technical program.

These research topics have already been established at BNC. A research program funded by the Hungarian Academy has been ongoing for 4 years, where an initial capability assessment of the techniques at BNC was completed. A dissertation is being prepared and planned to be submitted in 2024. Now, the topic can be expanded beyond neutron-based methods.



An EU grant application, REDIVIVA (Proposal ID 101069939, submitted in 2021), with the participation of BNC and RBI, was finally not accepted for funding.

We also mention the ReMade@ARI (REcyclable MAterials DEvelopment at Analytical Research Infrastructures) project (<u>https://remade-project.eu/</u>). CERIC-ERIC is formally a partner in this consortium, while BNC is also a beneficiary in its own right, coordinated by the LENS neutrons initiative. This project can also provide the opportunity and mobility funding to carry out experiments with measurement techniques unavailable within the CERIC consortium.

The CERIC network can contribute to finding appropriate industrial collaborators.

Study of the elemental composition of waste electrical and electronic equipment for circular economy (Principal investigator: Noémi Buczkó)

The proposed project aims to promote the efficient, economical, and environmentally friendly recycling of waste electrical and electronic equipment (WEEE) by developing methods for the comprehensive determination of the elemental composition of such waste. The amount of certified or standard reference materials available for the analysis of WEEE is very limited. Therefore, as a part of the tender, it is planned to develop in-house reference materials for the analysis of different ground WEEE (such as printed circuit boards, integrated circuits, LEDs, magnets from WEEE, solar cells, liquid-crystal displays, etc.). The developed in-house reference materials are planned to be used for calibration of equipment, for example, a handheld XRF spectrometer, suitable for industrial applications to determine the elemental composition of different ground WEEE with a particular focus on hazardous elements, valuable elements, or elements with a high supply risk. The examination of various complex WEEE (e.g. mobile phones, hard disk devices, etc.) will also be part of the research according to the plans. The aim here is to develop methods that are suitable for determining the internal structure and for determining in which parts the individual valuable and hazardous elements are concentrated. It will also be investigated how the methods can be adapted to an industrial environment, for example by using a neutron generator or industrial X-ray source.

5-year objectives of the proposal can be summarized as 4 main work packages (WP) as follows

- Preparation and analysis of ground and homogenized in-house reference materials using a combination of different analytical techniques, including INAA and PGAA available at BNC and PIXE and PIGE, available at Ceric partner Ruder Bošković Institute. (WP-1) (1-24 months)
- Development of industrially applicable techniques for the analysis of various ground and homogenized WEEE. (WP-2) (12-36 months)
- Determination of the internal structure of various complex WEEE with neutron radiography and tomography available at BNC, as well as X-ray imaging methods available at Ceric partner TomoLab Elettra Sincrotrone Trieste. Examination of the elemental composition of various complex WEEE and the spatial location of individual elements using neutron and X-ray based methods. (WP-3) (24-48 months)
- Development of methods applicable in industry, based on the results of measurements made at large-scale facilities, to determine the location of hazardous and valuable elements in components of complex WEEE. (WP-4) (36-60 months)

The 4 work packages of the research are strongly interconnected. WP-1 will be dedicated to produce and characterising in-house reference materials, WP-1 will be extensively used to validate the measurements made on complex and inhomogeneous samples in WP-3. The methods applied in WP 1 and 3 require expensive large-scale facilities, the results of these techniques will be especially used in WP 2 and 4 for the development and validation of cheaper, simpler, faster and even industrially applicable methods.

Development of silica aerogel-like nanomaterials and their composites (principal investigator Balogh Zoltán PhD student):

The proposed project aims to develop novel silica aerogel-like nanomaterials and their composites as highcapacity selective adsorbents for the recovery of precious heavy metals/ rare earth elements from aquatic environments and as non-toxic and biocompatible nanostructured drug carriers for potential medical and pharmaceutical applications by using different sol-gel strategies.

5-year objectives of the proposal can be summarized as 5 main work packages (WP) as follows:

- The synthesis of silica-based aerogel-like nanomaterials as novel adsorbents and drug carriers by sol-gel method (WP-1) (1-24 months)
- Physical, chemical, textural and microstructural characterizations of the adsorbents via conventional techniques (FTIR, SEM, TEM, nitrogen adsorption, thermal analysis, contact angle measurements) (WP-2) (1-36 months)
- Application of complementary characterizations (SANS, SAXS, XRD, NMR) (WP-3) (1-36 months)
- Performance evaluation of the synthesized materials as adsorbents in the liquid phase heavy metal (e.g. Pt, Pd, Hg, Ag, Cu, Ni, Co) /rare earth element (e.g. Nd, Eu, Ce, Y) sorption applications (WP-3) (24-60 months)
- Performance evaluation of synthesized materials as controlled-release carriers in pharmaceutical applications. (WP-3) (24-60 months)

WP-1-2 and 3 will be designed to be conducted simultaneously and the synthesis strategies will be developed constantly according to the feedback gained from characterization results. The on-site examination of the structure-property-activity relationship of the materials in a holistic, simultaneous, and integrative manner will allow us to ensure the continuity of the developed technology and will give the material the ability to be designed flexibly for any target application.

Annexe 1 – Human Resources: Resources connected to the activity of the required staff (total cost including overall estimated costs and use of the CERIC funding)

| CERTC | Total in Euro | | | | | | | | |
|--|---------------|--------|--------|--------|--------|--|--|--|--|
| CERIC | Year 1 | Year 2 | Year 3 | Year 4 | Year 5 | | | | |
| Consumables | 6000 | 6000 | 6000 | 6000 | 6000 | | | | |
| Personnel cost (PhD, researcher or technical staff) | 40000 | 40000 | 40000 | 40000 | 40000 | | | | |
| Travel costs | 4000 | 4000 | 4000 | 4000 | 4000 | | | | |
| Other costs (conference fees, publications, training, etc) | 3000 | 3000 | 3000 | 3000 | 3000 | | | | |
| TOTAL | 53000 | 53000 | 53000 | 53000 | 53000 | | | | |

Annex 2 – Infrastructure Development: Resources (including overall estimated costs and use of the required CERIC funding)

| CERTC | Total in Euro | | | | | | | | |
|----------------|---------------|--------|--------|--------|--------|--|--|--|--|
| CERIC | Year 1 | Year 2 | Year 3 | Year 4 | Year 5 | | | | |
| Equipment | 0 | 0 | 0 | 0 | 0 | | | | |
| Consumables | 0 | 0 | 0 | 0 | 0 | | | | |
| Personnel cost | 0 | 0 | 0 | 0 | 0 | | | | |
| Travel cost | 0 | 0 | 0 | 0 | 0 | | | | |
| TOTAL | 0 | 0 | 0 | 0 | 0 | | | | |

Appendix

The proposed topics align with the main research directions of CERIC, i.e., material science and the recent EU initiatives. During the proposed timeframe of 5 years, a young scientist can elaborate on the topic, establish partnerships within CERIC, as well as with the industry, and disseminate the results in the form of publications, and conference presentations, while also reaching out to policymakers and the general public.

Study of the elemental composition of waste electrical and electronic equipment for circular economy

Principal investigator: Noémi Buczkó

At BNC, the elemental composition of different waste electrical and electronic equipment (WEEE) was investigated as part of a PhD project even before this tender. During the previous research, one of the main research directions was the analysis of the elemental composition of ground printed circuit boards (PCBs) and integrated circuits (ICs), using neutron-based methods, such as prompt gamma neutron activation analysis (PGAA), instrumental and in-beam neutron activation analysis (INAA and in-beam NAA). The research was focused on valuable and hazardous elements, as well as on elements that are of high importance and at the same time a high supply risk for the European economy (critical elements). The advantages and limitations of each method were identified. Using a combination of methods, many valuable, critical, and hazardous elements (such as Au, Aq, Sb, various rare earth elements, Br, Cd, etc.) were identified. There were significant differences in the raw concentrations measured by different methods. The reasons for the discrepancies were identified, and corrections were applied for the measurements due to high boron concentration and oxygen that cannot be measured. The results of different techniques showed good agreement with using corrections. LED chips from LED light sources, that predictably contain large amounts of critical elements, were also analysed using neutron-based methods. The most important critical and valuable elements (e.g. Au, Ag, Ga, Y, Eu, Ce and Lu) were successfully quantified using a combination of individual methods, and low detection limits were achieved for the most important hazardous elements.

In the framework of the CERIC tender, it is planned to continue the research related to the circular economy. The amount of certified or standard reference materials available for the analysis of WEEE is very limited. Therefore, as a part of the tender, it is planned to develop in-house reference materials for the analysis of different ground WEEE (such as PCBs, ICs, LEDs, magnets from WEEE, solar cells, liquidcrystal displays, etc.). The knowledge and results obtained during the analysis of PCBs, ICs and LED chips will be used prominently. First time, the neutron-based methods (INAA and PGAA) available in the BNC will be used for the analysis of in-house reference materials. In addition to neutron-based techniques, it is also planned to involve other analytical techniques, to increase the accuracy of the results and the reliability of the in-house reference materials. For each element, the aim is to confirm the measured concentrations using more than one method. This CERIC tender offers the opportunity to access largescale analytical facilities for the analysis of in-house reference material. According to the plans, the CERIC partner Ruđer Bošković Institute will be prominently involved in the research. The methods available at this institute, are planned to be used, for example, to correct the distortion effect of individual elements on the PGAA method. The Rutherford backscattering spectrometry (RBS) and particle-induced gamma emission (PIGE) available at this institute, are among the few methods that are suitable for measuring light elements (e.g. Li, Be, C and O). In the case of the PGAA method, the undetected main components can cause analytical bias in the PGAA results, which causes an overestimation of the concentrations of all measured elements. WEEE frequently contains oxygen as a main component, for which only PGAA is suitable for detection among the methods available in the BNC. However, due to the too-high detection limit, it is typically not possible to measure the oxygen in WEEE. The measurement of carbon, which is also typically present in WEEE, is also problematic with neutron-based methods, the measured concentrations often have a high uncertainty, and/or the measurement requires a very long measurement time. With the PIGE and RBS techniques, it is expected that the carbon and oxygen content of the samples can be measured, so with the application of these methods, it will be possible to eliminate the distorting

effect of oxygen and carbon on the PGAA measurements. In addition, these two methods could be useful for the measurement of additional light elements present in some WEEE, considered important critical elements, such as lithium and beryllium, for which only a high detection limit is available with neutron-based methods. Furthermore, at the Ruđer Bošković Institute, particle-induced X-ray emission (PIXE) equipment is available, which also can be used to quantify additional important elements, that cannot or are difficult to measure with neutron-based methods. For example, lead is easily measurable with this method, which would be very important to measure due to its toxic effect. The developed in-house reference materials are planned to be used for calibration and verification of methods suitable for industrial applications, such as hand-held XRF spectrometry.

In the past, the element composition of hard disk devices was also investigated. The internal structure of this highly inhomogeneous waste type was successfully revealed by neutron and X-ray radiography. Various important valuable critical and hazardous elements were successfully identified with local PGAA measurements, and the spatial location of the identified elements was revealed by the joint interpretation of radiographic images and PGAA measurements. Based on the results of this research, it is planned to investigate the applicability of neutron and X-ray-based methods to determine the elemental composition of various complex and highly inhomogeneous WEEE types (e.g. mobile phones, components of computers, etc.) and to determine the spatial location of individual elements. Neutron-based imaging methods, available at BNC and the X-ray-based imaging methods, available at the CERIC partner, TomoLab, Elettra Sincrotrone, Trieste will be used to reveal the inner structure of the different waste, according to the plans. PGAA method, available in BNC, will be used for the elemental analysis. It is also planned to investigate the applicability of X-ray-based elemental analytical methods. The in-house grounded WEEE reference materials, presented in the previous chapter, will be extensively used to validate the results of the measurements made on complex and inhomogeneous samples. We want to focus the research on the measurement of hazardous elements such as Br, Cd, Hq, As, Pb, etc. Determination of the presence of these elements before recycling is very important to minimize the harmful effects of the recycling process, on the environment and human health. Determining the location of these elements within waste can promote environmentally friendly and economical recycling. In addition to the hazardous elements, it is also focused on the measurement of valuable and critical elements. The aim of the research is also to investigate how the methods can be extended to industrial scales, for example by using neutron generators and industrial X-ray sources.

As part of the research, we would like to pay special attention to the investigation of the waste containing batteries. The impact of waste batteries on the environment, as well as their environmentally friendly recycling, is receiving more and more attention nowadays. Knowledge of battery types is necessary for efficient recycling. One of the goals of the research is to develop a method that is suitable for the identification of different types of batteries [such as nickel metal hydride, different types of Li-ion batteries (for example lithium nickel cobalt aluminium oxide, lithium nickel manganese cobalt oxide, lithium iron phosphate etc.)]. For this task, it is planned to examine the applicability of the PGAA method, available at BNC, and X-ray-based methods. Also, the research aims to investigate the extensibility of the methods for industrial application.

First step of the collaboration plan:

The first visit would be to the Ruđer Bošković Institute to learn and perform PIXE and PIGE experiments on ground powder samples produced from printed circuit boards to produce in-house reference materials.



Strategy for the allocation of CERIC's membership fees in support of the integration of CERIC capabilities

Italian Partner Facility

Introduction

In its resolution 8th May 2023, the General Assembly (GA) agreed that as long as the contribution by the Host Member State of CERIC-ERIC allows covering the statutory operations fully, 90% of the Member's annual contributions are dedicated to supporting actions integrating the capabilities of the Member's Partner Facilities, **such as PhDs, post-docs, joint research projects, infrastructure investments and promotion of CERIC-ERIC Partner Facilities research offer.** These will be agreed upon by the GA, assuring that, over a 5-year average, this support to each Partner Facility will equal at least 90% of the cash contribution provided by the relevant Member during this period.

To enable the decision of the GA, the **Directors of the PFs should define the strategy and an annual program with a five-year outlook** for their own Facility within the CERIC collaboration framework and discuss it in the BoD for submittal to the GA through the ED, with the opinion of the ISTAC.

In the following, the PFs are requested to submit their proposal, possibly coordinated and agreed upon with other Partner Facilities, to allow for a discussion and development of a joint strategy at the October BoD meeting.

Proposing CERIC Partner Facility: Elettra Sincrotrone Trieste

Proposal summary (up to 200 words)

The Italian Partner Facility as part of Elettra Sincrotrone Trieste is currently undertaking a fundamental upgrade of its synchrotron facility, Elettra, toward a diffraction limited storage ring (DLSR), Elettra 2.0, planned to be open to all users in January 2027, after a 18-months dark-period. Elettra 2.0 will have improved brightness and coherence with respect to the present facility that will allow the construction of new beamlines that the present machine cannot support, such as micro X-ray diffraction (microXRD, IPF) and high-brightness SAXS (Austrian PF) served by in-vacuum undulators, as well as to improve the performances of existing beamlines, as in the case of the existing SAXS beamline toward a newer high-flux SAXS (HF-SAXS, Austrian PF). The aforementioned beamlines will give added value to the Life Science (LS) domain, complementing and strengthening the CERIC-ERIC LS program that, thanks to the project funded by the Italian government PRP@CERIC, will establish in Trieste a cryo-EM facility. In this framework, we aim to support implementation actions that promotes inter-PFs developments.

Specifically: i- the upgrade of control systems (332 K \in) of the new HF-SAXS and HB-SAXS beamlines at Elettra 2.0 and front-end of HB-SAXS (713.5 K \in), in collaboration with the Austrian PF; ii- the upgrade of the Cryo-EM facility and sample preparation laboratory with ancillary instrumentations and consumables (417,3 K \in), along with the training of new personnel across the cryo-EM and TEM facilities of SOLARIS and Elettra (230 K \in); iii-to in-kind contribute to CERIC-ERIC LS scientific programs in collaboration with the partner and associate facilities contributing, among the others, to osteoporosis program. The timeframe of the proposal perfectly fits with the ongoing upgrades, as it will be detailed in the

implementation plan.

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Section a: Current Status and future evolution of the PF

The Italian Partner Facility is located at the premises of the Italian Representing Entity, Elettra Sincrotrone Trieste.

Elettra Sincrotrone Trieste is a multidisciplinary international research center of excellence, specialized in generating high quality synchrotron and free-electron laser light and applying it for materials and life sciences. Its mission is to promote cultural, social and economic growth through:

- Basic and applied research
- Technology and know-how transfer
- Technical, scientific and management education
- Role of reference in the national and international scientific networks

The main assets of the research center are two advanced light sources, the electron storage ring Elettra and the free-electron laser (FEL) FERMI, continuously (H24) operated for light-matter interaction studies to more than 30 experimental stations. The experimental stations, also known as beamlines, enable the international community of researchers from academy and industry to characterize structure and function of matter with sensitivity down to molecular and atomic levels, to pattern and nanofabricate new structures and devices, and to develop new processes.

Every year scientists from more than 50 different countries compete by submitting proposals to access and use time on these experimental stations. Proposals are selected by peer-reviewed panels of international experts on the basis of scientific merit and potential impact, and the winners are granted free-of-charge access time as a contribution to their research. Because of its central location in Europe, Elettra Sincrotrone Trieste is increasingly attracting users from Central and Eastern European countries, where the demand for synchrotron radiation is in continuous growth, and is part of the primary network for science and technology of the Central European Initiative (CEI). But our outreach is far larger and reaches many more Countries in the world through long-term relations with the International Center for Theoretical Physics (ICTP) of UNESCO and the International Atomic Energy Agency (IAEA). The access by researchers from developing countries has tripled over the last few years, and the Indian research community is one of the largest users.

Users activities, joint research activities and collaborations among the laboratories allow to have an outstanding scientific production with more than 400 scientific papers published per year. Among these, about 30% are published on high-impact factor journals (IF>7). The most relevant scientific topics are in the fields of Functional Materials, Life Sciences, Environmental Sciences and Cultural Heritage, Low density and softs matter, Structure and Dynamics of systems, Surfaces and Interfaces but also Photon Sources and Instrumentation. For more details, please refer to Elettra Hiahliahts 2021-2022 (https://www.elettra.eu/images/Documents/SCIENCE/Elettra_HL_2022.pdf). The Elettra HL 2022-2023 will be published within November 2023.

Presently, the Italian Partner Facility consists of 14 beamlines, 2 offline instruments plus 2 laboratories:

- Band Dispersion and Electron-Phonon coupling beamline (BAEL)
- ESCA Microscopy beamline (ESMI)
- Gas Phase Photoemission beamline (GAPH)
- Inelastic Ultraviolet Scattering (IUVS)
- Materials Characterization by X ray diffraction beamline (MCX)
- Nanospectroscopy beamline (NASP)
- Synchrotron Infrared Source for Spectroscopy and Imaging beamline (SISSIBio)
- Synchrotron Infrared Source for Spectroscopy and Imaging beamline (SISSIMat)
- Spectromicroscopy beamline (SPEM)
- SuperESCA beamline (SUES)
- Synchrotron Radiation for Medical Physics beamline (SYRMEP)
- Soft X-ray Transmission and Emission Microscope beamline (TWINMIC)
- X ray Absorption Spectroscopy beamline (XAFS)

• X - ray Diffraction beamline (XRD1)

In addition, the IUVS and SISSIBio beamlines are available for experiments without synchrotron radiation with conventional light sources (IUVSOFF and SISSIBOFF) and the the Structural Biology Lab and the Nanoinnovation Lab are supporting the research. Their full integration to the CERIC-ERIC user offer is planned in the framework of the PRP@CERIC project (See section b for more details).

The aforementioned beamlines and Laboratories had / have /will have joint research programs with the other PFs. In the following a summary of them: Concluded projects: INTEGRA, Dyna Chiro, CEROP, RENEWALS, MAG-ALCHEMI

On going projects –OPV stability (XAFS, SISSI-Bio, SAXS) -PhDs Program, Battery lab upgrade program, ESBY project, STEAM project, FAITH project, BatERIC, CH-ERIC

Section b: Five-year development plan of the PF

The five-year objectives of the Italian Partner facility that reflect on the overall CERIC-ERIC consortium are: 1- the upgrade of the Elettra storage ring and 2- the strengthening of the LS activities.

1- Worldwide synchrotron facilities are nowadays implementing upgrades to Diffraction Limited Storage Rings (DLSRs). DLSRs, also known as ultra-low emittance storage rings or 4th generation SR facilities, are designed for achieving electron-beam emittance smaller or comparable to the emitted x-ray light. Presently, 4th generation SRs are operational in France (ESRF), Sweden (MAX IV) and Brazil (SIRIUS), while many more facilities are planning or are in the process of upgrading. Elettra is currently undertaking its upgrade to Elettra 2.0 DLSR as well. The project has been approved by the Italian Government in 2019 and, in accordance with the current implementation status, Elettra 2.0 is planned to be open to all users in January 2027, after an 18-months dark-period. Elettra 2.0 will be in the same building and it will have the same ring circumference (259.2 m) of the present 3rd generation source, while improving brightness and coherence thanks to the replacement of the existing symmetric double bend achromat (S2BA) storage ring layout with a new symmetric six bend achromat-enhanced (S6BA-E) one. Elettra 2.0 upgrade program is progressing with the upgrade of the existing beamlines, such as SAXS beamline toward a high flux more performant beamline (HF-SAXS, Austrian PF), while the brilliance and coherence of the new machine will allow the construction of new beamlines that the present machine cannot support, for micro X-ray diffraction, micro X-ray fluorescence, high-brightness SAXS (Austrian PF) and Coherent Diffraction Imaging. The first three will be served by in-vacuum undulators, while super-bends will be the source of the upgraded X-ray tomography beamline (SYRMEP-LS), of the XAFS and Xpress beamline, for X-ray absorption spectroscopy and X-ray diffraction at extreme conditions, respectively.

The upgrade of Elettra to Elettra 2.0 is intrinsically a project that will be beneficial also for the other CERIC-ERIC PFs, with special reference to the Austrian Partner Facility and the Czech Partner Facility. The present project naturally fits and integrate the projects submitted by the aforementioned PFs.

2- The Italian PF is investing in the life science domain. The most relevant action is the crucial involvement in the "Pathogen Readiness Platform for CERIC-ERIC Upgrade" (PRP@CERIC), funded through the NEXT-GENERATION EU program. The project aims to create an "Integrated macro-platform of biophysics and structural biology" that merges and harmonizes two platforms: 1- the "Integrated structural biology platform", geographically located at the Trieste node, that in the short-term integrates established X-rays synchrotron based structural characterization tools (XRD1, XRD2, SAXS beamlines) with the newly establishing cryo-EM facility and, in the medium-term, the future micro-focusing MX beamline (micro-XRD) and HB-SAXS and HF-SAXS beamlines at Elettra 2.0; 2- The "Sample preparation and characterization platform", of the Structural Biology Laboratory.

As can be appreciated, the direction taken to boost the LS domain intrinsically matches with the future plans of the Austrian PF, and complement the CERIC-ERIC already available facilities at SOLARIS. The cryo-EM system in Trieste will not duplicate the one at SOLARIS, being a 200KV machine, while the scientific direction is to integrate the two instruments. This action has been already taken in the framework



of the INTEGRA project, and it will be further pursued with the present one, by potentiating the sample preparation Lab at Elettra, at the Structural Biology Laboratory, and training new personnel at the two PFs, able to support the integration action.

In addition to these main directions, it is noteworthy to mention that a general upgrade also of SISSI-Bio and IUVS beamline is ongoing, as well as of the NanoInnovation Laboratory. All these Labs are deeply involved in the LS research and, with special reference to the NanoInnovation Lab in addition to the Structural Biology Lab, support the proposal of the Slovenian PF.

Despite both the upgrade of Elettra 2.0 and the LS-implementations at Elettra relies on funded projects, an extra budget is needed for actively supporting both of them in the direction of integration with the other PF involved.

Section c: Rationale and Scientific and technical description of the proposal

Considered the five-year development plan of the Italian PFs, the present proposal proposes actions that promote inter-PFs developments in the LS domain supporting: i- the upgrade of control systems for the new HF-SAXS and HB-SAXS beamlines at Elettra 2.0, as well as the front-end of HB-SAXS; ii- the upgrade of the Cryo-EM facility and sample preparation laboratory with ancillary instrumentations and consumables;

1- Small Angle X-ray scattering at Elettra2.0 for Life Sciences: High Brightness SAXS (HB-SAXS) e High Flux SAXS (HF-SAXS) beamlines (BLs)

HB-SAXS and HF-SAXS of the Austrian PF will have an important performance advantage by Elettra 2.0, given by an efficient use of the high intensity and high brilliance of the synchrotron upgrade. For exploiting this potential, it is needed:

1.A To design, purchase and install the frontend of HB-SAXS

BL performances will be improved by an in-vacuum undulator source providing a very high flux, but at the same time a high thermal power. The new high-power load front-end (FE) will provide the connection between the DLSR and the BL. The budget allocated for the FE will cover the following elements:

1) Manual vacuum valve to divide storage ring from FE.

2) Pumping unit to provides pumping capacity and vacuum measures to the FE zone next close to the SR. In particular, this unit shall pump down the outgassing generated by the mask.

3) Fixed mask to cut off the part of the photon beam emitted from ID that will not be used by the. This element defines the maximum aperture available for the BL and reduces the heat load on all downstream elements.

4) X-ray Beam Position Monitor or XBPM, a diagnostic element providing information regarding the position of the photon beam.

5) Photon shutter to block completely the synchrotron radiation beam. A pump is needed for absorbing the radiation outgassing together with local vacuum readings.

6) Fast closing shutter, a fast-reacting element that protects the SR vacuum integrity from any accident occurring in the BL. The trigger gauges controlling the actuation of this element will be installed on the Trigger unit. Fast closing shutter acts as a conductance restriction system but it is not vacuum tight.

7) Pneumatic vacuum valve, an additional standard gate valve vacuum tight actuated together with fast closing shutter.

8) Primary slits: they allow the BL users to define the photon beam dimensions within the aperture defined by the fixed mask.

9) Bremsstrahlung Stopper, to block the high-energy radiation (gas bremsstrahlung radiation,) directed towards the BL. It consists of a pneumatically actuated block of tungsten alloy. This unit shall also provide pumping capacity and vacuum readings.

12) Wall pipe, a vacuum pipe providing the connection between the SR tunnel and the BL.

13) Trigger unit, to provide pumping capacity, vacuum readings, and allocates at least one of the two trigger gauges in charge of activating the upstream fast closing shutter.

14) Pneumatic vacuum valve, an additional standard gate valve vacuum tight to separate front-end and beamline vacuum.

The cost of the FE components fabrication, design and installation can be been estimated to be about $500.000 \in (VAT \text{ included})$, while the vacuum elements will be $213.500 \in (VAT \text{ included})$.

1.B To develop HB-SAXS and HF-SAXS control systems and personal safety systems

The budget for each the beamline is justified as follows:

• Hardware costs, amounting to 91000 € (VAT included) for each beamline, cover a range of essential equipment and materials. These include control racks and accessories, PDUs, a switch for the controls network, interface computers of various types, Serial-Ethernet converters, a workstation with dual monitors, a server for data acquisition, and PLCs for interlock, vacuum control, and safety. These components are crucial for the efficient operation and control of the beamlines, ensuring accurate data acquisition and maintaining the safety of the facility and its personnel. The cost also includes materials for cabling and consumables, which are necessary for the installation and maintenance of the control systems.

• The human resources costs, for the two beamlines, are 150.000 € (3 years FTE), are allocated for software development. This includes mandatory software development, which is essential for the operation of the beamlines, software development for FAIR data HDF, which will ensure that the data generated by the facility will Findable, Accessible, Interoperable, and Reusable (FAIR), thereby maximizing its utility for researchers, and finally software development for acquisition and experiment control, which is crucial for the efficient operation of the beamlines and the accurate collection of data.

In conclusion, the total cost of for HB-SAXS and HF-SAXS control systems and personal safety system's developments it is 332.000 €. It is justified by the need for high-quality hardware, efficient and reliable software, and the safety of the facility and its personnel. The personnel, coordinated by Elettra ICT group, will ensure quality and standardization fundamental to the efficient and safe operation of the beamlines. This investment will ensure the successful operation of the HF-SAXS and HB-SAXS beamlines and the production of high-quality data for research.

2- Cryo-EM facility & Preparation Laboratory

The new cryo-EM facility of PRP@CERIC, that will be set by CNR-IOM, will be a new instrument part of the scientific offer of the Italian Partner Facility and open to CERIC-ERIC users. The facility, that will be installed at the IPF premises and co-managed and maintained by the two Institutions, will be equipped with a state-of-the-art 200 KV cryo-EM for single particle analysis and cryo-ET. The installation is scheduled at the beginning of the second semester 2024. A cross-beam SEM-FIB-iFLM, two vitrification systems and a cryo-confocal fluorescence microscope (CERIC-ERIC internal project ESBY) are also part of the facility. The facility will be supported for the sample preparation and pre-characterization part by the Structural Biology Laboratory at Elettra, that in the framework of PRP@CERIC project will be set an user-dedicated facility for sample preparation and pre-characterization. To further strengthen the upgrade programs, the present project encompasses:

1- Two postdoctoral fellowships who will be involved in LS activities of protein expression, purification, crystallization and cryo-EM preparation, to strengthen the cross-talk between NMR-SAXS-Macromolecular crystallography-Cryo-EM. Specifically, the postdocs will be trained on the cryo-EM utilization exploiting the existing collaboration between Elettra and SOLARIS, to better complement the two instruments for the CERIC offer and to grow a new generation of microscopists. Special emphasis will be given to the expression of proteins that interact with DNA/RNA hybrids, R-loops, D-loops, triple helices and DNA/RNA G-quadruplexes, to the characterization of the interactions from the biochemical and biophysical perspective for the selection of the best complexes for structural analysis, working in close collaboration with CERIC PFs for the osteoporosis research activities. Considering 2 postdoctoral fellows for 2 years (4 FTE 200.000 €) and about 15.000 € each for training at other PFs, the estimated cost is 230.000 €.

2- Cryo-EM sample preparation, pre-characterization, characterization and storage demands for a number of ancillary tools and consumables for making the integrated structural biology platform fully functional. The budget is considered for the following items: Lab furnitures, incubators and purification

systems, add-ons for fermentators, imaging system to visualise and analyse gels, ultrafreezers at -80°C, consumables (grids, tweezers, etc...), maskless photopatterning system for prototyping and engineering custom in vitro microenvironments.

Section d: Impact

Life Sciences in one of the CERIC-ERIC identified priorities. The present proposal perfectly fits with the mission, harmonizing the upgrade programs of the IPF with the ones of the other CERIC-ERIC partners. The proposed investments in the direction of control systems of HB-SAXS and HF-SAXS, and of the frontend of the in-vacuum-undulator HF-SAXS match with the proposal of the Austrian PF, but, in a more general perspective, the Elettra2.0 program will support also the upgrade plans and proposal of the Czech PF.

Elettra 2.0 program also bridges the PRP@CERIC project, and the present proposal will made the synergy even more solid. The proposed investments for the Structural Biology Laboratory will support cryo-EM sample preparation and pre-characterization, providing a preparation environment functional also to the cryo-EM facility of SOLARIS. With the intent to enforce the cross-talk among the two instruments, 2 postdoc fellows will be hired, and trained at both PFs. The scientific activities of the fellows will encompass the expression of proteins that interact with DNA/RNA hybrids, R-loops, D-loops, triple helices and DNA/RNA G-quadruplexes, the characterization of the interactions from the biochemical and biophysical point of view, the select the best complexes for structural analysis, taking adavantage from the expertiese of the Structural Biology laboratory and working in close collaboration with CERIC PFs. Indeed, noncanonical nucleic acid structures are emerging as important players not only in modulating a variety of cellular processes, but also in the development and progression of many human diseases, including cancer and degeneration. Preliminary evidence suggests that these structures also play a role in the expression of osteoporosis-related genes. A number of helicases under study at the Structural Biology laboratory have been associated with osteoblast maturation, osteosarcoma or osteoporosis. In particular RecQ4 is required for normal osteoblast expansion and its mutations give a strong predisposition to develop osteosarcoma; whereas mutation in the Werner and RTEL1 helicase cause premature aging and osteoporosis. Therefore, a clear bridge exist and it is inteded with the Slovenian PF proposal.

Finally, the implemtation of teh cryo-EM facility with a maskless photopatterning system goes in the direction to improve microfabrication capabilities of CERIC-ERIC consortium and optimize the planned investements of the CERIC-ERIC internal project ESBY, that will allow to install a cryo-confocal microscope in Trieste, for cryo-ET and cellular analysis in general, being beneficial also for SR-imaging approaches, such as at TwinMic and SISSI-Bio beamlines, but also for the pro'poses of the AFM analysis at the NanoInnovation laboratory.

Section e: Description of the implementation

The project implementation will be performed according to the following actions:

- 1- Implementation of the structural Biology Laboratory for sample preparation, pre-characterization, characterization and storage (M1-M12);
- 2- Hiring and training of 2 FTE postdoctoral fellows involved in LS activities for two years (M12-M36);
- 3- Hiring of 1 FTE for 3 years for hardware and software implementation of the control systems of HB-SAXS and HF-SAXS (M24-M60);
- 4- Hardware components for the implementation of the control systems of HB-SAXS and HF-SAXS (M36-M60);
- 5- Hardware and vacuum components for HB-SAXS frontend (M48-M60);
- 6- Maskless photopatterning system for prototyping and engineering custom in vitro microenvironments and consumables for cryo-EM sample preparation (M48-M60)

Assuming the project start in 2024, during this year Elettra will be still operative (until the first semester 2025). Taken into consideration that the cryo-EM facility will be installed in the second half of 2025, action
1 at year-1 is intended to be ready with the upgraded Structural Biology laboratory on time with the cryo-EM facility. During the second year (2025), two FTE postdoctoral fellows will be hired, trained at the Structural Biology Laboratory at SOLARIS, for being ready to work on collaborative research during the second year of the contract (2026). In 2026 Elettra will be in the dark-period and installation phase. A new FTE will be hired in 2026 for the hardware and software implementation for both HB- and HF-SAXS beamlines. Taking advantage from the experience already gained by the collogues, the hardware and software will be tuned on the two beamlines in 2026. The hardware components will be then purchased in 2027 and beginning 2028, then assembled. In 2027 is expected the delivery of the vacuum components and frontend elements for HB-SAXS, and their installation as well, according with the dark period scheduling. In 2028, it is expected to reach a maturity state of the operation for the cryo-EM facility for single-particle analysis. In order to better bridge also the cellular community for cryo-ET and beyond, we plan to improve the cryo-EM facility with a maskless photopatterning system for micropatterning, hydrogel polymerization and microfabrication, to create in vitro cellular microenvironments and get better cell models for both cell biology experiments or cryo-ET studies. In addition, consumables for cryo-EM experiments (such as grids, small tools non-durable, solvents, bio-reagents, fluorophores, etc...) will be purchased for supporting inter-PFs research and user's activities.

Annex 1 – Human Resources: Resources connected to the activity of the required staff (total cost including overall estimated costs and use of the CERIC funding)

| CEDIC | | Total in Euro | | | | | | | |
|---|--------|---------------|----------|--------|--------|--|--|--|--|
| CERIC | Year 1 | Year 2 | Year 3 | Year 4 | Year 5 | | | | |
| Consumables | | | | | | | | | |
| Personnel cost (PhD, researcher or technical staff) | | 100,000€ | 100,000€ | | | | | | |
| Travel costs | | 15,000 € | 15,000€ | | | | | | |
| Other costs (conferences fees, publications, training, etc) | | | | | | | | | |
| TOTAL | | 115,000€ | 115,000€ | | | | | | |

Annex 2 – Infrastructure Development: Resources (including overall estimated costs and use of the required CERIC funding)

| CERTC | Total in Euro | | | | | | |
|----------------|---------------|--------|---------|----------|----------|--|--|
| CERIC | Year 1 | Year 2 | Year 3 | Year 4 | Year 5 | | |
| Equipment | 219,000€ | | | 804,500€ | 211,000€ | | |
| Consumables | | | | | 78,346€ | | |
| Personnel cost | | | 50,000€ | 50,000€ | 50,000€ | | |
| Travel cost | | | | | | | |
| TOTAL | 219,000€ | | 50,000€ | 854,500€ | 339,346€ | | |



Strategy for the allocation of CERIC's membership fees in support of the integration of CERIC capabilities

Polish Partner Facility

Introduction

In its resolution 8th May 2023, the General Assembly (GA) agreed that as long as the contribution by the Host Member State of CERIC-ERIC allows covering the statutory operations fully, 90% of the Member's annual contributions are dedicated to supporting actions integrating the capabilities of the Member's Partner Facilities, **such as PhDs, post-docs, joint research projects, infrastructure investments and promotion of CERIC-ERIC Partner Facilities research offer.** These will be agreed upon by the GA, assuring that, over a 5-year average, this support to each Partner Facility will equal at least 90% of the cash contribution provided by the relevant Member during this period.

To enable the decision of the GA, the **Directors of the PFs should define the strategy and an annual program with a five-year outlook** for their own Facility within the CERIC collaboration framework and discuss it in the BoD for submittal to the GA through the ED, with the opinion of the ISTAC.

In the following, the PFs are requested to submit their proposal, possibly coordinated and agreed upon with other Partner Facilities, to allow for a discussion and development of a joint strategy at the October BoD meeting.

Proposing CERIC Partner Facility: SOLARIS

Proposal summary (up to 200 words)

SOLARIS postulates to reinvest its CERIC contribution to strengthen SOLARIS manpower by financing three FTEs. We strongly believe that this will strengthen CERIC, create synergy, provide integration and open new area for collaboration between SOLARIS and other CERIC PFs.

The main objective of the CERIC 2 FTE @ SOLARIS will be:

to enhance integration with other CERIC PFs in the area of development and realization of joint research projects with the focus on two new SOLARIS infrastructures (however not exclusively):

• NAP-XPS branch of the PHELIX beamline – involvement of Czech, Austrian, Slovenian and Italian PFs have been declared

• STXM facility at DEMETER beamline branch – involvement of Italian and Austrian PFs so far have been declared

b. Deliver new initiatives regarding joint CERIC projects

c. Provide new technical and scientific know how in order to support new research projects as well as users

We propose to devote the 3rd FTE to the following administrative tasks:

a. promotion of CERIC PFs amongst the scientific communities in the Member Countries open access, diversity of infrastructures, available support.

- b. Promoting projects and stimulating new ones
- c. Involvement in CERIC common actions e.g.: collaboration with industry, open data, EOSC ...
- d. Improving links with the CERIC seat

Section a: Current Status and future evolution of the PF

Provide (1-2 page):

- a brief summary of the present status of the PF, listing

- all its present research activities and programmes, including those not reported within CERIC (but a part of the PF);

- resources (main instruments, collaborating staff and all funding sources).

- list of the publications in the last two years.

- an outline on how the PF intends to evolve, particularly in collaboration/integration with the rest of CERIC. Briefly list the already ongoing activities with other CERIC Partner facilities. This should help to define the ongoing and future strategy.

- the possible need for new resources to make the PF more effective and visible, including administrative support to provide annual accounts. Please also explicitly refer to organisational needs within your hosting institution, allowing for a better definition and identity of the PF and its operation, its reporting and integration within CERIC...etc.

SOLARIS, since joining CERIC-ERIC in 2016, has been continuously developing its research infrastructure offer. In 2024, access to 6 beamlines and 2 cryo-EM microscopes is available. Recently new naming standard has been introduced where beamlines are called after entries in science-fiction/fantasy tales. Currently they are: ASTRA – dedicated to X-ray absorption spectroscopy (XAS) and related techniques in 1 keV to 15 keV energy range; DEMETER – operating in 100-2000eV range, where two measurement branches equipped with PEEM STXM microscopes are available; PIRX- dedicated to spectroscopy in the soft X-ray energy range 100-2000eV; PHELIX- offering Soft X-ray Angle Resolved Photoelectron Spectroscopy (SX-ARPES), XAS, TEY, CD, Res-PES measurements in 40-1500eV range; POLYX- a compact beamline for X-ray microimaging and X-ray microspectroscopy in the energy range 4-15 keV; URANOS- offering Angle-Resolved PhotoElectron Spectroscopy (ARPES) technique in the range from 8 to 170 eV with any selectable polarization. Two diagnostic beamlines LUMOS and PINHOLE have also been installed to monitor the synchrotron performance. SOLARIS complementary Cryo-EM Facility provides access to two high-end cryo-electron microscopes dedicated to determining structures of biomacromolecules. Single particle analysis (SPA), cryo-electron tomography (cET) and microcrystal electron diffraction (MicroED) techniques to analyse specimens at atomic resolution are available.



Vigorous infrastructural development has resulted in the constant growth of SOLARIS users' community. In 2023, SOLARIS recorded 1333 registered users which submitted 370 research projects from 70 Polish and foreign universities and research institutes. The amount of requested beamtime exceeded the available access by about 50%.





Due to the overbooking only 200 proposals were granted by the International Evaluation Committee on the grounds of their superior excellence. Around 700 scientists visited SOLARIS to perform their measurements covering many disciplines of science.

SOLARIS performance indexes over the last 5 years

SOLARIS Users and Statistics





SOLARIS Users and Statistics







Section b: Five-year development plan of the PF

The proposers should describe (1 page maximum):

- 5-year objectives of the PF (what it wants to achieve in 5 years in collaboration with the other CERIC PFs) and an outline of a program to reach the objectives.

- key needs of the PF within the next five years (where possible, refer to the ISTAC recommendations) and how the proposal fits within this five-year program and with a joint program with the other CERIC PF's

SOLARIS plans for the next two years include the construction of new beamlines. To accommodate these infrastructures an extension of the experimental hall has been completed at the end of 2023 increasing its area by 2800 m2 and allowing also for building auxiliary laboratories and offices for SOLARIS users and employees. Financing has been secured for building three new beamlines at different stages of construction. The most advanced is CIRI beamline: Chemical InfraRed Imaging which should be commissioned in 2024. It is a specialized research installation using SR in the infrared region. CIRI will ultimately be equipped with three end stations for imaging in micro- and nanometric spatial resolution. First one, FT-IR microscope equipped with two types of detectors: MCT detector used for single-point measurements and mapping and FPA detector (Focal Plane Array) for imaging. The second end station - microscope SNOM/AFM-IR- is dedicated to experiments with spatial resolution below the diffraction limit of infrared light. The third planned end station is the O-PTIR microscope (Optical Photothermal Infrared) which in addition to using IR SR source will be equipped with 532nm laser. CIRI is going to be one of the few most advanced infrastructures utilizing synchrotron IR Radiation. CIRI Another two constructed beamlines are SOLCRYS and SMAUG with planned commissioning in 2025. SOLCRYS (MX) is very much anticipated by the Polish scientific community a wiggler-based, high energy X-ray beamline for structural studies of proteins, nucleic acids and small molecules. The planned research capabilities of the MX end station include wavelength tunability for multiwavelength anomalous diffraction (MAD) experiments and a high flux mode for standard (routine) diffraction data collection for protein crystals.

SMAUG beamline (Small Angle X-ray Scattering) is the bending magnet-based beamline using the hard X-rays in the range of 6 to 16 keV. The planned research capabilities of the end station will offer measurement capabilities in the following techniques: bio-SAXS (studies of biological systems in solutions), SEC-SAXS (combined SAXS studies with simultaneous chromatographic separation), SAXS static measurements (including tests at low and high temperatures, magnetic or electric field) and SAXS liquid measurements at high pressures.



Figure 1 SOLARIS @ the end of 2025

Long-term development plans include construction of portfolio of new beamlines @ all available SR ports. Continuing our collaborative approach, talks with research institutions in Poland are in progress, some in advanced stage. Separately, responding to CERIC initiatives would be appreciated.

Modification of the linear accelerator to provide full energy injection at 1.5 GeV enabling top-up operation mode is alos on the table. Such modernization will allow the synchrotron to deliver constant intensity beam round the clock without any interruptions. Eventually, the quality of research will substantially improve. Consecutively construction of an ultra-short soft X-ray pulse facility for studying fast transient processes is envisaged.

Section c: Rationale and Scientific and technical description of the proposal

The Proposal should concisely describe its rationale and, how it fits in the five-year outlook, how the scientific and technical quality will be assured. For proposed PhD students, list also the University(ies) awarding the degree and the name of the proposed supervisor (s) (maximum 1 page).

Facing the introduction of cash contribution by the CERIC members and resulting reinvestment in the PFs the SOLARIS management has performed analysis of the best usage of the money in order to enable better integration and collaboration with CERIC. Below we present the results and the proposal.

SOLARIS in CERIC - constraints analysis

1. SOLARIS has been set up and financed as the open and free of charge infrastructure facility where the primary mission is to answer the demands of research community and provide operational spectrum of advanced research techniques installed at the synchrotron beamlines with all the necessary support for external users. This includes, amongst the others, construction of new infrastructures, maintenance and development of the existing ones in such areas of hardware, controls, data acquisition and storage, data processing software. Users' support and assistance is of another priority.

Hence the employed staff is focused on providing the above service mission – where the scientific division plays the leading role and is exceptionally charged with a broad spectrum of duties.

Nevertheless, SOLARIS management is fully aware that the scientific division should be involved in research project (also the in-house ones) – not being reduced to delivering services and support to external users. Finding the necessary balance between these activities is challenging and in many cases depends on the expertise and knowledge of the employed scientists. It is also affected by the obligation of supplying functional infrastructure for the users. Development of in- house research activities at the cost of the user's services can disturb that balance and affect the cause for financing the center.

Unfortunately current SOLARIS limited human resources do not allow for engagements in ambitious research projects organized by CERIC where other PFs are involved. This applies to either involvement in the already running projects or to the constructing new initiatives. We would like to address this shortfall.

2. Since 1st of March 2016 SOLARIS Has joined CERIC as Polish Partner Facility. One of the main mission of CERIC is to offer for external research groups multidisciplinary and multitechnique research options available at the broad spectrum of all CERIC Partner Facilities. One of the Key Performance Indexes of CERIC is number of users of the consortium Partner Facilities. Looking from the perspective of each CERIC member country this index has a big impact on the local decisionmakers. In our context number of Polish groups performing research at CERIC PFs abroad is important. This becomes is even more essential when cash contributions are being introduced. Despite the constant growth of the number of users SOLARIS management reckon that there is room for improvement and promotional activities are needed to increase the awareness of CERIC offer of free of charge, multitechnique measurements at different PFs.

Proposed solution

To address the above shortcomings SOLARIS postulates to reinvest its CERIC contribution to strengthen SOLARIS manpower by financing three FTEs. We strongly believe that this will create synergy, provide integration and open new area for collaboration between SOLARIS and other CERIC PFs. The main objective of the CERIC 2 FTE @ SOLARIS will be:

a. to enhance integration with other CERIC PFs in the area of development and realization of joint research projects with the focus on two new SOLARIS infrastructures (however not exclusively):

- NAP-XPS branch of the PHELIX beamline involvement of Czech, Austrian, Slovenian and Italian PFs have been declared
- STXM facility at DEMETER beamline branch involvement of Italian and Austrian PFs so far have been declared
- b. Deliver new initiatives regarding joint CERIC projects
- c. Provide new technical and scientific know how in order to support new research projects as well as users
- We propose to devote the 3rd FTE to the following administrative tasks:
- a. promotion of CERIC PFs amongst the scientific communities in the Member Countries e.g. open access, diversity of infrastructures, available support.
- b. Promoting projects and stimulating new ones
- c. Involvement in CERIC common actions e.g.: collaboration with industry, open data, EOSC ...
- d. Improving links with the CERIC seat

We strongly believe that our proposal should work as a test case for the CERIC consortium for better collaboration and administrative integration of the partner facilities into CERIC.

During deliberations on our proposal, SOLARIS's in kind contribution should be taken into account. SOLARIS has been offering 10% of its infrastructure for CERIC users. This offer has been constantly increasing with the development of new beamlines and experimental stations. One can transfer our contribution into 10% of our running costs, but also one should consider the manpower involved. Currently we have 120 employees which, results in 12 FTE provided to CERIC activities.

Section d: Impact

The Proposal should describe (0,5 page maximum) its expected impacts on the overall scientific and technical quality and capability of CERIC. How the proposal complements and fits in common developments with other activities both at the PF and in other PFs, aimed at integrating the facilities and overall strengthening of CERIC.

Our proposal of devoting the funds to cover 3 FTEs is based on the belief that such enhancement of the SOLARIS team will provide better services and support for the users and increase the recognition of the CERIC facilities in the CERIC-ERIC landscape. At least @SOLARIS we gain satisfaction from the number of users and delivering the best support. Also; we strongly believe that our proposal will integrate CERIC PFs and stimulate collaboration and further research projects.

Section e: Description of the implementation

This section should describe (1 page maximum) in a clear way the maturity and implementation of the project and its timeframe. Please also describe a possible time-line of the proposed investment e.g. how the investment will accumulate over the 5 years after the contributions commence (2024). For proposals, including the hiring of personnel, outline the research/technical program.

We are proposing to use the CERIC funds for strengthening the expert manpower @SOLARIS hence @ CERIC. The rationale is presented in section c above. The tasks/duties are generally described also there. Nevertheless, for obvious reasons they will need to be defined in the details upon implementation of the reinvestment scheme.

Regarding the infrastructures we define as needing support in order to explore their research potential – the following two:

NAP-XPS – Near Ambient Pressure XPS System at PHELIX beamline

- Photon enery: 50-1500eV
- Beam size: 100 × 50 μm2
- Sample environment: UHV 50 mbar, temp up to 700°C (resistive heating)
- Solid-gas interface

Near-ambient pressure X-ray photoelectron spectroscopy (NAP-XPS) is a chemically sensitive technique, which probes both the surface structure and interfaces between solids, liquids and gases. The NAP-XPS

station, operating at elevated pressure, will allow processes to be followed under real working conditions (in situ/operando studies) of relevance to catalysis and photocatalysis, nanomedicine or new energy sources.

In particular, NAP-XPS demonstrates its significance for probing active sites and unravelling surface reaction mechanisms in heterogeneous catalysis during in-situ/operando investigations.

The use of NAP-XPS to investigate electrochemical interfaces e.g. during oxygen evolution reaction (OER). OER is a bottleneck in electrochemical energy conversion and storage, which are crucial to the solutions to the current global energy challenges.

STXM - Scanning Transmission X-ray Microscopy @ DEMETER Beamline

- Photon enery: 200-2000eV
- Base resolution ~30 nm
- Working modes: transmission and fluorescence
- Working presure 10-7 mbar to 1100mbar (He atm.)
- 2 image acquisition modes (point by point, line by line)

The STXM microscope is dedicated to imaging local changes in the sample. By combining microscopy and spectroscopy, we are able to obtain chemical information from the imaged region (30nm). The advantage of this technique is sensitivity to different chemical forms of the same element.

Environmental tests - both organic and inorganic materials. Catalysis and electrochemistry. Batteries. Biology and biomedical. Magnetism.

Further development required to enable ptychography and fluorescence measurements.

Annex 1 – Human Resources: Resources connected to the activity of the required staff (total cost including overall estimated costs and use of the CERIC funding)

In accordance with the regulations introducing Members' cash contributions, the SOLARIS input is assumed @ 141 kEUR/year. Following pt.7 of the document (90% of the Members annual contributions is dedicated to supporting actions integrating the capabilities of the Members Partner Facilities, such as PhDs, post-docs, joint research projects, infrastructure investments and promotion of CERIC-ERIC Partner Facilities research offer) we assumed reinvestment in SOLARIS @ 125 kEUR/year. Below we present the relevant budget of our proposal.

| | Total in Euro | | | | | |
|---|---------------|--------|--------|--------|--------|--|
| CERIC | Year 1 | Year 2 | Year 3 | Year 4 | Year 5 | |
| Consumables | 5000 | 5000 | 5000 | 5000 | 5000 | |
| Personnel cost (PhD, researcher or technical staff) | 100000 | 100000 | 100000 | 100000 | 100000 | |
| Travel costs | 10000 | 10000 | 10000 | 10000 | 10000 | |
| Other costs (conferences fees, publications, training, etc) | 10000 | 10000 | 10000 | 10000 | 10000 | |
| TOTAL | 125000 | 125000 | 125000 | 125000 | 125000 | |

Annex 2 – Infrastructure Development: Resources (including overall estimated costs and use of the required CERIC funding)

| CERTC | Total in Euro | | | | | | |
|----------------|---------------|--------|--------|--------|--------|--|--|
| CERIC | Year 1 | Year 2 | Year 3 | Year 4 | Year 5 | | |
| Equipment | _ | _ | _ | _ | _ | | |
| Consumables | _ | _ | _ | _ | _ | | |
| Personnel cost | _ | _ | _ | _ | _ | | |
| Travel cost | _ | _ | _ | _ | _ | | |
| TOTAL | | | | | | | |



Strategy for the allocation of CERIC's membership fees in support of the integration of CERIC capabilities

Romanian Partner Facility

Introduction

In its resolution 8th May 2023, the General Assembly (GA) agreed that as long as the contribution by the Host Member State of CERIC-ERIC allows covering the statutory operations fully, 90% of the Member's annual contributions are dedicated to supporting actions integrating the capabilities of the Member's Partner Facilities, **such as PhDs, post-docs, joint research projects, infrastructure investments and promotion of CERIC-ERIC Partner Facilities research offer.** These will be agreed upon by the GA, assuring that, over a 5-year average, this support to each Partner Facility will equal at least 90% of the cash contribution provided by the relevant Member during this period.

To enable the decision of the GA, the **Directors of the PFs should define the strategy and an annual program with a five-year outlook** for their own Facility within the CERIC collaboration framework and discuss it in the BoD for submittal to the GA through the ED, with the opinion of the ISTAC.

In the following, the PFs are requested to submit their proposal, possibly coordinated and agreed upon with other Partner Facilities, to allow for a discussion and development of a joint strategy at the October BoD meeting.

Proposing CERIC Partner Facility: NIMP-LASDAM

Proposal summary (up to 200 words)

NIMP represents a flagship of the Romanian research in materials science through the quality of the research infrastructure, human resources and the obtained results. NIMP was invited by ISTAC to join CERIC-ERIC in 2014 as Representing Entity of Romania, founding member, along with similar research entities across Central Europe. By joining valuable scientific competences and advanced research equipment, during its almost 10 years of activity CERIC-ERIC gained a worldwide reputation and attractivity for external users. This achievement can only be sustained and improved by continuously maintaining and upgrading the infrastructure and human resources while permanently optimising the consortium administrative activities. This proposal aims to strengthen the NIMP-LASDAM participation in CERIC-ERIC by contributing to the upgrade of the existing HRTEM and EPR research infrastructure, in order to maintain at the highest level both the scientific and technical quality standards of NIMP-LASDAM and the CERIC-ERIC. On the other hand, this proposal will contribute to better adapting the NIMP-LASDAM investigation capabilities to the research programs initiated by CERIC-ERIC on materials for batteries and fuel cells. The 345000 Euro procurement budget, distributed over 5 years, is based on the NIMP-LASDAM annual membership fee within CERIC-ERIC. The associated implementation costs will be covered by NIMP-LASDAM.

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Section a: Current Status and future evolution of the PF

The Romanian Partner Facility in CERIC is the Laboratory of Atomic Structures and Defects in Advanced Materials (LASDAM) within the National Institute of Materials Physics appointed as Representing Entity on behalf of Romania as CERIC Member. The research activity of LASDAM is directed towards the investigation and manipulation of physical properties at nanometric and atomic scale with the goal to develop new materials (dielectrics, semiconductors, alloys, ceramics) for applications in the semiconductor industry (gas sensors, optical sensors, memories, radiation detectors), telecommunications, energy conversion, health and environment.

Main instruments

LASDAM includes equipment for materials synthesis, processing and characterization among which: - analytic aberration-corrected high-resolution transmission electron microscope JEM ARM 200F provided with JEOL EDS and Gatan EELS spectrometers;

- analytic high-resolution transmission electron microscope JEM 2100 provided with JEOL EDS spectrometer and precession electron diffraction unit;

- analytic SEM-FIB Dual System Tescan Lyra III XMU provided with EDS, EBSD units;

- laboratory for TEM/SEM specimen preparation using precision mechanical processing, ion milling, plasma etching, electrochemical etching;

- pulsed X-band EPR Spectrometer Bruker ELEXSYS E580 with accessories for ENDOR and ELDOR (5 - 300 K);

- continuous wave Q-band EPR Spectrometer Bruker ELEXSYS E500Q with accessories for ENDOR (5 - 300 K);

- continuous wave X-band EPR Spectrometer Bruker EMXplus (80 - 300 K);

- Cryomech LHeP18 liquid He plant with helium recovery system;

- magnetron sputtering installation, provided with in situ surface analysis by AES, LEED and ellipsometry;

- laboratory for chemical synthesis of nanostructured materials by coprecipitation and hydrothermal growth;

experimental chains for electrical and photoelectrical measurements under continuous and modulated illumination (10 – 500 K), magnetoresistance and Hall measuring chains (up to 2.5 T; 4 – 300 K);
gas mixing station and measuring chain for characterizing electrical/electronic properties of materials under controlled atmosphere for gas sensing applications.

The infrastructure for high-resolution transmission electron microscopy (HRTEM) and electron paramagnetic resonance (EPR) spectroscopy has been selected for open access within CERIC.

<u>Staff</u>

LASDAM counts 32 members among which 28 research personnel and 4 technical support.

Funding sources

The funding sources consist in RD projects granted within the national and international programs such as the National Core Program, the National RD Plan through calls like "Exploratory Research" (PCE), "Experimental Demonstration Project" (PED), "Young Research Teams" (TE), post-doc (PD), "Competitiveness Operational Program" (POC), M-ERA.NET, EEA Grants.

List of publications in the last 2 years

The scientific production of LASDAM counts in average 60 publications in ISI journals each year.

| Year | Total | Q1 | Q2 | Q3 | Q4 |
|------|-------|----|----|----|----|
| 2021 | 69 | 44 | 19 | 5 | 1 |
| 2022 | 50 | 30 | 17 | 3 | |

The full list of publications each year is published on the laboratory webpage https://infim.ro/lab-70/publications/

Prospective evolution of LASDAM in collaboration/integration with CERIC partners

Romania through NIMP-LASDAM is founding member of CERIC-ERIC strongly committed to support CERIC by actively taking part in the regular CERIC activities in collaboration with external users as well as in internal programmes initiated by CERIC-ERIC. NIMP-LASDAM participate in CERIC projects submitted by external users mainly with in-depth microstructural and spectroscopic characterisation of advanced materials using modern techniques of data acquisition and processing installed on the mentioned HRTEM and EPR instruments. In addition, NIMP-LASDAM takes part to CERIC internal programs such as the ongoing CERIC-ERIC PhD Programme, internal research projects along with other CERIC PFs (e.g. Renewals – Graphene for Water in Life Sciences) or the recently launched CERIC initiatives on materials for batteries and fuel cells.

The NIMP-LASDAM proposal for the allocation of CERIC's membership fees in support of the integration of CERIC capabilities is based on the two CERIC-ERIC initiatives with respect to materials for batteries and fuel cells. Our proposal aims at the development of the current HRTEM & EPR infrastructure available at NIMP-LASDAM in order allow for in situ and operando investigations on the mentioned types of materials. In a synergetic approach along with other CERIC PFs, these developments are in line with the already existing in situ and operando characterization facilities at the ELETTRA XAFS beamline and at Charles University with the NAP-XPS and the EnviroESCA instruments allowing for indepth analysis of catalysts, in liquids or at liquid-solid interfaces.

Moreover, this investment will contribute to a better integration of NIMP-LASDAM within CERIC-ERIC regarding the CERIC participation in the Horizon Europe project IMPRESS. The in situ / operando HRTEM system under implementation at NIMP-LASDAM is currently oriented towards studies on solid-state batteries. Accordingly, new methods of microfabrication need to be put in place to produce thin TEM samples with the functionality of a solid-state battery (half cells or full micro-battery) and to enable atomic-resolution microstructural and spectroscopic studies on the electrochemical processes at the electrode-electrolyte interfaces during the charging/discharging cycles.

This investment will contribute to creating a solid platform for microstructural (HRTEM) and spectroscopic (EPR0 investigations on batteries and fuel cells offered to external users, but will also strengthen the research opportunities among the CERIC PFs. We mention here the existing collaboration with Charles University based on several CERIC projects on catalysts for fuel cells, work visits of Romanian PhD students for NAP XPS experiments at Prague and a common M-ERA.NET application which could ne reiterated either on a future call or as an in-house CERIC project along with other partners involved in in situ and operando characterization such as the ELETTRA XAFS beamline or associated partners like LISA.

Section b: Five-year development plan of the PF

One of the strategic objectives mentioned in the Strategic Development Plan of NIMP is represented by strengthening the NIMP participation in large research infrastructures such as C-ERIC, CERN, ITER, or ELI-NP. The evolution perspective of NIMP-LASDAM in connection with CERIC takes into consideration the ISTAC recommendations following the last periodic evaluation of the NIMP-LASDAM activity within CERIC (October 26th 2022).

The 5-year development plan of NIMP-LASDAM in relation to CERIC-ERIC concerns the instrumentation, the human resources including the research and the administrative personnel, as well as the organizational needs, aiming at reaching the following objectives:

1. Maintain the current HRTEM and EPR instrumentation at a world-class level.

2. Extend the current HRTEM infrastructure in order to allow for in situ and operando atomic-resolution investigations.

3. Extend the current EPR capabilities by improving the working conditions at cryogenic temperatures and the pulsed EPR techniques.

4. Implement CERIC's FAIR and Open Data policy.



In order to achieve the above-mentioned objectives, the following key needs are considered for the next five years:

1. Financial resources to cover maintenance and repair services costs provided by the HRTEM and EPR equipment manufacturers.

2. Extension of the HRTEM facility with a dedicated system for in situ heating and electrical biasing of the thin specimen during TEM observation

3. Upgrade of the SEM-FIB instrument with a high-precision nanomanipulator allowing for nanoscale sample translation and rotation under the electron/ion beam.

4. Upgrade of the EELS spectrometer installed on the HRTEM instrument with Dual EELS, fast Spectrum Imaging capabilities.

5. Upgrade of the EPR spectrometers with dedicated equipment for measurements at cryogenic temperatures, including a cryostat for X-band cavities, automatic helium purifier, cryogen free variable temperature cryostat.

6. Extension of the EPR experimental capabilities with an electrochemical cell.

The envisaged infrastructure development is being considered based on NIMP-LASDAM participation in research projects focused on materials for batteries and fuel cells, according to the strategic initiatives of CERIC-ERIC, but also with respect to the research topics approached by NIMP and LASDAM within the national research projects. The necessary funding will be provided both from allocation of CERIC's membership fees in support of the integration of CERIC capabilities and from national projects developed at NIMP.

Section c: Rationale and Scientific and technical description of the proposal

NIMP represents a flagship of the Romanian research in materials science through the quality of the research infrastructure, human resources and the obtained results. It is the very reason why NIMP was selected by ISTAC and invited to join CERIC-ERIC along with similar research entities across Central Europe. By joining valuable scientific competences and advanced research equipment, during its almost 10 years of activity CERIC-ERIC gained a worldwide reputation and attractivity for external users. This achievement can only be sustained and improved by continuously maintaining and upgrading the infrastructure and human resources while permanently optimising the consortium administrative activities.

This proposal aims to strengthen the NIMP-LASDAM participation in CERIC-ERIC by contributing to the upgrade of the existing HRTEM and EPR research infrastructure, in order to maintain at the highest level both the scientific and technical quality standards of NIMP-LASDAM and the CERIC-ERIC attractivity with respect to external users. On the other hand, this proposal will contribute to better adapting the NIMP-LASDAM investigation capabilities to the research programs initiated by CERIC-ERIC in the field of materials for batteries and fuel cells.

Upgrade of the EPR facility

The upgrade of the current EPR spectrometers with dedicated equipment for measurements at cryogenic temperatures and the extension of the experimental capabilities with an electrochemical cell are considered by this proposal.

The EPR investigations of both paramagnetic centres of interest in materials science (point defects, dopants, radicals etc.) and their host material properties at atomic level (local structure, lattice dynamics, structural and compositional transformations, magnetic properties etc.) often require measurements at variable temperature down to the liquid helium temperature. This proposal intends to extend the existing equipment for measurements at cryogenic temperatures by acquiring a cryostat for rectangular and cylindrical X-band resonators, an automatic helium purifier for the helium recovery system, and a cryogen free variable temperature cryostat for the continuous wave and pulse experiments on the ELEXSYS E580 spectrometer. The envisaged extension of the existing low temperature facilities will considerably improve the cost-effectiveness and duration of the low temperature experiments and increase the range of continuous wave and pulse EPR investigations offered to the CERIC-ERIC users.

The acquisition of an electrochemical cell designed for working on an X-band spectrometer concerns the development of an experimental setup for in-situ EPR observations, especially for applications in batteries and fuel cells.

Upgrade of the HRTEM facility

The upgrade of the current TEM specimen preparation techniques and the extension of the available in situ HRTEM conditions are considered by this proposal.

The first condition to be satisfied in order to conduct relevant undistorted microstructural investigations by HRTEM is to be able to prepare thin specimens (below 50 nm thickness) without inducing artefacts or transforming the original microstructure of the sample. A wide range of techniques and instruments have been developed along the time for the preparation of thin specimens, covering a large spectrum of sample types spanning from fragile nanostructures (nanowires, nanotubes, 2D materials, nanoparticles) to thin and ultrathin films, complex heterostructures, composite materials, ceramics, alloys or intermetallic compounds. The preparation methods may involve mechanical microprocessing, ion milling, electrochemical chemical etching, plasma treatment, each of which carrying advantages and disadvantages or being appropriate to one or more types of samples. Ultramicrotomy is a purely mechanical method, allowing for cutting ultrafine slices from a sample which can then be observed in a TEM, with an extremely low if any probability of specimen altering by contamination or surface modification. This proposal intends to reinforce the laboratory for TEM specimen preparation at NIMP-LASDAM by acquiring an ultramicrotome that will be applied to an extremely large variety of samples, from biological matter, like animal or plant tissue to inorganic or organic materials such as nanostructures, rocks, semiconductors, metallic samples or polymers in accordance to the diversity of samples arriving via the CERIC-ERIC proposals.

A second investment pertaining to the development of the NIMP-LASDAM HRTEM facility regards the currently available experimental conditions for in-situ TEM observations. A dedicated set up is now in place allowing for TEM observations under variable temperature or under an electrical bias applied to the specimen. The envisaged acquisition represents an upgrade of the current set up that will allow for simultaneously heating and biasing the specimen during the TEM observation. This facility will be used for investigating the morpho-structural effects on battery materials during charging-discharging cycles in various temperature conditions.

Section d: Impact

The new technical features of the upgraded systems will open additional possibilities to investigate the microstructural properties of materials in correlation with their functional characteristics close to the normal operating conditions in practical devices. The proposed upgrades for in situ and operando TEM, electrochemical cell and cryogenic accessories for EPR spectroscopy address solid-state materials for advanced applications in energy storage where the correlation between the electrical, thermal and structural properties at nanometric and even atomic scale needs to be established. This is in line with CERIC's internal program for research on new materials for batteries and fuel cells, with a generous opening towards related materials for the semiconductor industry. The proposal will impact on the further increase of the scientific quality of the papers published in partnership with CERIC users in journals like Advanced Functional Materials (IF 19.924), Energy Storage Materials (IF 17.789), Energy & Environmental Materials (IF 13.443), ACS Applied Materials & Interfaces (IF 9.229). Another positive impact will concern the increase of the NIMP-LASDAM research quality in European projects stemmed from successful collaborations within CERIC, such as the M-ERA.NET project in collaboration with the University of Minho (grant agreement No 958174).

Demonstrating a prolific activity within CERIC-ERIC, NIMP managed to attract at the end of 2020 a substantial financial support for the participation in CERIC-ERIC through the national grant "Consolidating NIMP participation in the CERIC-ERIC consortium", co-funded from the European Regional Development Fund through the Competitiveness Operational Program 2014-2020 (contract POC no. 332/2020). As this contract has recently come to an end, a new competition for similar proposals has been launched in September 2023, where NIMP-LASDAM will take part with high chances to obtain a new grant

for the next 3 years, from which additional resources will be considered to co-fund the necessary investments described in this proposal.

Section e: Description of the implementation

The EPR spectroscopy and TEM infrastructure at NIMP-LASDAM has known a significant qualitative leap in 2010 with the commissioning of state-of-the-art instruments which have been further appointed for the Romanian participation in CERIC-ERIC. Progressive and sustainable investments have been made ever since from local resources and with significant contributions from CERIC-ERIC in order to extend their initial capabilities. The most recent such investment regards the upgrade of the HRTEM facility with the implementation of in situ TEM techniques and the upgrade of the EELS spectrometer and of the SEM-FIB instrument. The project is currently being implemented, with the necessary financial resources provided mostly by CERIC-ERIC and locally from national projects.

This proposal comes in line with the development projects so far, being organized in two distinct work packages according to the following infrastructure items to be acquired:

| WP1. | Activity 1.1 - Bruker ESR900 cryostat for X-band cavities |
|---------------|---|
| EPR upgrade | Activity 1.2 - Automatic Helium Purifier |
| | Activity 1.3 - Cryogen Free Variable Temperature Cryostat for EPR |
| | Activity 1.4 - Electrochemical cell for EPR |
| WP2. | Activity 2.1 - Ultramicrotome |
| HRTEM upgrade | Activity 2.2 - Extension of the in situ TEM system for specimen heating & biasing |

The two work packages will be organized according to the following Gantt chart.

| Activity | Year 1 | Year 2 | Year 3 | Year 4 | Year 5 |
|--------------------|--------|--------|--------|--------|--------|
| WP.1 EPR upgrade | | | | | |
| A1.1 | | | | | |
| A1.2 | | | | | |
| A1.3 | | | | | |
| A1.4 | | | | | |
| WP.2 HRTEM upgrade | | | | | |
| A2.1 | | | | | |
| A2.2 | | | | | |

The project budget as detailed in Annexes 1 and 2 contains only the amounts committed to equipment procurements, to be allocated from the annual Romanian membership fees. All the personnel costs will be covered by NIMP-LASDAM. The procurement budget has been organized in such a way that the annual amount allocated to NIMP-LASDAM will represent a certain fraction only from the annual membership fee. This will allow for the amount capitalization towards the end of the 5-year period, with the aim of purchasing the most expensive items in the final part of the contract.

Annex 1 – Human Resources: Resources connected to the activity of the required staff (total cost including overall estimated costs and use of the CERIC funding)

| CEDIC | | Total in Euro | | | | | | | |
|---|--------|---------------|--------|--------|--------|--|--|--|--|
| CERIC | Year 1 | Year 2 | Year 3 | Year 4 | Year 5 | | | | |
| Consumables | 0 | 0 | 0 | 0 | 0 | | | | |
| Personnel cost (PhD, researcher or technical staff) | 0 | 0 | 0 | 0 | 0 | | | | |
| Travel costs | 0 | 0 | 0 | 0 | 0 | | | | |
| Other costs (conferences fees, publications, training, etc) | 0 | 0 | 0 | 0 | 0 | | | | |
| TOTAL | 0 | 0 | 0 | 0 | 0 | | | | |

Annex 2 – Infrastructure Development: Resources (including overall estimated costs and use of the required CERIC funding)

| CERTC | Total in Euro | | | | | | |
|----------------|---------------|--------|--------|--------|--------|--|--|
| | Year 1 | Year 2 | Year 3 | Year 4 | Year 5 | | |
| Equipment | 30000 | 35000 | 20000 | 150000 | 110000 | | |
| Consumables | 0 | 0 | 0 | 0 | 0 | | |
| Personnel cost | 0 | 0 | 0 | 0 | 0 | | |
| Travel cost | 0 | 0 | 0 | 0 | 0 | | |
| TOTAL | 30000 | 35000 | 20000 | 150000 | 110000 | | |



Strategy for the allocation of CERIC's membership fees in support of the integration of CERIC capabilities

Slovenian Partner Facility

CERIC Partner Facility: Slovenian NMR Centre, National Institute of Chemistry, Slovenia

Proposal summary

<u>Osteoporosis</u> is a bone disease characterized by low bone mass, resulting in increased bone fragility and hence susceptibility to fracture. In this project, we would like to investigate if and how different noncanonical DNA/RNA structures formed within promoter regions and 5'-UTR influence the expression of osteoporosis-related genes. Additionally, we would like to focus on 3'-UTR regions of these genes to disclose the mechanisms by which miRNAs recognize mRNA regions of these genes and influence their functions.

The proposed project represents an integrated approach of studying the structural mechanisms of osteoporosis and includes the cooperation of <u>six partner (PF) and associated facilities (AF) within</u> <u>CERIC</u>. Next to *Slovenian PF (SLONMR)*, that will offer <u>NMR</u> insight into DNA/RNA secondary structures and their interactions with protein partners, protein/NA interactions will be studied with complementary methods available within CERIC, such as <u>SAXS</u> (*Graz University of Technology*), <u>crystalography and helicase activity tests</u> (*Elettra, Structural Biology Laboratory*), <u>AFM in liquid state and FRET</u> (*Elettra, NanoInnovation Laboratory*), <u>SPR</u> (*JRC Nanobiotechnology Laboratory*) and <u>EELS-STEM-EFTEM</u> (*Bio Open Lab, Salento*). The intention to collaborate on the project with *MS* has also been indicated at *Bio Open Lab, Salerno*. We believe our work within this CERIC project will provide important information about the genes suitable to be exploited for medicinal purposes in the development of drugs that would in the future allow to treat/prevent occurrence of osteoporosis.

PFs involved in the project:

- Slovenian PF (SLONMR)
- Austrian PF (Graz University of Technology)
- Italian PF (Elettra)

AFs involved in the project:

- JRC Nanotechnology Laboratory, Ispra
- Bio Open Lab, Salento
- Bio Open Lab, Salerno

Glossary of the abbreviations: PF = Partner Facility AF = Associated Facility NMR = Nuclear Magnetic resonance SAXS = Small Angle X-ray Scattering AFM = Atomic Force Microscopy FRET = Förster Resonance Energy Transfer SPR = Surface Plasmon Resonance EELS = Electron Energy Loss Spectroscopy STEM = Scanning Transmission Electron Microscopy EFTEM = Energy-Filtered Transmission Electron Microscopy MS = mass spectrometry

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Section a: Current Status and future evolution of the PF

The Slovenian NMR Centre (SLONMR) is a national research facility that coordinates a high number of scientific projects and activities at the international level. Additionally, SLONMR provides support to numerous academic research groups and industrial partners in Slovenia and abroad. The personnel of SLONMR consists of 13 scientists with Ph.D. and postdoctoral experience abroad that provide a breadth of scope and focus. We operate several high-field NMR spectrometers, namely one 400, three 600 and one 800 MHz spectrometers for studies in solution that are indispensable for detailed structural studies of macromolecules. Next to CERIC ERIC membership since 2014, we are members of COVID-19 NMR consortium headed by University in Frankfurt, partners of pan-EU R-NMR project. We have been involved in several MSCA projects, including LightDyNAmics and NeurodegRBPs. In recent years we hosted numerous Ph.D. students and postdoctoral fellows for several months, and professors on their sabbatical from all over the world. We collaborate with pharmaceutical and chemical companies in Slovenia and in the region, particularly Krka, Lek, Helios, Melamin, Belinka, Jub, FerroČrtalič, Pliva and INA.

Our studies are focused on structure and dynamics of biomolecules as well as their interactions and NMR method development for studies of small and larger systems in solution and solid state. Understanding the roles of nucleic acids and proteins in living organisms requires insights into intricate relationships between their biological function and structure. NMR is an excellent tool for studies of structure and conformational changes of DNA, RNA and proteins as well as their interactions with ligands and cations under conditions, which are close to physiological states. The subjects of our studies are most often regions of DNA and RNA, which can due to sequential prerequisites form non-B DNA secondary structures, which can influence the expression of related gene or function at telomeric ends of chromosomes. Guanine rich (G-rich) DNA and RNA sequences, for example, have been shown to form G-quadruplexes, while different tandem repeats sequences may form other noncanonical structures. In recent years, our group reported several novel DNA and RNA structures with repetitive sequences that are intricately related to specific diseases or influence basic cellular processes. For example, we demonstrated that the G-rich sequence from the 5'-UTR region of the RANKL gene is able to form Gquadruplexes that may have implications on the severity of osteoporosis by affecting RANKL protein levels in the cell or significantly influence binding of transcription factors. Related to ALS and FTD, our group have shown that K⁺ ions, which are abundant in the intracellular environment, induce higher-order species by stacking of two tetramolecular G-quadruplex units, which could potentially affect genomic stability and the pathophysiology of these diseases. In other studies, we investigated the influence of oxidative byproduct 8-oxoguanine (^{oxo}G) on formation of G-guadruplexes. We have shown that introduction of single ^{oxo}G does not necessary prevent G-quadruplex formation. Additionally, using d(TG₄T) analogues, we demonstrated that G-quartets can be fully substituted with ^{oxo}G nucleobases to form an ^{oxo}G-quartet. Although, the formation of ^{oxo}G-quartet influences hydrogen-bonding scheme and dimensions of the central cavity, formed G-quadruplexes retain their relatively high thermal stabilities. Understanding the mechanism by which biological macromolecules fold into their functional native conformations represents a problem of fundamental interest. For two DNA oligonucleotides derived from human telomeric repeat we have in detail described their folding mechanisms through pre-folded structures, stabilized by formation of guanine base triples in K⁺-independent manner. Next to folding mechanisms, we focus on interaction studies of Gguadruplexes with different ligands. In our most recent study, we revealed that Phen-DC₃ causes complete rearrangement of G-quadruplex fold from so called hybrid-1 to an antiparallel chair-type structure. The ligand intercalates into the G-core and ejects one potassium ion.

Interestingly, G-rich sequences are able to form structures that fundamently differ from Gquadruplexes as well. We described a novel structural family formed by oligonucleotides containing GGGAGCG repeats, named **AGCGA-quadruplexes**. It is especially interesting that even though guanine residues are very common in these repeats, AGCGA-quadruplexes do not contain G-quartets and are, in contrast to G-quadruplexes, insensitive to the presence of different cations such as Na⁺ and K⁺. In contrast to majority of telomeric repeats from different species that form G-quadruplexes, we showed that G-rich oligonucleotide derived from yeast telomeric DNA forms a **G-hairpin**. Detailed insights into structural characteristics of G-hairpins could have relevance for the development of pharmaceuticals, genetic engineering and DNA-based nanotechnology. From the point of view of nanostructures consisting of continuous stacks of G-quartets, we revealed the exact mechanism of how short, G-rich oligonucleotide

self-assemble into **G-wire** at molecular level. Furthermore, we showed that we can closely control the properties of desired G-wires (length and thermal stability) by changing the type of loop residues.

Recently, we are focusing on conformational and dynamic states of **pre-miRNAs**, which could potentially be utilized for tumor suppression and structural characterization of mitochondrial transfer RNAs (**mt-tRNAs**) and their fragments. We believe that high-resolution structures of pre-microRNAs and mt-tRNAs will provide unprecedented information about the structure-function relationship in the biogenesis of miRNAs and mechanisms of mitochondrial translation machinery, respectively.

Several high impact publications were published in journals with impact factors above 12 in the last two years, *i.e. Nat. Commun., Nucleic Acids Res.* and *Angew. Chem.*, some of which were highlighted as a cover story. The list of 10 publications in the last two years: 1.) M. Ghezzo, M. Trajkovski, J. Plavec and C. Sissi, *Angew. Chem. Int. Ed.* **2023**, 62, e202309327; 2.) V. Štih, H. Amenitsch, J. Plavec, and P. Podbevšek, *RNA* **2023**, 29, 1520-1534; 3.) M. Zalar, B. Wang, J. Plavec and P. Šket, *Int. J. Mol. Sci.* **2023**, 24, 13437; 4.) Novotny, J. Plavec and V. Kocman, *Nucleic Acids Res.* **2023**, *51*, 2602–2613; 5.) K. Peterková, M. Stitch, R. Boota, P. A. Scattergood, P. I. P. Elliott, P. Podbevšek, J. Plavec and S. J. Quinn, *Eur. J.* **2023**, 29, e202203250; 6.) M. Marušič, M. Toplishek and J. Plavec, *Curr. Opin. Struct. Biol.* **2023**, 79, 102532; 7.) Q. Li, M. Trajkovski, C. Fan, J. Chen, Y. Zhou, K. Lu, H. Li, X. Su, Z. Xi, J. Plavec and C. Zhou, *Angew. Chem. Int. Ed.* **2022**, *61*, e202201848; 8.) S Aleksič, P. Podbevšek and J. Plavec, *Biochemistry* **2022**, *61*, 2390-2397; 9.) A. Ghosh, M. Trajkovski, M.-P. Teulade-Fichou, V. Gabelica and J. Plavec, *Angew. Chem. Int. Ed.* **2022**, *61*, e202207384; 10.) D. Pavc, N. Sebastian, L. Spindler, I. Drevenšek-Olenik, G. Koderman Podboršek, J. Plavec and P. Šket, *Nat. Commun.* **2022**, *13*, article number: 1062.

In the future, we would like to focus on research of genes related to bone diseases (more specifically osteoporosis). Several genes involved in signaling pathways connected with osteoporosis susceptibility were already identified. Additionally, it has been shown that bone remodeling can be regulated on posttranscriptional level through miRNAs. Although extensive molecular and genetic studies in recent years untangled various factors affecting the homeostasis of bone, structural insights that would in detail explain the causes of osteoporosis are still unexplored. In the next five years we tend to characterize non-canonical DNA/RNA structures that can influence osteoporosis-related gene expression and their potential interactions with protein partners. Moreover, we would like to uncover the structural principles that drive miRNA recognition element of mRNA regions of osteoporosis-related genes. We believe our work within this CERIC project will provide important information about the genes suitable to be exploited for medicinal purposes in the development of drugs. We want to connect the expertise of the SLONMR on structural characterization of nucleic acids and their interaction with protein partners with **NMR** spectroscopy with **complementary methods offered by CERIC PFs** that allow detailed investigation of the overall shape and structure of proteins and their complexes with different biomolecules (*i.e.* X-ray, SAXS, Cryo-EM, EELS-STEM-EFTEM, SPR, FRET, AFM).

Section b: Five-year development plan of the PF

Within the framework of five-year development plan, we will focus on different regulatory regions of osteoporosis-related genes:

<u>A) PROMOTER AND 5'-UTR REGIONS:</u> Characterization of non-canonical DNA/RNA structures that can influence osteoporosis-related gene expression and their interactions with protein partners

In promoters and 5'-UTR regions of many genes, we can find G-rich sequences that are able to adopt tetra-stranded DNA/RNA structures, such as G-quadruplexes. In this part of the project, we will focus on promoter and 5'-UTR regions of some of the most important genes involved in bone remodeling (among others *SOST*, *LRP4*, *LRP5*, *DKK*) and structurally characterize potential GQ structures formed by their G-rich regions (years 1-3). Furthermore, we would like to investigate the interaction of GQs with related transcription factors and other protein partners (such as Osx, Runx2, and FOXO1) in collaboration with other CERIC PFs (years 2-4). Within the project, the influence of gene variants (SNPs) on the stability of non-canonical structures and their ability to bind to protein partners will be studied as well (years 4-5).

Knowledge gained from this part of the project: suitable protein targets for aptamer development (aptamers are oligonucleotide sequences that can mimic monoclonal antibodies, which is one of the main strategies of osteoporosis treatment today – denosumab; aptamer would bind to the target protein and prevent its activity).

<u>B) 3'-UTR REGIONS:</u> Disclosure of structural principles that drive miRNA recognition elements of 3'-UTR mRNA regions of osteoporosis-related genes

miRNA are short non-coding RNAs that directly bind to the 3'-UTR regions of mRNA in a sequencecomplementary manner to inhibit translation and facilitate degradation of their target transcripts. They play critical roles in all stages of bone formation and resorption.

Within the proposed project, we would like to gain structural insights into miRNA recognition of 3'-UTR regions of selected osteoporosis-related genes and how different gene variants (SNPs or post-transcriptional modifications) influence the binding of miRNA (for example *DKK1*-miR-335-5p or *RANKL*-miR-29a) (years 1-3). We would also like to uncover which chemical modifications of miRNA can stabilize the interaction with its target 3'-UTR region (years 2-4) and how these changes influence its recognition by protein binding partners (years 2-5), especially RNA-induced silencing complex (RISC).

Knowledge: discover of suitable miRNA platforms that can be used for the development of siRNAbased therapeutics that would mimic miRNA-binding mechanisms, use the same recognition elements, and by binding to mRNA molecules of osteoporosis-related genes influence the amount of translated proteins.

Key needs: human resources within Slovenian PF – PI, post-doc, two PhD students (one working on part A, one on part B); infrastructure: NMR spectrometers and oligonucleotide synthesizer within Slovenian PF; SAXS, Cryo-EM, EELS-STEM-EFTEM, MS, SPR, FRET, AFM, protein production in collaboration with CERIC PFs (for details see Section e).

Collaboration with CERIC PFs: WPA2, WPA3, WPB3 (for details see Section e).

Section c: Rationale and Scientific and technical description of the proposal

Osteoporosis is a bone disease characterized by low bone mass, resulting in increased bone fragility and hence susceptibility to fracture. International Osteoporosis Foundation (IOF) estimated that in 2019 around 25.5 million women and 6.5 million men aged +50 across Europe had osteoporosis, while just in 2019 total direct cost of osteoporotic fractures was around 57 billion euros for 27 countries of the EU together with Switzerland and UK. In the proposed project, we would like to connect different CERIC PFs in one joint goal - use our expertise in structural biology and available infrastructure to in detail explain molecular mechanisms of bone remodeling and connect structural insights with the functions of important genetic targets. We believe our work within this CERIC project will provide important information about the genes suitable to be exploited for medicinal purposes in the development of drugs against the disease that is on the rise due to aging society.

Main objectives of the proposal (part A and part B) include synthesis of studied oligonucleotides and their purification and folding in a way, suitable for NMR spectroscopy. All oligonucleotides can be produced in-house – we routinely synthetize DNA/RNA oligonucleotides up to 100 nucleotides. Our expertise includes synthesis of isotopically labeled oligonucleotides and oligonucleotides with chemically modified phosphoramidites. NMR spectroscopy will be used as a key method to gain insights into structure and dynamics of nucleic acid targets. SLONMR stuff operates five high-magnetic field NMR spectrometers that can be used for structural studies of biomolecules in solution. Additionally, we are one of the leading laboratories in Europe in the field of structural biology of noncanonical DNA and RNA structures. However, successful realization of the proposed project would need the involvement of various infrastructures located at different CERIC-representing entities. We believe that other CERIC PFs can offer their expertise in complementary methods that allow detailed investigation of the overall shape and structure of proteins and their complexes with different biomolecules (*i.e.* X-ray, SAXS, Cryo-EM, EELS-STEM-EFTEM) and production of investigated protein partners.

State of the art research will reflect in a number of high-impact journal publications, which will improve the success rate of future project applications. Challenges arising from experimental work on protein-nucleic acids interactions will incite a more advanced use of the research infrastructure already available within CERIC and will undoubtedly provide a multidirectional transfer of knowledge between CERIC PFs. Coupling of NMR spectroscopy with SAXS, Cryo-EM, AFM, SPR and EELS-STEM-EFTEM will lay the groundwork for future projects dealing with protein-DNA/RNA complexes and will establish CERIC as a consortium, which will in the future be able to routinely offer such services to internal and

external users. Diversification of CERIC services will contribute to its international success and increase research impact and quality of member facilities. The knowledge acquired during the proposed project could be disseminated in the form of workshops and seminars available to members from CERIC PFs. Additionally, promising results will encourage investments into major upgrades of research infrastructure at host and PFs and stimulate joint research grant applications through various funding schemes.

The workflow at SLONMR will be monitored and guided by PI and one post-doc researcher and requires employment of two PhD students (each working on one part of the project). Both students will be enrolled in study program at the University of Ljubljana with dr. Martina Lenarčič Živković as a proposed supervisor.

Section d: Impact

NMR studies of structure as well as conformational and stereochemical features of oligonucleotides under (close to) physiological conditions, performed at SLONMR, importantly contribute to the unravelling of the intricate relationships between DNA/RNA structure and their biological function. Additionally, structural details help us to define novel therapeutic targets and strategies. We believe that our work on regulation of osteoporosis-related genes in the next few years will serve as a springboard in the development of new therapeutic strategies in combat against osteoporosis, which affects more than 200 million people worldwide. High-resolution G-quadruplex structures can represent suitable platforms for the design of highly specific ligands with anti-osteoporotic function or initial structures to develop aptamers that would bind important protein targets. Additionally, miRNA platforms can be used for the development of siRNA-based therapeutics that would mimic miRNA binding mechanisms, use the same recognition elements, and by binding to mRNA molecules of osteoporosis-related genes influence the amount of translated proteins.

The work packages within the proposed project will connect different CERIC PFs, which can also invite their academic partners to participate in the project and by this expand CERIC outreach. Next to established experts in the field of structural biology, we expect that we will engage two Ph.D. students. The project will thus provide a platform for a new generation of researchers at the beginning of their careers, whose education process will be decisively entangled with CERIC.

Section e: Description of the implementation

A) Promoter and 5'-UTR REGIONS

Main aim: to find suitable protein targets for aptamer development

WPA1: This part of work will be performed on SLONMR, where the synthesis and purification of samples will take place. Next, we will collect sets of 1D and 2D NMR spectra to establish, which samples will be suitable for WPA2 and WPA3. Additionally, we will structurally characterize important nucleic acid (NA) targets (years 1-3)

WPA2: In collaboration with other CERIC PFs we will study interactions between suitable NA targets and their protein partners. Part of the work will be performed on <u>SLONMR</u>, while <u>CERIC PFs and AFs</u> will be engaged for complementary studies (years 2-4):

- <u>Graz University of Technology (Prof. Heinz Amenitsch):</u> The Austrian PF has a strong experience on structural characterization of the DNA/RNA structures and their binding with proteins with SAXS. Here the structural results of SLONMR from WPA1 (and the other PFs) will be complemented by the SAXS measurements (batch or SEC-mode) and the subsequent determination of low-resolution models of the overall structure at various conditions.
- 2.) Structural Biology Laboratory, Elettra Sincrotrone Trieste (Prof. Silvia Onesti): Within Structural Biology Laboratory at Elettra Silvia Onesti is actively working on the interactions between GQs and various DNA/RNA-binding proteins. An important line of their research is focusing on the selectivity and specificity of DNA helicases belonging to the human RecQ family towards DNA GQs found in the promoter regions of different genes. A number of helicases under study at the Structural Biology laboratory have been associated with osteoblast maturation, osteosarcoma or osteoporosis. In particular RecQ4 is required for normal osteoblast expansion and its mutations give a strong predisposition to develop osteosarcoma; whereas mutation in the Werner and RTEL1 helicase cause premature aging and osteoporosis. Part of the WPA2 will include structural studies of DNA/RNA GQs identified by WPA1 and their potential interaction with osteosarcoma-connected helicase RecQ4. Additionally, Italian PF will offer their expertise on protein production and protein



crystallography.

- 3.) <u>NanoInnovation Laboratory, Elettra Sincrotrone Trieste (Prof. Loredana Casalis)</u>: The NanoInnovation Laboratory of ELETTRA will share their expertise in advanced AFM imaging modes in liquid environment, to highlight structural details of protein/NA interaction, at a single molecule level. Additionally, they can provide large-scale protein expression/purification equipment and different biophysical and biochemical approaches to characterize proteins and protein/protein interactions (FRET).
- 4.) JRC Nanobiotechnology Laboratory (Prof. Pascal Colpo): Within WPA2 JRC from Ispra will be using surface plasmon resonance (SPR) to study affinity and kinetics of interactions between biomolecules. They will analyze interaction between transcription factors and other protein partners and GQs that will be identified within WPA1. Investigated oligonucleotides will be immobilized on a SPR sensor using specific surface chemistry (by using a biotin tag on the oligonucleotides and a streptavidin coated sensor) and partner proteins will be incubated at different concentrations to study protein/NA interactions. Modified oligonucleotides with biotin entities will be synthesized by SLONMR facility. JRC facility will provide in kind contribution by hosting visiting scientists/students from PFs for performing experiments with their instrumentation with support of JRC staff.
- 5.) Bio Open Lab (Prof. Lucio Calcagnile): The Applied Physics Group at the University of Salento, Italy will be involved on structural characterization by providing structural, morphological and spectroscopical characterizations at atomic resolution by means of EELS-STEM-EFTEM, EDX and Raman spectroscopy, using the electron microscopy facilities at the Department of Mathematics and Physics of University of Salento. Other groups at the Department of Mathematics and Physics and the Department of Biology of the same University will be involved in the project with complementary facilities related useful to reach the goals of the project. Information about the composition of samples can be found throughout the electron energy loss spectrum. The low loss spectrum (0–20 eV) contains fine structure arising from excitations of molecular energy levels, which can be used to estimate the relative amounts of water, proteins, nucleic acids, and other components in frozen hydrated preparations. The low loss spectrum also provides a simple way of determining the specimen mass per unit area. Signals from core edges provide quantitative information about a range of endogenous elements within organic macromolecules. For example, phosphate groups can be revealed in nucleic acids or phosphorylated proteins, just as the presence of cysteine or methionine residues in proteins can be related to the presence of sulphur, and sulphate groups to carbohydrates. Other techniques such as Energy dispersive X ray emission by using two different windowless detectors will be used to investigate elements at atomic level inside the samples down to atomic number Z=5 (boron) even with the possibility of elemental mapping of the cells. Raman spectroscopy or other imaging techniques will provide the possibility to integrate the investigation at molecular level.

WPA3: Different gene variants of suitable NA targets and their influence of interaction with protein targets will be tested. Work will be performed on <u>SLONMR and different CERIC PFs</u>. Work within WPA3 is linked to WPA2 – here we will mainly focus on protein/NA complexes examined in WPA2 and evaluate the influence of SNPs on their interaction. Comprehensive study within WPA3 will be accomplished by collaboration between SLONMR (NMR insight into influence of SNPs on DNA/RNA secondary structures and their interaction with protein partners) and other CERIC PFs: <u>Graz University of Technology with SAXS</u> measurments, Structural Biology Laboratory at Elettra with crystallography, NanoInnovation Laboratory at Elettra with AFM, JRC Nanotechnology Laboratory with SPR and BOL with EELS-STEM-EFTEM.

B) 3'-UTR REGIONS

Main aim: to find suitable miRNA platforms that can be used for the development of siRNA-based therapeutics against selected bone-remodeling-connected genes

WPB1: This part of work will be performed on SLONMR, where the synthesis and purification of RNA oligonucleotides will take place. Next, we will collect sets of 1D and 2D NMR spectra to establish, which samples will be suitable for WPB2 and WPB3. Additionally, we will structurally characterize important RNA targets (years 1-3)

WPB2: Studies in this part will include introduction of different chemical modifications of miRNA that can stabilize their interaction with its target 3'-UTR region and can offer valuable information for the development of siRNA-based therapeutics (years 2-4)

WPB3: In collaboration with other CERIC PFs we will study interactions between suitable initial RNA targets, their modified counterparts and related protein partners. Part of the work will be performed on SLONMR, while CERIC PFs will be engaged for complementary studies (years 2-5):

- 1.) <u>Graz University of Technology (Prof. Heinz Amenitsch)</u> with SAXS measurements (batch or SEC-mode) and the subsequent determination of low-resolution models of the overall structure at various conditions.
- 2.) <u>Structural Biology Laboratory, Elettra Sincrotrone Trieste (Prof. Silvia Onesti)</u> with evaluation of the influence of miRNA chemical modifications on the interaction with protein partners. Additionally, PF will offer their expertise on protein production and protein crystallography.
- 3.) <u>NanoInnovation Laboratory, Elettra Sincrotrone Trieste (Prof. Loredana Casalis)</u> with advanced AFM imaging modes in liquid environment, to highlight the influence of chemical modificastions of miRNA on their interaction with protein partners, at a single molecule level.
- 4.) JRC Nanobiotechnology Laboratory (Prof. Pascal Colpo) using surface plasmon resonance (SPR) to study affinity and kinetics of interactions between biomolecules. The same principle of specific surface chemistry (biotin-streptavidin) will be applied as in WPA2 and WPA3 to characterize the interaction between miRNA and 3'-UTR mRNA regions of osteoporosis-related genes. Modified oligonucleotides with biotin entities will be synthesized by SLONMR facility.
- 5.) **Bio Open Lab (Prof. Lucio Calcagnile)** will provide structural characterization at atomic resolution by means of EELS-STEM-EFTEM, EDX and Raman spectroscopy, using the electron microscopy facilities at the Department of Mathematics and Physics of University of Salento.

| | 2024 | 2025 | 2026 | 2027 | 2028 |
|--|------|------|------|------|------|
| A) Promoter and 5'-UTR REGIONS | | | | | |
| WPA1: Characterization of noncanonical DNA/RNA structures | | | | | |
| WPA2: Interactions between suitable nucleic acid targets and | | | | | |
| their protein partners | | | | | |
| WPA3: Influence of gene variants (SNPs) | | | | | |
| Collaboration with other CERIC PFs and AFs | | | | | |
| Graz University of Technology | | | | | |
| Structural Biology Lab., Elettra | | | | | |
| NanoInnovation Lab., Elettra | | | | | |
| JRC Nanobiotechnology Lab. | | | | | |
| BOL, Salento | | | | | |
| B) 3'-UTR REGIONS | | | | | |
| WPB1: Structural studies of targets and their interaction with | | | | | |
| suitable miRNA | | | | | |
| WPB2: In search of chemical modifications of miRNA | | | | | |
| WPB3: Influence of chemical modifications on recognition of | | | | | |
| mRNA by protein binding partners | | | | | |
| Collaboration with other CERIC PFs and AFs | | | | | |
| Graz University of Technology | | | | | |
| Structural Biology Lab., Elettra | | | | | |
| NanoInnovation Lab., Elettra | | | | | |
| JRC Nanobiotechnology Lab. | | | | | |
| BOL, Salento | | | | | |
| Management, coordination and dissemination | | | | | |



Personnel requirements:

| | 2024 | 2025 | 2026 | 2027 | 2028 | | | | |
|--|-------------------|------|------|------|------|--|--|--|--|
| SLONMR | | | | | | | | | |
| PI (Martina Lenarčič Živković) | | | | | | | | | |
| Post-doc (Peter Podbevšek) | | | | | | | | | |
| PhD student A ^a | From Oct. 2024 | | | | | | | | |
| PhD student B ^a | From Oct. 2024 | | | | | | | | |
| Graz University of Technology | | | | | | | | | |
| PhD student ^b | From Oct. 2024 | | | | | | | | |
| Structural Biology Lab., Elettra | | | | | | | | | |
| | | | | | | | | | |
| NanoInnovation Lab., Elettra | | | | | | | | | |
| | | | | | | | | | |
| JRC Nanobiotechnology Lab. | | | | | | | | | |
| In kind contribution of performing experiments with support of JRC staff | | | | | | | | | |
| BOL, Salento | | | | | | | | | |
| PhD student ^c | | | | | | | | | |

^aStudy program at University of Ljubljana. ^bStudy program at Graz University of Technology. ^cStudy program at the University of Salento.

Annex 1 – Human Resources: Resources connected to the activity of the required staff (total cost including overall estimated costs and use of the CERIC funding)

The costs considered in the table below refer only to the expected resources from the CERIC membership fee of Slovenian PF.

| CERIC | | Total in Euro | | | | | | |
|---|--------|---------------|--------|--------|--------|--|--|--|
| CERIC | Year 1 | Year 2 | Year 3 | Year 4 | Year 5 | | | |
| Consumables | 10000 | 10000 | 10000 | 10000 | 10000 | | | |
| Personnel cost (PhD, researcher or technical staff) | 19000 | 19000 | 19000 | 19000 | 19000 | | | |
| Travel costs | 2000 | 2000 | 2000 | 2000 | 2000 | | | |
| Other costs (conferences fees, publications, training, etc) | 5000 | 5000 | 5000 | 5000 | 5000 | | | |
| TOTAL | 36000 | 36000 | 36000 | 36000 | 36000 | | | |

Resources needed for successful implementation of the proposed project (Slovenian PF only)

| CERIC | Total in Euro | | | | | |
|---|---------------|--------|--------|--------|--------|--|
| | Year 1 | Year 2 | Year 3 | Year 4 | Year 5 | |
| Consumables | 50000 | 50000 | 50000 | 50000 | 50000 | |
| Personnel cost (PhD, researcher or technical staff) | 90000 | 120000 | 120000 | 120000 | 105000 | |
| Travel costs | 20000 | 20000 | 20000 | 20000 | 20000 | |
| Other costs (conferences fees, publications, training, etc) | 10000 | 30000 | 30000 | 30000 | 30000 | |
| TOTAL | 170000 | 220000 | 220000 | 220000 | 205000 | |

Resources for specific partner of this proposal:

Graz University of Technology

NOTE: The costs considered in the table below refer only to the expected resources from the CERIC membership fee of the Austrian PF and are replicated in the form of the Austrian Partner facility. Consumables/Travel costs/other costs will be covered by the partner facility.

| CERIC | Total in Euro | | | | | |
|---|---------------|--------|--------|--------|--------|--|
| | Year 1 | Year 2 | Year 3 | Year 4 | Year 5 | |
| Consumables | | | | | | |
| Personnel cost (PhD, researcher or technical staff) | 11500 | 45000 | 45000 | 33500 | | |
| Travel costs | | | | | | |
| Other costs (conferences fees, publications, training, etc) | | | | | | |
| TOTAL | 11500 | 45000 | 45000 | 33500 | | |

JRC Nanobiotechnology Laboratory

In kind contribution by hosting visiting scientists/students from PFs for performing experiments with their instrumentation with the support of the JRC staff.