ALBA II
PRE-WHITE PAPER

ALBA Team
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ALBA Synchrotron is developing the next generation of advanced instruments and methodologies to enhance the Spanish and international scientific and industrial capacities for solving the pressing societal challenges, while applying conscious and sustainable use of resources.

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ALBA CURRENT AND FUTURE ROLE IN THE SPANISH AND EUROPEAN RESEARCH INFRASTRUCTURE AREA

Over the past decade, ALBA *(1)* has become an important pillar of the Spanish and European Research Area, providing extended research capabilities and a wide range of state-of-the-art instrumentation to academic and industrial users. It delivers to the Spanish research and policy community another gate to the larger European research network and infrastructures from its current chairing of LEAPS, the *League of European Accelerator-based Photon Sources (2)* and its positioning in the incoming Horizon Europe programs. ALBA industrial program directly impacts the economic growth by showing industrial leaders of Spain new development opportunities and ultimately windows of innovation for their businesses. ALBA plays today an influential role in science tutoring and education, contributing to dual professional training, preparing and enabling young scientist and engineers for their national and international career, and seeding the inquisitiveness for rational cognizance and the scientific perspective in the youngest generations. In other words, ***ALBA has proven to be a resilient essential part of the Spanish research landscape*** and ALBA staff has shown their social and innovation responsibility corroborating ALBA as an important asset in Spain.

Significant progress in accelerator design, X-ray optics, detection technology, and Information Technology (IT) infrastructure drives worldwide the evolution of synchrotron light sources to the ***4th generation***, with cutting-edge research instruments opening ***new windows to the exploration of inner details of matter, devices, and their functionality***. Photon brilliance (photons per unit time, per unit area, per unit solid angle and per unit spectral bandwidth) and the coherent fraction of the photon flux are increased by orders of magnitude, providing the ground for unmatched analytics tools, ultimately leading to develop new approaches and technologies for a sustainable, clean and smart economy and a more efficient health system. The first 4th generation operating light source is MAX IV *(3)* and all new synchrotrons in construction belong to the new generation. ESRF has been the first 3rd generation light source upgrading to the ESRF-EBS *(4)* project, setting the example for many others, who will upgrade during the next decade their facilities.

ALBA is ready to leap from the 3rd to the 4th generation and give birth to ***ALBA II***, by combining the partial substitution of the accelerator with the upgrade of the existing instrumentation and the addition of new and fully optimized beamlines, thus maintaining the prominent position within the European and worldwide scenario and providing a crucial competitive advantage for the Spanish innovation ecosystem.

ALBA vision is twofold: to provide tools to users to ***develop green technologies***, and to make ALBA a ***green infrastructure*** itself. CELLS will implement specific actions and policies to bring ALBA and its working environment to the next level of sustainable use of resources and social responsibility. A continuous assessment process will be implemented and an effective transversal investment program will be pushed forward. The holistic approach will comprise taking concrete action in relation to external cooperation, research programs and projects, and is aligned to national and international green policies with special attention to research and innovation related to health, environment and energy economy. ***ALBA will be positioned in Europe and worldwide as a positive example for a self-aware and environmental best practice facility***.

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HOW ALBA II HELPS TO SOLVE THE PROBLEMS OF THE 21TH CENTURY

Most urgent challenges in the world are related to health, climate change, environment and energy. Solutions require the visualization of complex systems and understanding how subsystems work together on different length scales. Promoting ALBA to a 4th generation light source will enable imaging tools with enhanced resolution capacity and allow lensless imaging techniques with near atomic resolution. It will also provide more powerful instruments to probe the structural and electronic changes under *operando* conditions with higher-energy X-rays. The combination of advanced data analysis algorithms with the increased volume of the data acquired will reveal correlations between changes and functions, and will make our microscopic information available to the big-data world, closing the loop between the micro and macro scales.

The current ***health*** threat of the COVID-19 pandemic shows the paramount importance of fast and safe drug and vaccine developments not only to save the lives of thousands, but also to allow life quality and a thriving economy. Macromolecular crystallography (MX), one of our tools, has always been one of the key components in this fight, solving the structures of proteins involved in the infection processes. Using high-resolution data, active sites can be identified and infection processes can be understood, revealing ways to block the infection. In combination with big-data science, this structural information can be the basis for screening hundreds of existing drugs and participating in the activities for development of vaccines and optimized medicaments. ALBA II with its laboratory support structure and much reduced photon beamsize will relax the requirements on the protein crystal to the micrometer and sub-micrometer size, a significant enabler for fast response, and will combine a wide range of techniques including serial MX, *in-situ* crystallization experiments, and high throughput fragment screening, all tools providing fast insights in the infection mechanism. Beyond this, the interplay of the different microscopy tools, as the present transmission microscopy beamline and the cryo-electron microscopy being installed in 2021, will add information on how the potential medication or vaccine interact with membranes, individual cell organelles, and cells (as an example, see figure 1).

Rational governance for ***climate change control, environment safeguard and sustainable agriculture*** requires the understanding of complex systems and their interdependences, involving a wide range of length scales, human behavior patterns and global economic drivers.

The obvious grand challenge is to visualize and understand on an atomistic level the chemistry, structure, and dynamics of the entangled and intricated subsystems and provide quantitative models and simulations which predict impacts of factors like fertilization, environmental hazards, water supply or erosion on all length scales. Such a toolbox will bring a scientific base to the development of new approaches and policies, will allow to tune these to the local conditions, ultimately creating a sustainable, practical, and thrifting economy and guaranteeing a healthy environment.

Synchrotron related research has demonstrated the power of multi-length scale imaging, by providing models of the speciation and transport of elements from the atomic level using high resolution microscopy techniques to the macroscopic scale using "clever" sample and subsystem selection combined with state-of-the-art data mining approaches. More efficient catalysis processes, detection of undesired environmental waste elements like nano-plastics and heavy metals, or bio-uptake of desired nutrients by the plants are examples of current ALBA contributions.

ALBA II with its significantly improved brilliance will push the microscopic resolution to the nanometer range and at the same time the detection limit and the ability to study systems as plants *in vivo* and in their natural soil environment. A new instrument, the scanning hard X-ray nano probe will work in concert with the already existing soft transmission X-ray microscope, electron microscopy and a new large field-of-view, high energy tomography system with sub micrometer resolution. In combination, a 3-D model of macroscopic objects with atomic resolution is sculped, allowing to understand the underlaying chemical processes and structure relationships which go hand in hand with transport of pollutants, trace elements, and nutrition. ALBA II's optimized data management will enable the researchers to connect these models to the larger data mining world, empowering system relevant research.

Green energy transition will only happen with the development of new materials for efficient generation-, storage-, conversion-, and ultimately transport of energy. The technologies of interest span a wide range, including photovoltaics, wind turbine, fuel cells, batteries, superconducting transport, generation and conversion, and specifically the full H_2 and CH_4 cycle. A large fraction of current ALBA user community works in these fields. The impact of ALBA II will be pronounced in the understanding of catalytic reactions which are enablers in most of these technologies. A catalyst is a complex system in which the substrate and the actual catalytic particle have multiple functions like the splitting of molecules, the storage and activation of the reactants, and ultimately the reaction to the final product. ALBA II will improve the information on the catalyst defect structure and structural changes at the atomic level which are driving forces of this complex process.

Whereas ALBA can currently follow macroscopically averaged structural and electronic changes, ALBA II will image these changes with near atomic resolution and study its dynamics with advanced time resolution, utilizing the high flux of transversally coherent X-ray. Coherent diffraction imaging and ptychography are two recent experimental techniques well adapted to the new generation light sources, which allow to achieve nanometric resolution in amorphous materials. Moreover, in partially crystalline samples, Bragg Coherent Diffraction Imaging allows determining shape and structure changes, the strain and defects with atomic resolution and assess their impact on the chemical reactions providing unique insights into the functionality of complex systems. In addition, the temporal evolution of the diffraction patterns will provide the underlying dynamics of these changes.

ALBA II, with the large data volume that will be generated and with its multimodal ansatz, will ***help to solve the challenges of this century*** and will ***be a part of the digital transformation in the Spanish research landscape***. All the data generated and data analysis tools will contribute to the future European Open Science Cloud (EOSC *(5)*). Providing FAIR data, e.g. data which meet principles of Findability, Accessibility, Interoperability, and Reusability, will warrant their future universal use. And, from this solid basis, Artificial Intelligence and data mining techniques will exploit the multimodal and multiple-length scale imaging concept.

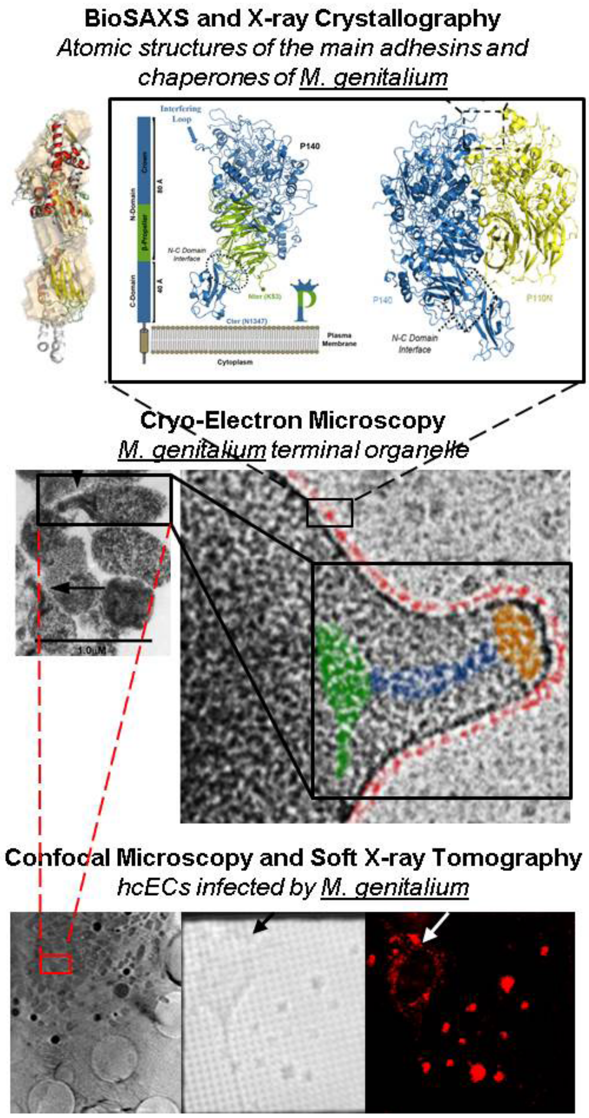

Figure 1 - The infection by Mycoplasmas, an emergent human pathogen for its resistance to antibiotics and responsible to a wide range of diseases like cervicitis and pelvic inflammatory disease in women or a range of respiratory diseases, is visualized to reveal the infectivity mechanism and to identify new potential targets for vaccines or drugs. Such data can be derived by applying a multilength scale imaging approaches by combing atomic resolution molecular structure models, simulations and fragment screening with three-dimensional models of infected cells *(6-10)*.

3

ALBA II TECHNOLOGICAL DEVELOPMENTS

The core of the upgrade of a light source from 3rd to 4th generation is the ***increase of brilliance and coherence fraction of the photon beam***, which enhances the resolving power and analytical capabilities for investigating matter to ultimate performances. The ***minimization of emittance of the electron beam*** (horizontal dimension x horizontal divergence) in the main accelerator, the storage ring is the starting point for such evolution, combined with the upgrade of beamline optics and technologies and completed with new state-of-the-art beamlines, fully conceived to take advantage of the new source parameters and complementing the existing instruments.

A simplified representation of the physical evolution of the facility is shown in Figure 2: the arcs of the storage rings will be substituted with new structures where the bending magnets will be more distributed, thus producing an emittance smaller by at least a factor of 20 with respect to the present one, and complemented with new vacuum chambers and corresponding diagnostic systems.

The design, the construction and part of the installation of ALBA II systems will be carried out while operating the facility with its present beamlines during the next eight years (2021-28). Then, the facility will be shut down during one year for the installation of the new storage ring components and another year will be dedicated to commissioning of the accelerator and of the new beamlines. This extremely cost-effective intervention will equip the scientific and industrial community with a state-of-the art light source for the thirties.

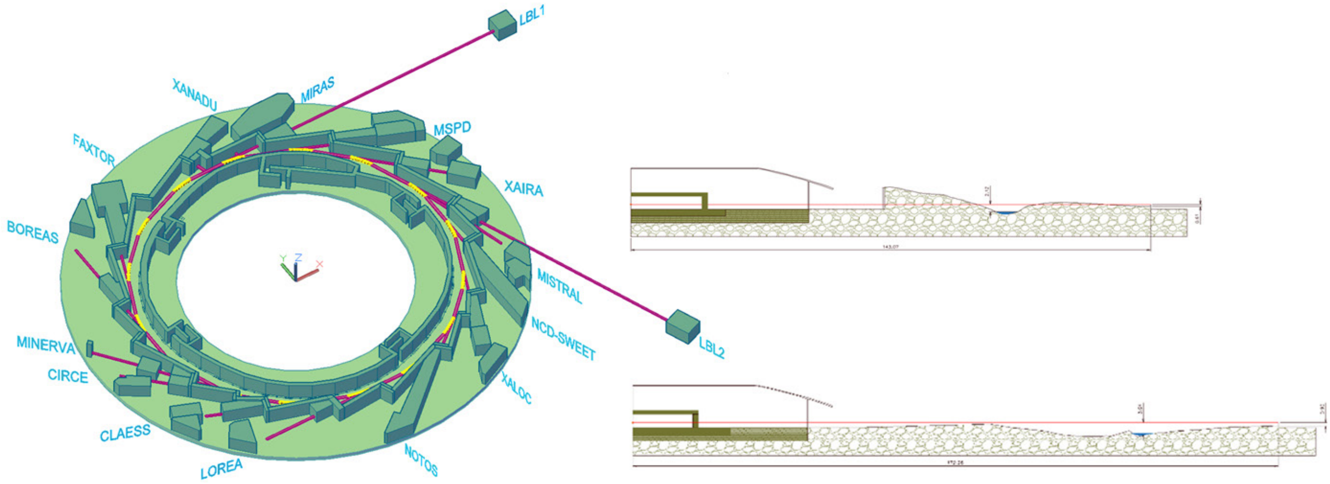

Figure 2 – Schematic representation of ALBA Synchrotron and its beamlines with ALBA II modifications in yellow.

Figure 3 shows the change in the transverse section of the photon beam in one of the present beamlines: the horizontal dimension will be reduced by a factor of about ten. The brilliance increase, as shown in Figure 4 for the present ALBA photon sources ranges from a factor of ~10 for wigglers up to a factor ~70/80, in the case of in vacuum undulators, what opens the possibility of using the range of higher energy X-rays in the beamlines equipped with this type of insertion devices. Development of technologies for pushing the photon energies even further are on-going in collaboration with other LEAPS facilities.

Some of the new beamlines will be built with long optical paths from the light source to the end stations to provide the high optical-demagnification which reduces the photon beam spots down to the nanometric dimensions. At least two of the end-stations will be located in a plot next to ALBA parcel, which is part of the location foreseen for the ASTIP park (ALBA Science, Technology and Innovation Park, see below).

The integration in the scientific hub will enhance the ***opportunities for collaboration with the participating institutes***, streaming from the Advanced Microscope Platform now in construction at ALBA which hosts instrumentation owned by several research institutions. The hub will host also the data center PIC (Port d'Informació Científica *(11)*), a great opportunity for enlarging the data storage and on-line capacities of the ALBA IT infrastructure. ALBA has just joined the EOSC Partnership *(5)*, assuming the data curation responsibility, and the data stewardship role, which ensures that the quality of the data and its associated metadata fully comply with the FAIR principles.

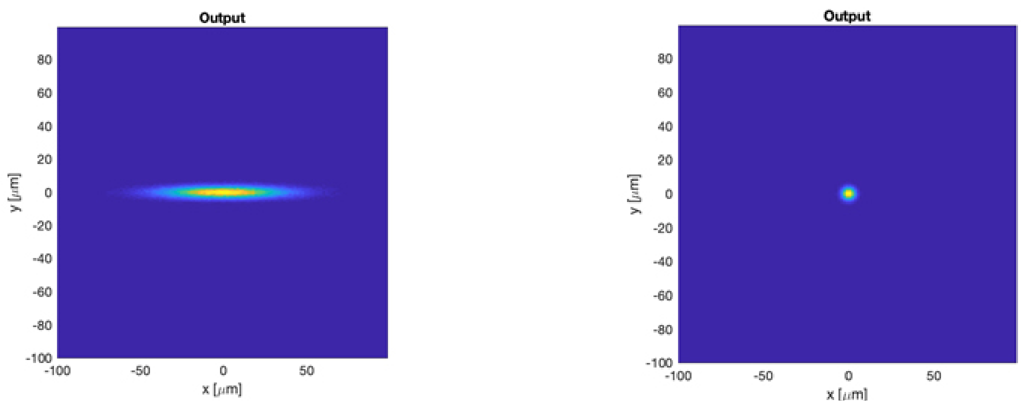

Figure 3 – Photon beam at the sample position at XALOC Beamline with ALBA and ALBA II (simulations): while the vertical dimension is not changing since already near the diffraction limit, the horizontal beam size is reduced by more than a factor of 10.

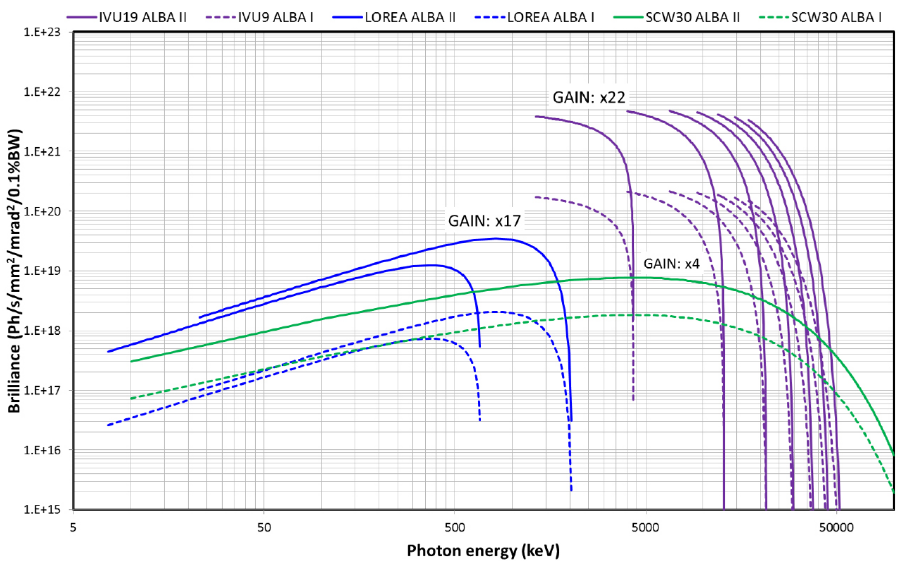

Figure 4 – Brilliance of three different types of ALBA Insertion Devices as today (dashed lines) and at ALBA II (solid lines), calculated with a reference electron beam current of 100 mA.

4

ASTIP
THE ALBA SCIENCE, TECHNOLOGY AND INNOVATION PARK

The proposal of developing ***a new scientific and technological center in the vicinity of ALBA*** aims at activating the evolution from the original synchrotron facility to a center of excellence for synchrotron radiation science with enhanced capacities in research and innovation.

ALBA Science, Technology and Innovation Park purpose is the establishment of an ecosystem where scientific research, technology development and industrial innovation are integrated to create a resilient, resource-efficient and competitive environment focused on ***green energy, digital transition and health***. ASTIP nucleates around the ALBA Synchrotron and its upgrading to ALBA II, and encloses the key actors involved in the innovation value chain located in the Barcelona area, including several leading research institutions, the Universitat Autònoma de Barcelona (UAB) *(12),* and the Eurecat technology center *(13)*.

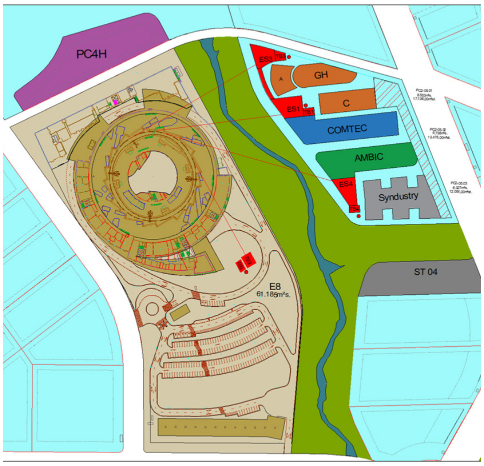

Figure 5 – ALBA II and ASTIP preliminary layout. The four long beamlines paths are sketched for showing all the future possibilities

ASTIP will be an ***interdisciplinary innovation hub*** that blends a unique combination of imaging and characterization tools for complex materials and for biological systems, material growth and detector and device fabrication facilities, big-data and data-mining capabilities with innovation driving synergies. ASTIP shall not only spearhead its own research programs, but shall provide various user modes tailored to, and accessible for, the experienced and early-career scientific researcher and, at the same time, the innovating developer. It will be a portal of access for the industry to these singular scientific and technological capabilities, accelerating knowledge-based innovation and targeting the local and national industrial ecosystem.

ASTIP will be located in a new complex adjacent to the ALBA Synchrotron (see Figure 5), within the Parc de l'Alba *(14)* and has the support of ALBA Synchrotron, of the UAB with its departments and institutes, of the Cerdanyola del Vallès City Council and of the institutions with which the participant centers are associated, in particular CSIC *(15)*, CERCA *(16)* and BIST *(17)*. The initial list of research institutions includes IBMB (Institut de Biologia Molecular de Barcelona (*18*) - CSIC); ICMAB (Institut de Ciència de Materials de Barcelona (*19*) - CSIC); ICN2 (Fundació Institut Català de Nanociència i Nanotecnologia (*20*)- CERCA, BIST member, UAB, CSIC); and IFAE (Institut de Física d'Altes Energies (*21*), CERCA, BIST member, UAB), which includes the PIC. ASTIP is meant to be inclusive and open to more national and international institutes who can profit from the proximity of the research environment to a large research infrastructure.

ASTIP includes ***three new centers*** and the new ALBA II beamlines which enhance ASTIP scientific reach. The centers are the Complex Materials and Technologies Center (***COMTEC***), the Advanced Multiscale Bio Imaging Center (***AMBIC***), and the Innovation Hub (***SYNDUSTRY***, Synchrotron light-based R&D towards new industrial applications). Combining the optimization of already existing resources with state-of-the-art instrumentation fully profiting of the enhanced properties of the synchrotron, will make this center almost unique worldwide. One example is the fully integrated biosafety level-3 environment connected to one of the new beamlines, enclosing the imaging and sample preparation instrumentations and a strong data-driven bio-computational: it will allow *in-situ* infection studies, essential to understand all steps of the infection pathway and will provide insights in the pathological changes of cells, tissues and even organs, empowering clinical researchers for a fast response to health threats or crises.

The center will exploit existing local and urban infrastructures and boost the research and training vocation of Cerdanyola del Vallès to a new level and will include a large auditorium and a guest house. ASTIP possible construction schedule and costs are not included in this document.

5

TIMELINE

ALBA II will be developed in parallel with the operation of the present ALBA facility, and with the upgrade and construction of new beamlines. Let's recall that in 2021 ALBA is operating 10 beamlines and has three more in construction which will enter in operation in 2022 and 2023.

In a nutshell, the White Paper (WP) will be prepared during 2021. Three years will be then dedicated to the Technical Design Report (TDR) definition, so that the construction of the new accelerator systems can start in 2025, to be finished in 2028, installed in 2029, and commissioned in 2030. Once the main parameters of the source are defined by 2022, it will be possible to start the upgrade of the present beamlines and the definition and construction of up to four new ones. Their construction start-up dates can follow the rule of one per year, as successfully tested during the last few years at ALBA for the Phase II and III beamlines. The first two new beamlines could enter in operation using ALBA source even if optimized for the future ALBA II one. All new beamlines characteristics will be determined by the Science Case, defined together with the present and future user community.

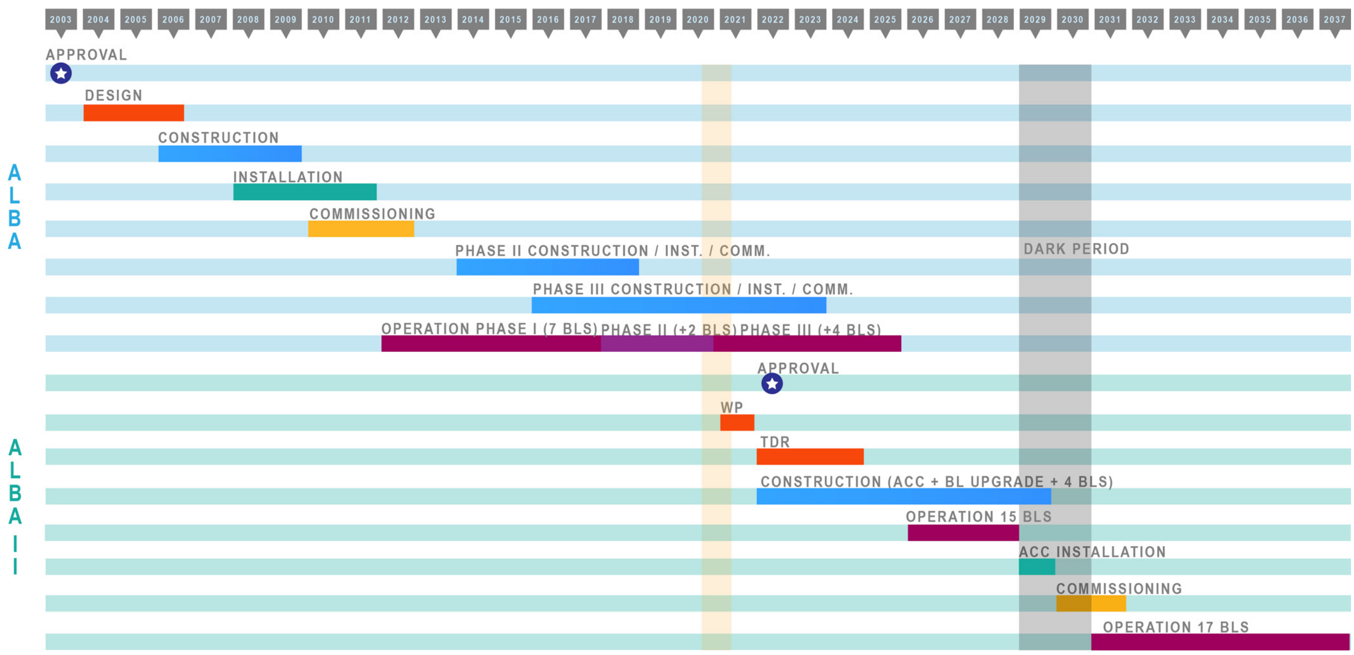

Figure 6– ALBA II timeline. The dark time corresponds to the period with no operation, used for installation and commissioning.

6

COST

The evolution of ALBA from the 3rd to 4th generation is an extremely ***cost-effective project***: it will boost the capacity of the research infrastructure after almost twenty years of operation to a superior level, with a moderate increase in the investments if compared to the overall budget needed to continue ALBA operation without the upgrade.

6.1 OVERALL BUDGET

The tentative budget has been estimated for a 15 year period (2023-2037), which covers the time span for the next two European programs. Costs include personnel, operation and maintenance, plus investment programs. ASTIP is not included.

The difference between upgrading the facility or investing only in operation, maintenance and building new beamlines, is an extra cost over the whole period of only + 13%. The extra staff capacities include updated and extended accelerator technology capacities, extended optics development capacities, specialized staff for the long beamlines, extended scientific data management capacities and adjusted support and maintenance services.

Table I summarizes the integrated cost of ALBA II.

The investment programs include

- ***Accelerator Upgrade***: prototypes and final components for updated accelerators, including additional temporal manpower for installation.
- ***Beamline construction***: construction of four new beamlines, at least two of them with long optical path with the end station in a separated building.
- ***Beamline refurbishment***: modernization of already operational beamlines to current state of technology. The program takes into account the new accelerator configuration.
- ***Transversal investments***: terrains, extended auxiliary buildings, general technical infrastructure for ALBA II and the sustainability subprogram. Contributions to strategic collaborations ALBA Scientific Pole are also included.

	Budget 2023 - 2037	ALBA-II 4th Gen.
	ALBA-II INVESTMENT PROGRAMS	209
Prog.1	Accelerator Upgrade	77
Prog.2	BL construction	44
Prog.3	BL upgrades	25
Prog.4	Transversal	63
	OPERATIONS & MAINTENANCE	309
Ope.1	Energy, gas, water	120
Ope.2	Maintenance	46
Ope.3	Other current cost	68
Ope.4	Financial	3
Ope.5	Users and other transfers	10
Ope.6	General and replacement investments	62
	PERSONNEL COST	360
Pers.	Personnel	360
	TOTAL	878

Table 1 – ALBA II Tentative budget in M€.

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CONCLUSIONS

By building on ALBA culture, ***ALBA II will be one important answer for growing research demands caused by the ecological and economical challenges of the 21th century and the aftermath of the current COVID-19 crisis***.

Upgrading the storage ring, the photon sources, and completing the optimized instrumentation will significantly ***increase the number of photons on the sample and at the same time increase the spatial resolution***, it will push the available energy range to higher energies, and will provide remarkable coherent flux in the tender to hard X-ray range.

With respect to 2021, in 2032 ALBA will have ***increased the operating beamlines from 10 to 17***, proportionally increasing the number of beamtime hours provided to users. The staff will increase by 50%.

This will drive ALBA to ***the top of leading synchrotron facilities worldwide*** enhancing the supportive role for the Spanish community and will translate to many research areas enabling technologies and game changing opportunities.

In combination with ASTIP, the science park built to foster research and create innovation and economic growth based on the research enabled by ALBA II, ***a unique high-tech incubator for Spain and specifically for the Barcelona area*** will be provided.

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