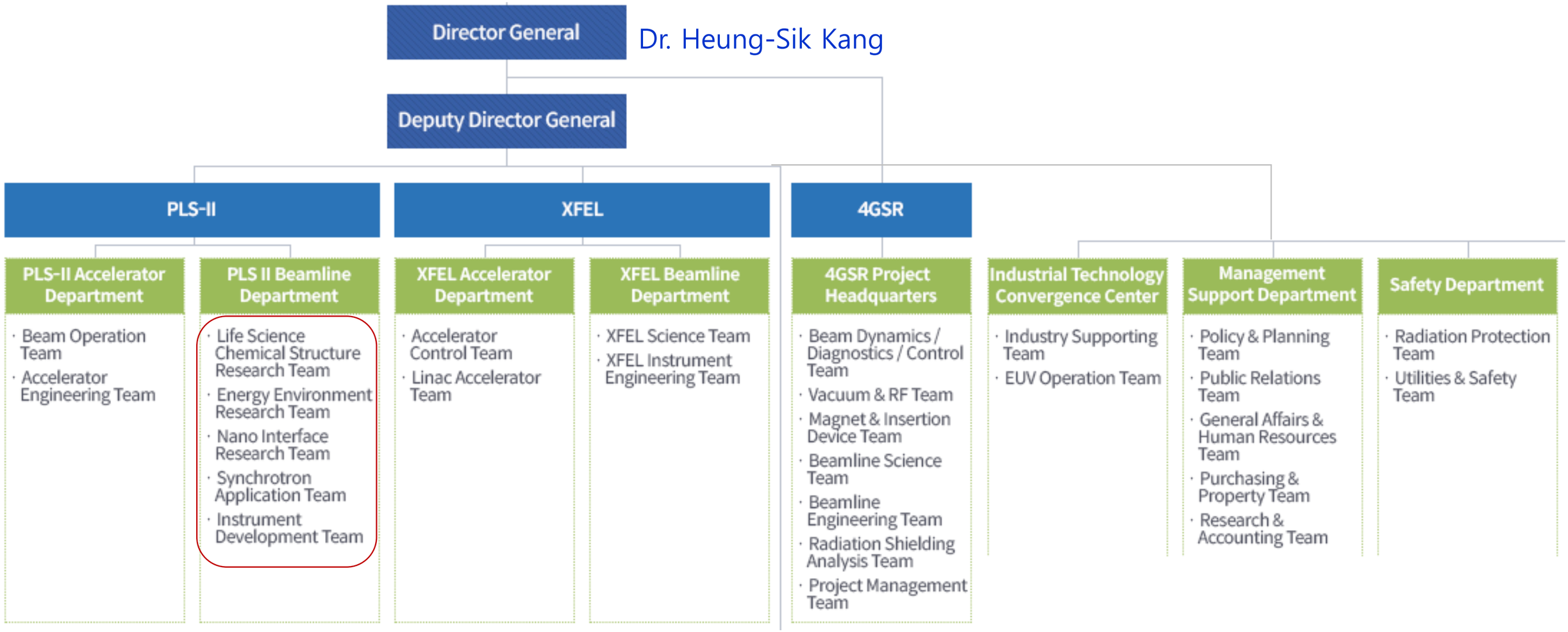
Overview of PLS-II Beamlines

Hyun Hwi Lee

November 13, 2023

PAL Organization Chart

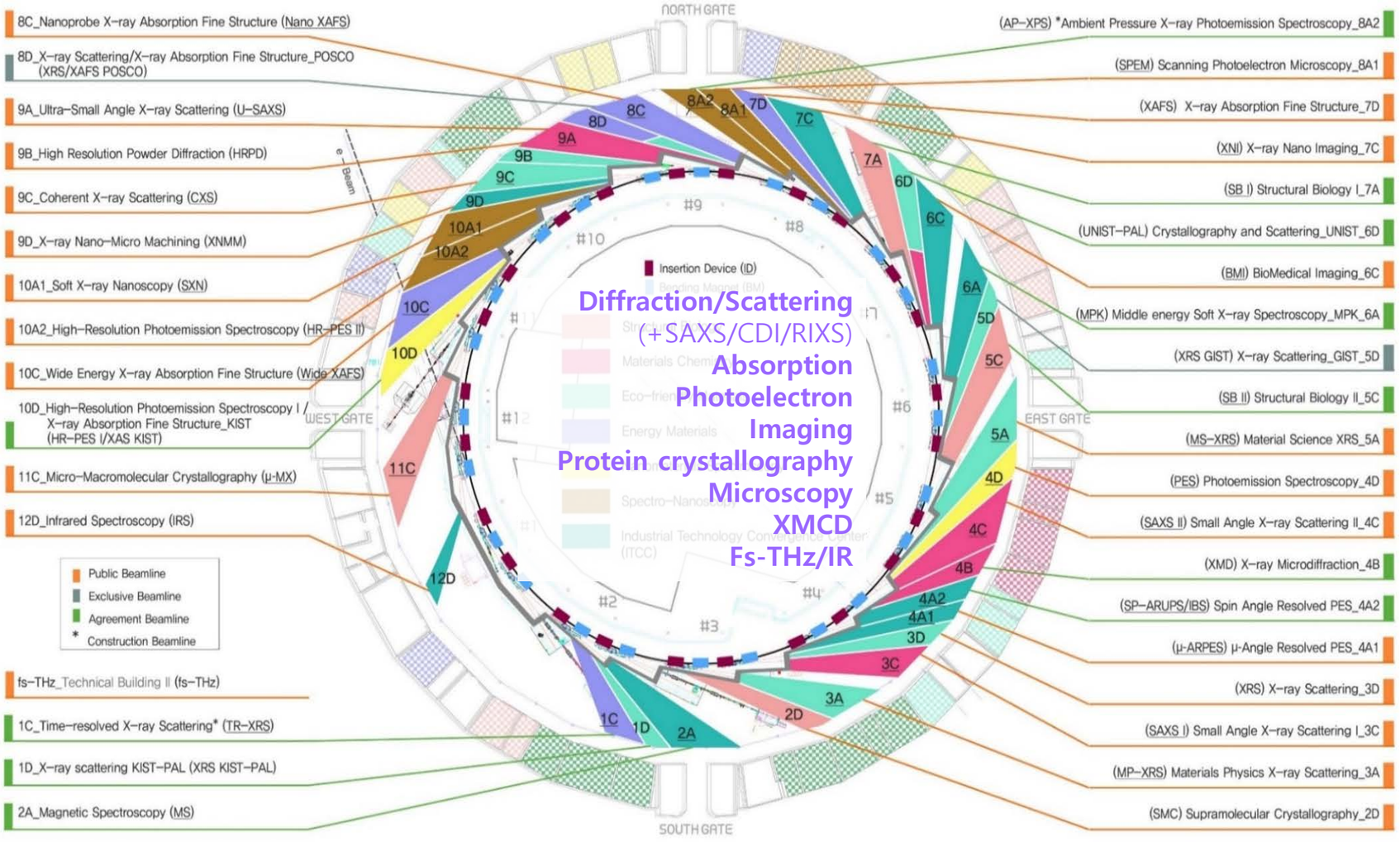
POHANG ACCELERATOR LABORATORY



PLS-II Beamlines and Research Area

POHANG ACCELERATOR LABORATORY

Beamline Map (36 BLs)

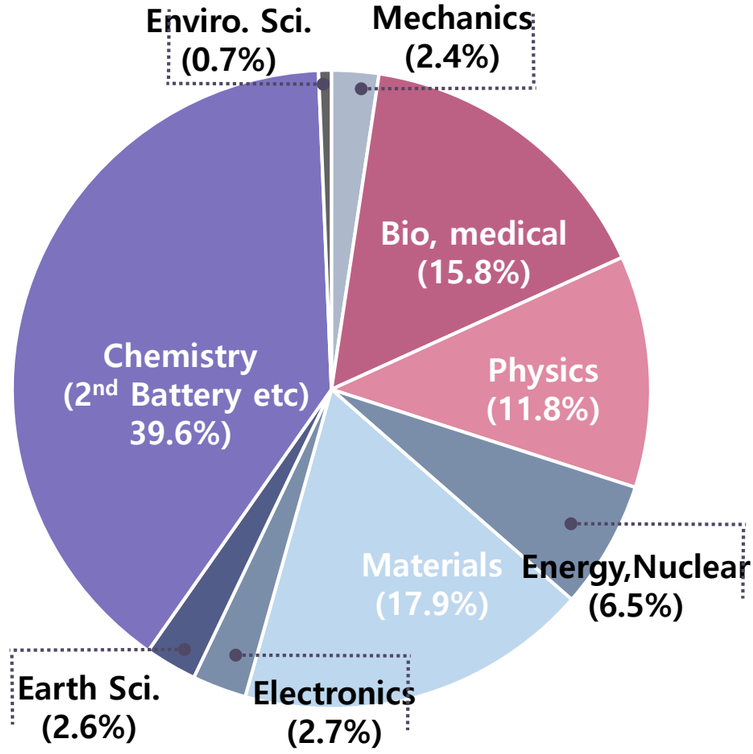


Storage Ring

- Electron beam energy: **3 GeV**
- Ring current: **400 mA, Top-up mode**
- User beamtime: 190 days/year

Research Area

► Based on assigned proposals at year 2022



Assigned Beamtime Statistics

Year	Domestic			International	Total
	Univ.	Institute	Industry		
'21	1,539 (82.3%)	234 (12.5%)	52 (2.8%)	46 (2.4%)	**1,871**
'22	1,691 (84.2%)	220 (11.0%)	73 (3.6%)	25 (1.2%)	**2,009**

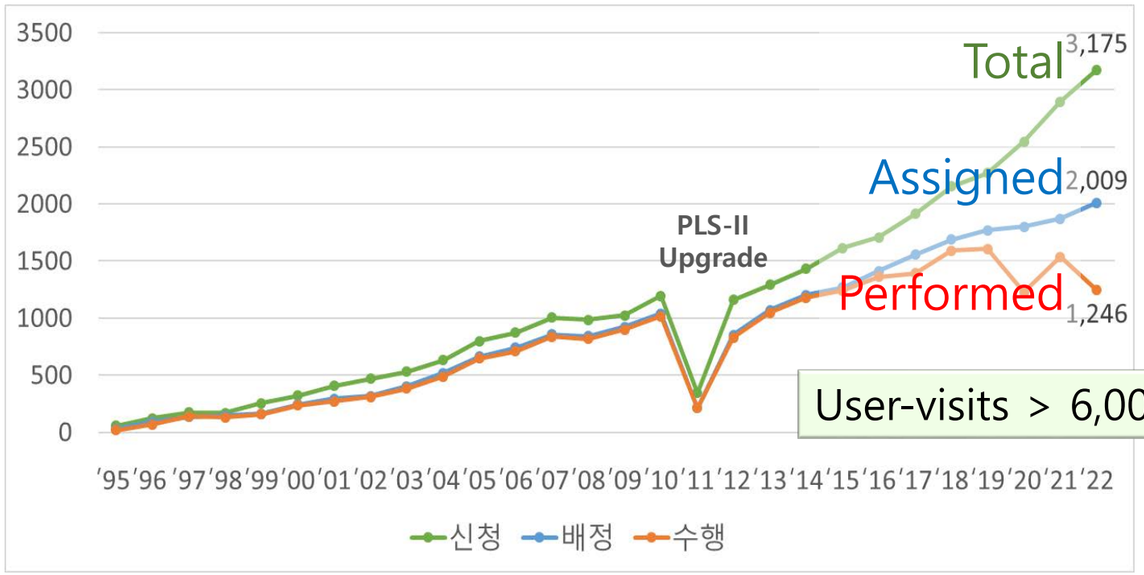
PLS-II User Statistics & Publications

POHANG ACCELERATOR LABORATORY

No. of Beamtime Proposals

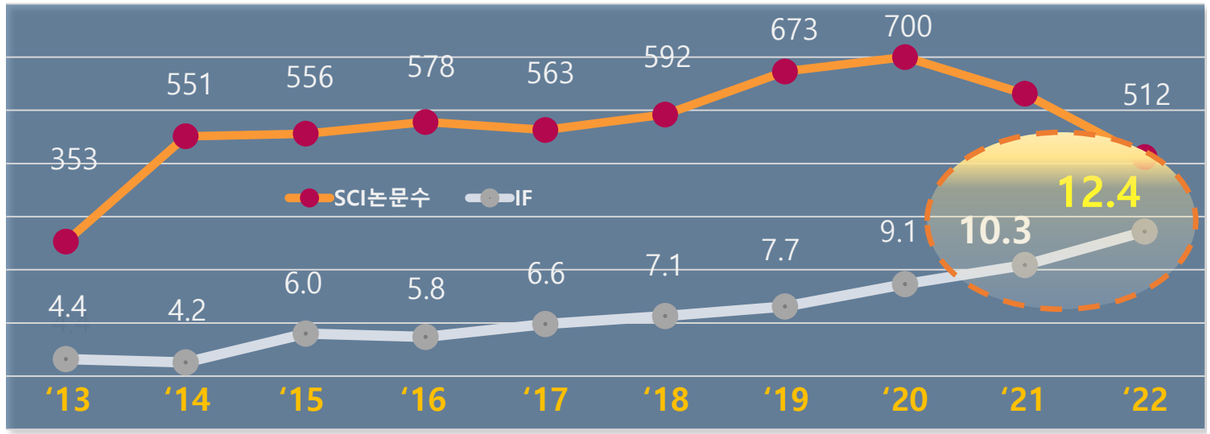
Statistics of PLS-II Experiments and Proposals('22)

(@ Sep '22)



Year	'18	'19	'20	'21	'22
Target Proposals	1,500	1,600	1,600	1,600	**1,600**
Total Proposals	2,152 (Int. 112)	2,271 (Int. 122)	2,545 (Int. 100)	2,897 (Int. 92)	**3,175 (Int. 48)**
Accepted Proposals	1,686 (Int. 71)	1,768 (Int. 81)	1,802 (Int. 57)	1,871 (Int. 46)	**2,009 (Int. 25)**
Performed Proposals (Users)	1,592 (5,877)	1,607 (6,096)	1,224 (3,109)	1,538 (5,132)	**1,246 (3,717)**
Competition Rate	1.3:1	1.3:1	1.4:1	1.5:1	**1.6:1**

SCIE Papers (PLS-II+PAL XFEL)



- Averaged IF for all Korean Scientists is 3.9.
- The decrease in 2019-2020 was due to COVID-19 and reduced beamtime schedule (SRF issue)

User Satisfaction Survey

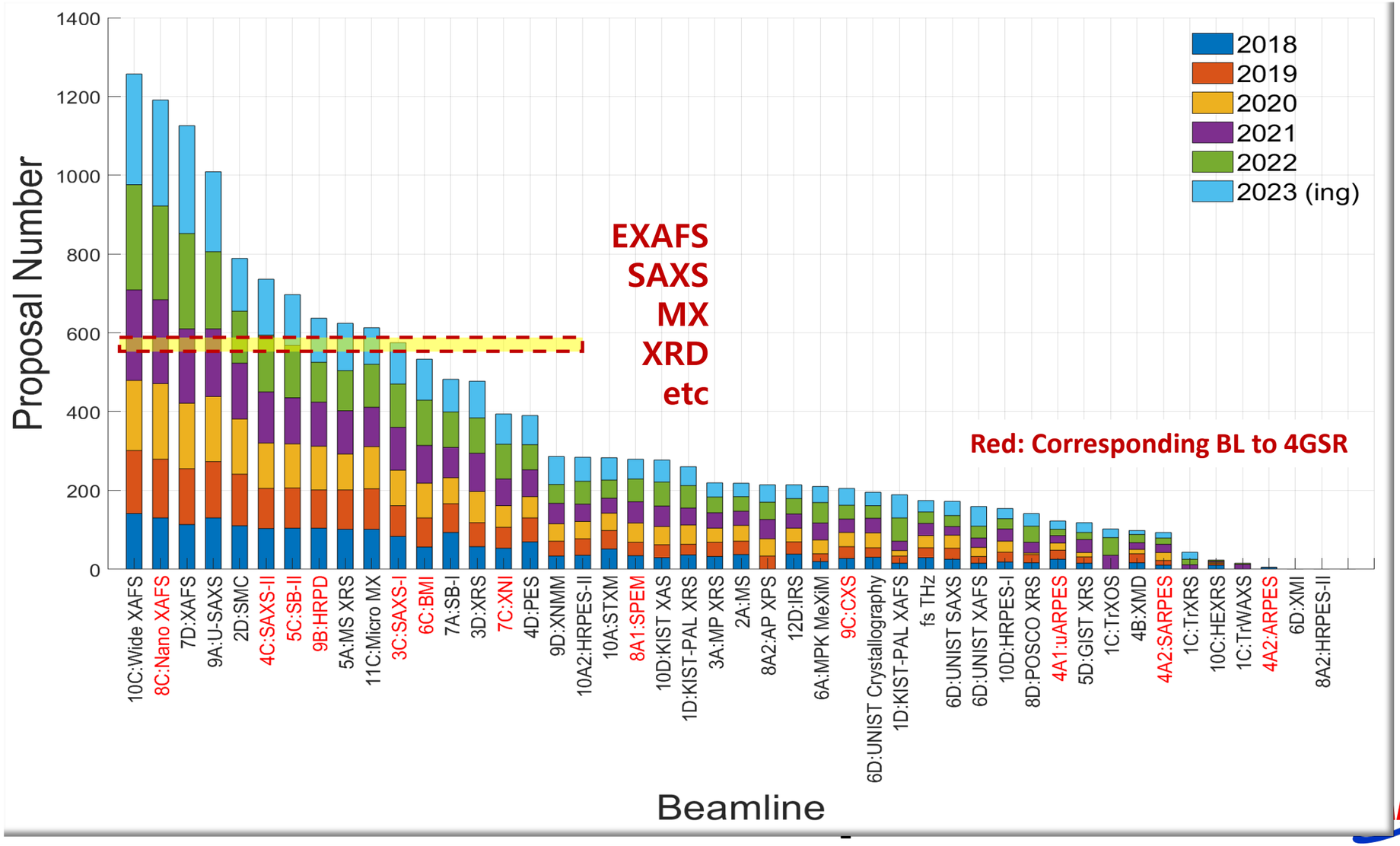
Statistics of PLS-II ('22)

* Surveyed 440 people in '22 (~9/30)

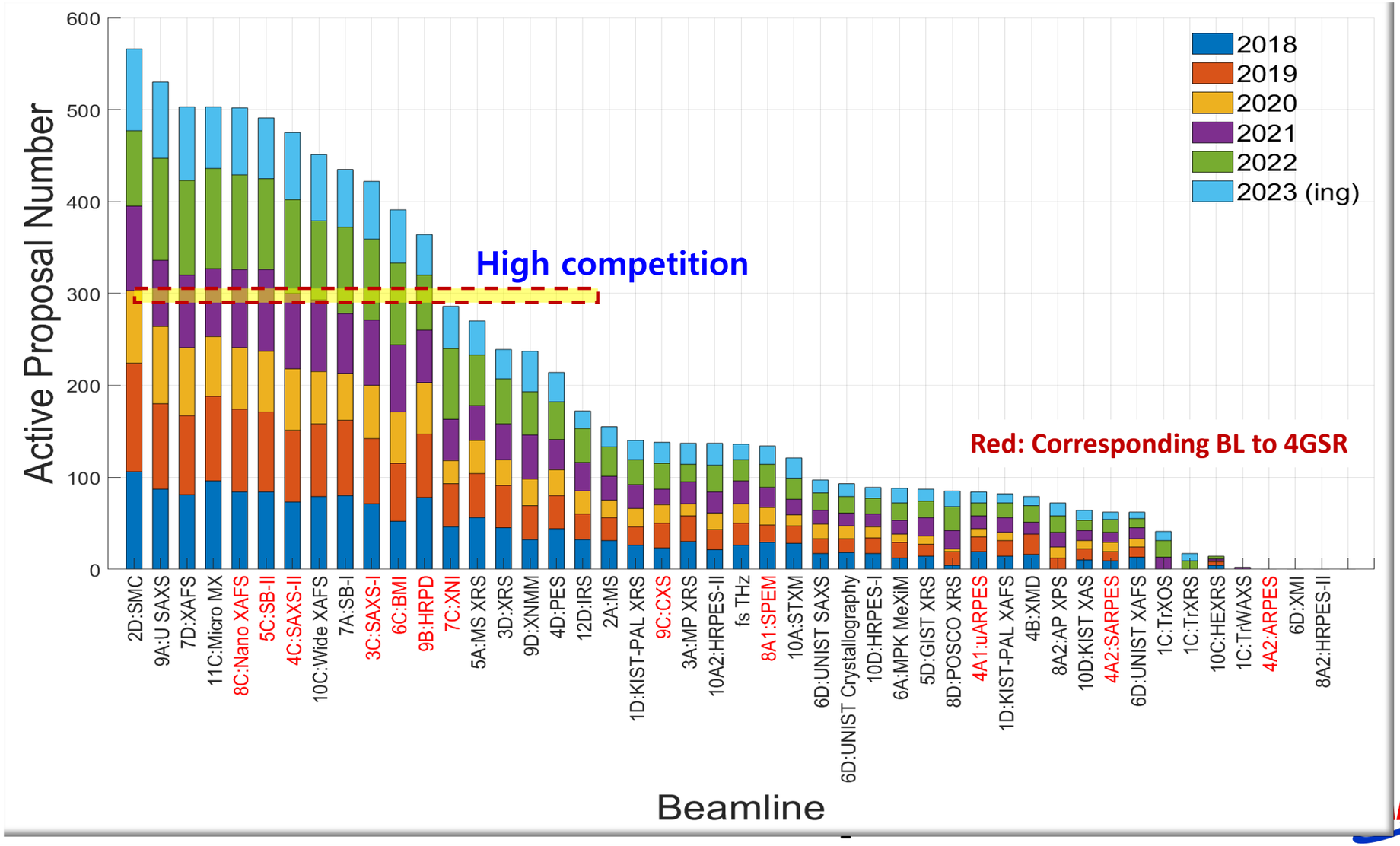
Category	Satisfaction Rate					S.R. (higher than 4)	(Compare) '18-'21 Satisfaction			
	5	4	3	2	1		2018	2019	2020	2021
Beam Quality	69.0%	20.2%	9.6%	0.5%	0.7%	89.2%	80.2%	85.8%	85.6%	85.9%
Beamline	72.5%	18.3%	8.2%	0.7%	0.2%	90.8%	86.8%	89.0%	88.0%	87.1%
Exp. Data	61.0%	27.5%	11.0%	0.2%	0.2%	88.5%	84.4%	87.0%	87.1%	85.6%
Staff Support	73.9%	15.5%	9.6%	0.5%	0.5%	89.4%	85.1%	87.0%	88.0%	87.8%
Service	66.9%	22.8%	9.4%	0.5%	0.5%	89.7%	83.1%	87.3%	86.4%	87.5%
Average	68.7%	20.8%	9.6%	0.5%	0.4%	89.5%	84.0%	87.2%	87.0%	86.7%

Satisfaction Rate higher than 3: 99.1%

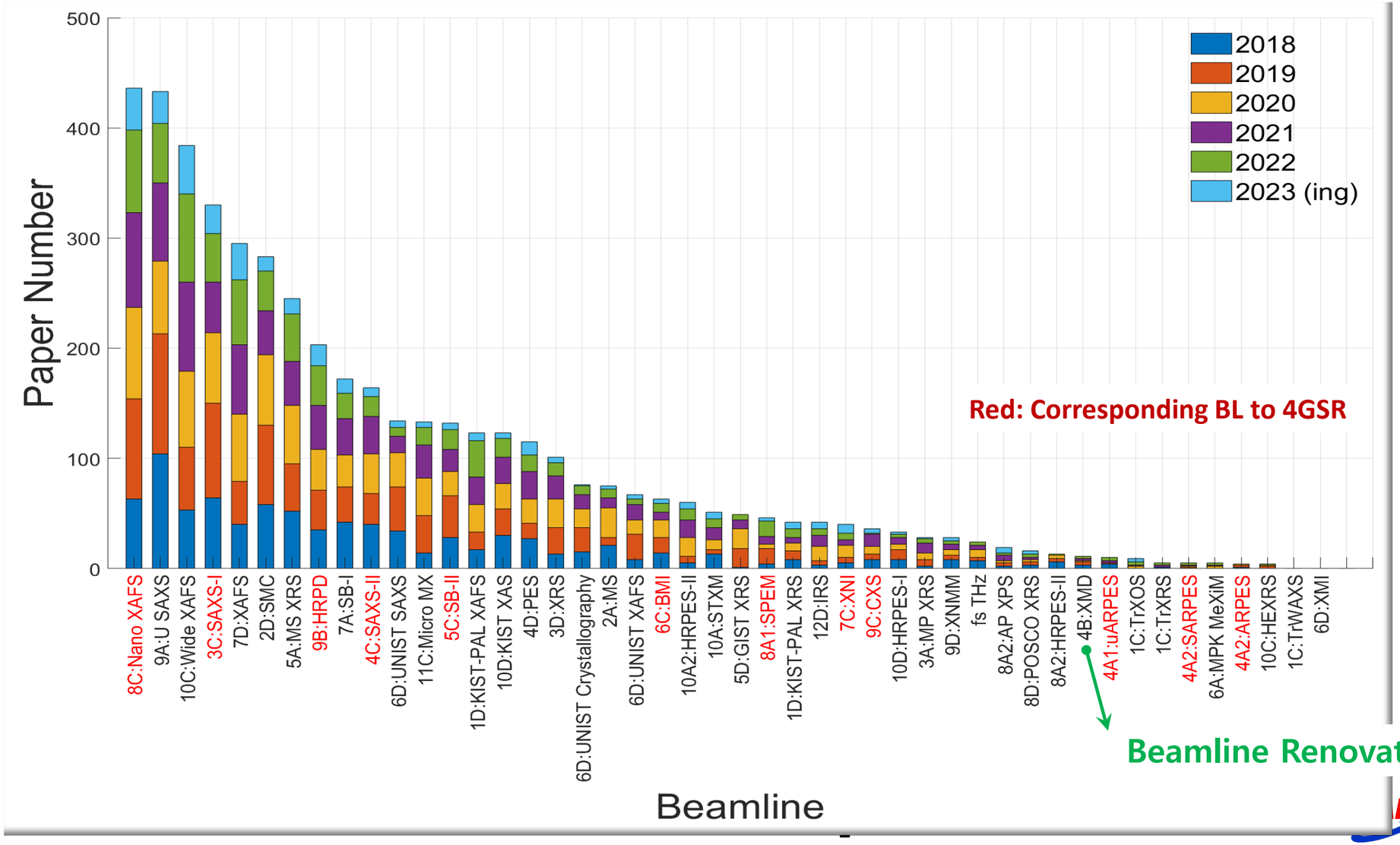
Beam-time Proposals for recent 5-years



Performed propsals for recent 5-years



Scientific Achievement(SCIE) for recent 5-years



Beamline Renovation / 4B HRPD-II

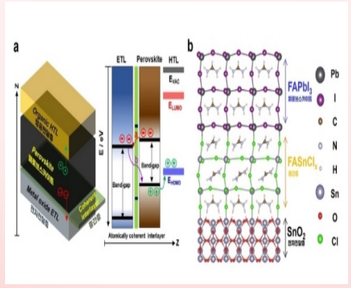
Research Highlights of PLS-II and PAL

POHANG ACCELERATOR LABORATORY

Journal paper

PLS-II, 10C

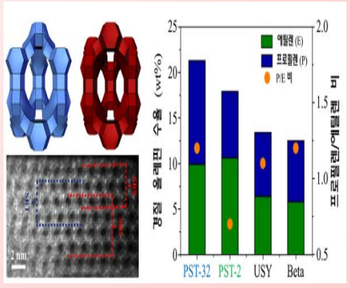
the world's highest efficiency (25.8%) perovskite solar cell



NATURE 2021

PLS-II, 9B,5A,2D

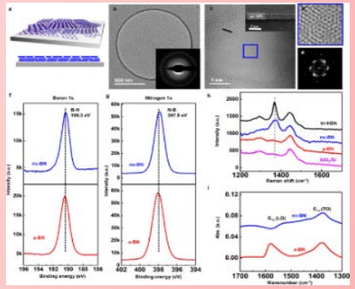
New discovery of zeolite catalyst for petroleum catalytic cracking



SCIENCE 2021

PLS-II 4D, 6D, 10A2

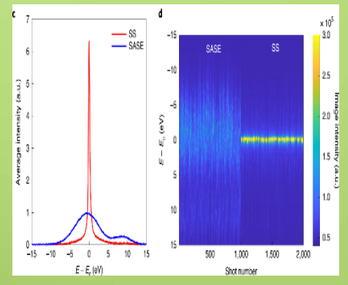
Semiconductor device Material "Amorphous Boron Nitride" insulator development



Nature 2021

PAL-XFEL, NCI-SFX

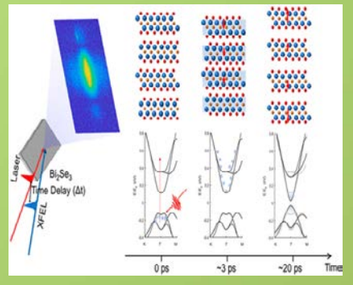
Creating the world's brightest light using self-seeding



Nature Photonics 2021

PAL-XFEL, XSS-FXS

Real-time (fs) measurement of ultrafast structural changes in the crystal lattice caused by excited electrons



Nano Letters 2021

PAL-XFEL, XSS

Observation of non-freezing water and phase transition at -70℃

SCIENCE 2020

industry results

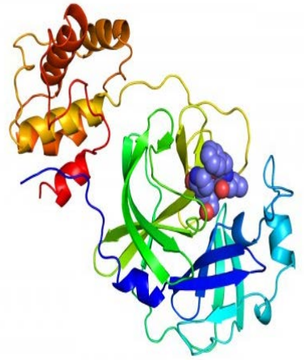
Development of injectable COVID-19 treatment

identify the therapeutic agent (CT-P59) and the COVID-19 protein binding structure at a resolution of 0.27 nm

⇒ Confirm that the therapeutic agent binds correctly to the surface of the spike protein

* Nature Communications('21.1)

Discovery of edible candidates for COVID-19 treatment



Discovery of new drug candidates that inhibit '3CL protease', an essential protein for virus proliferation

⇒ Identification of the 3D atomic structure of 3CL protease and inhibitors with a resolution of 1.6Å

* under Preclinical trial

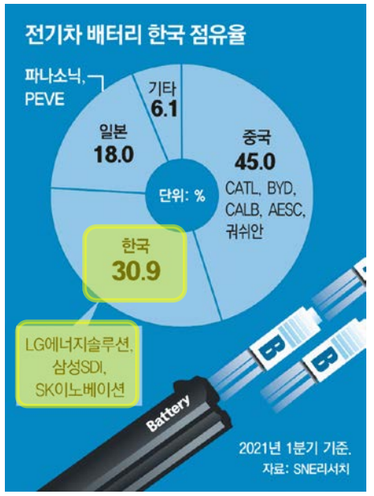
National Core Industries, B-B-C (Industry-Academy-Gov)

BBC?

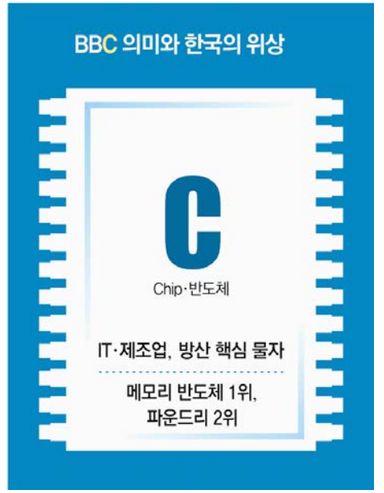
- Bio, Battery, and Chip(semicon) are 3-major industries of global hegemony (war)
- Key industries that hold the key to the future
- U.S. President Joe Biden Orders BBC To Check Supply Chain In Four Areas With Rare Earths After Inauguration

• Bio

• Battery (energy)



• Chips (Semicon)

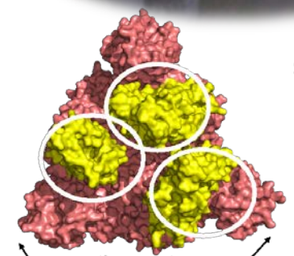


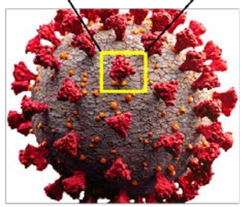
동아일보 21-05-17, 22-09-13
뉴스타운경제 22-09-13 (기사를 발췌한 것임)

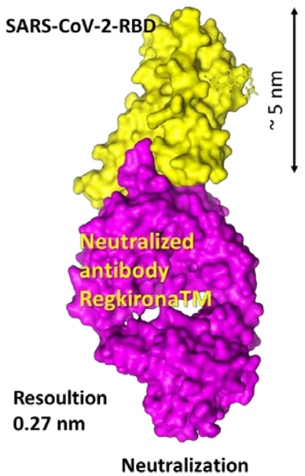
PAL Research Highlights (BBC – The Korean power)

POHANG ACCELERATOR LABORATORY

• Bio Research



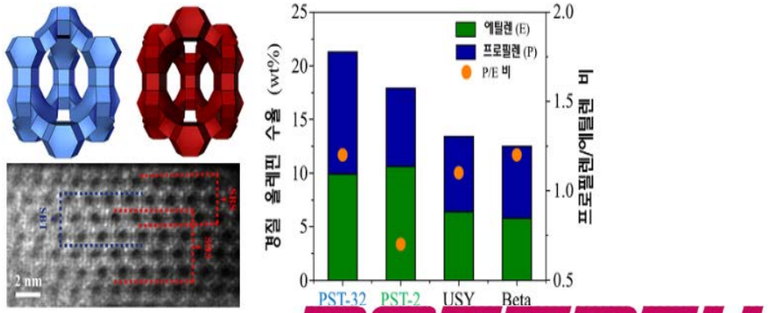




Celltrion Inc.
Neutralized antibody RegkironaTM
* Nature Communications 2021, 12(1):288

• Battery & Energy Research

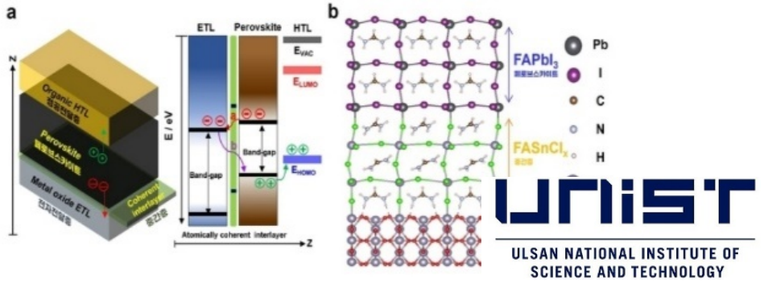
Development of New Zeolite Catalysts for Petroleum Contact Cracking



SCIENCE ('21)

POSTECH
POHANG UNIVERSITY OF SCIENCE AND TECHNOLOGY

Development of World's highest efficiency (25.8%) perovskite solar cells



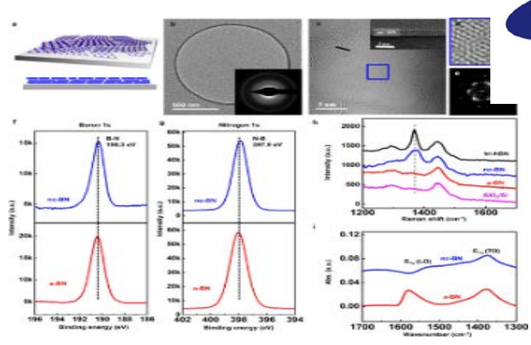
UNIST
ULSAN NATIONAL INSTITUTE OF SCIENCE AND TECHNOLOGY

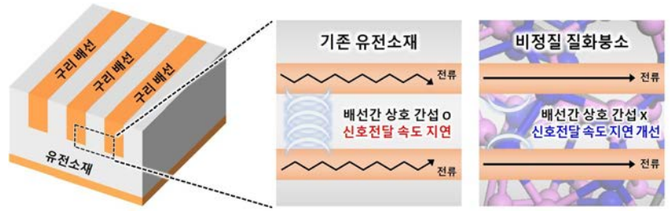
NATURE ('21)

• Chip(semicon.) Research

Semiconductor device Material "Amorphous Boron Nitride" insulator development

SAMSUNG ELECTRONICS



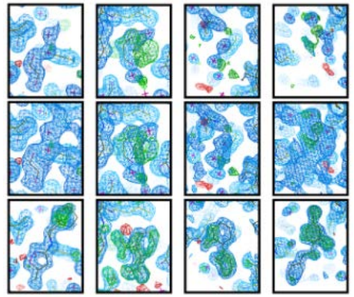


NATURE ('20)

Future Strategy of PLS-II (beamlines)

• Bio Research

- **FBDD program (5C)**
- **Micro MX program (11C) /**
- **General MX program (7A)** / Detector Upgrade

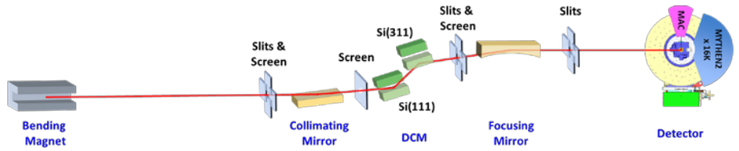


• **FBDD: 300 fragment screening/day**

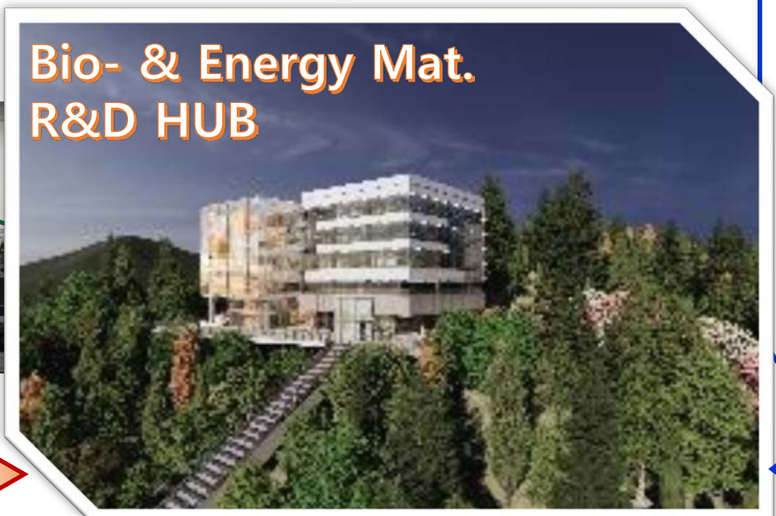
- 2nd XFEL Beamline ('24~'26)

• Battery & Energy Research

- New Beamline: **Multimodal program**
  : 2C HEXA (on-going)
- Beamline Renovation: **High-throughput**
  : 4B HRPD-II (on-going)



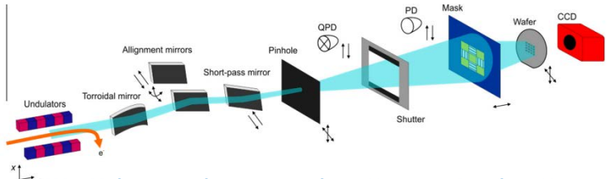
- Tender X-ray Beamline **(planning)**
  : To extend measurable elements
  : Si, P, S, Cl etc
  : New or renovation



• Chip(semicon.) Research

- Tender X-ray Beamline: **(planning)**
  : To cover missing elements and doping elements / Si, P, S etc
  : New or renovation (planning)

- EUV Beamline @ PLS-II: **(planning)**
  : New or renovation



• XIL-II beamline at the Swiss Light Source

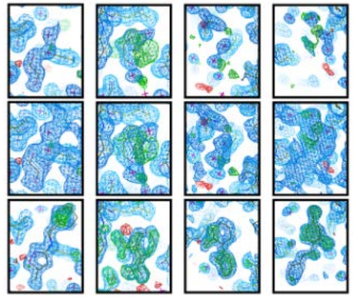
- **Upgrade of Imaging beamlines**

- Future EUV Beamline @ EUV **(on-going)**

Future Strategy of PLS-II (beamlines)

• Bio Research

- FBDD program (5C)
- Micro MX program (11C) /
- General MX program (7A) / Detector Upgrade



• FBDD: 300 fragment screening/day

- Solution SAXS

- Bio-medical Imaging

FBDD program (5C)*: 300 crystals → 600 crystals/day
- Improve beam flux ~x20 and auto-imaging performance

General MX (7A)*: Macro & Supra Molecular program
- Improve both Optics & End-station
→ Merge Supra-molecule Crystallography (SMC) program
→ High throughput and Remote Access program

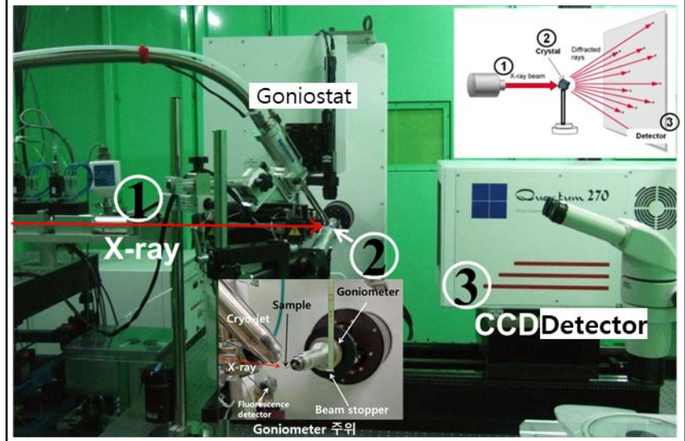
Solution SAXS (4C): Real-time & multimodal program
→ High-throughput (solution) SAXS by Rapid SDD changing
→ New science discovery by real-time & multimodal program

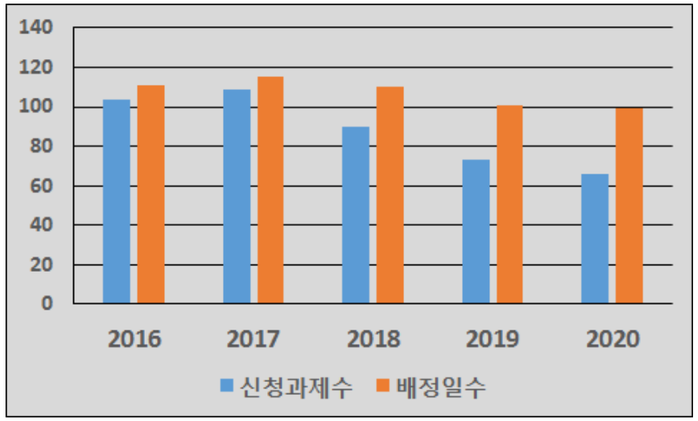
Bio-medical Imaging (6C): Specializing in Medical imaging
- New technique (Edge-enhanced → Quantitative phase imaging)
- Long-term) SC-3pW source & long beamline transfer

Red: Corresponding BL to 4GSR

MX-SMC Program (BL7A)

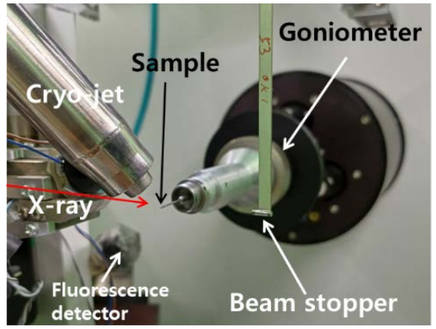
Experiment hutch



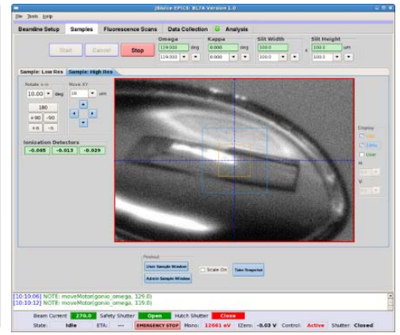


(Goniostat)

➢ Goniostat
- Goniometer
  : single omega axis/kappa axis)
- Camera
  : placing crystals to X-ray
- Performance
  : Sphere of confusion: ~ 5 μm
  : Mechanical poor translation
  : No suitable for small crystal
  (less than ~ 10 μm)



Around sample



Centered crystal

(CCD Detector)

ADSC Quantum 270 CCD detector

➢ Slow data acquisition
- Read time: 2 s

➢ Less sensitive than pixel detector (Dectris)

MX-SMC Program (BL7A)

Upgrade in this year

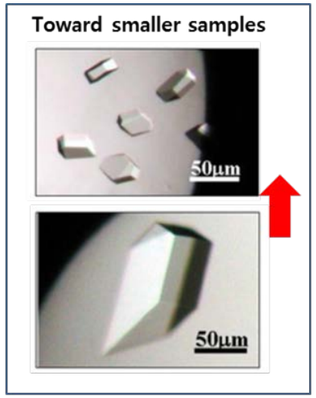
MX (Macromolecular X-ray diffraction)

- **Instrumentations**
  Routine single crystal X-ray diffraction
- **Specifications**
  - *Upgrade in progress*
    : **Large sensitive 2D pixel detector (Eiger2 S 9M)**
  - After upgrade
    : Fast data collection within ~ 5 min (1°/1s: total 360)
    : Semi-high throughput
    : Expansion of sample size space to less than 20 μm)

Current Q270 CCD detector
27 cm x 27 cm
(ADSC, 2010)

Eiger2 S 9M (Decteris)
23.3 cm x 24.4 cm

- Large Fast pixel detector -



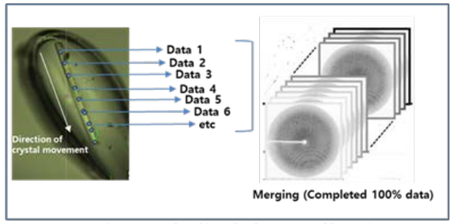
Expansion of routine sample size
(Middle (50 μm) to Micro-crystal (20 μm))

Further plan

General MX-SMC Program (Supramolecular Crystallofraphy)

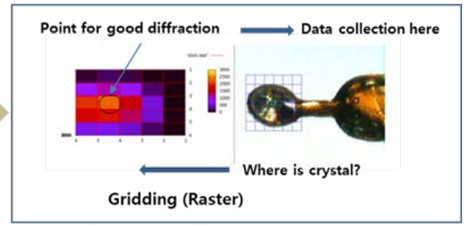
- **Instrumentations**
  Single crystal X-ray diffraction for challenging samples like 10 μm membrane protein crystals
- **Specifications**
  - **High accuracy goniometer**
    : MD3-up

Tools for challenging samples



Line or helical data collection

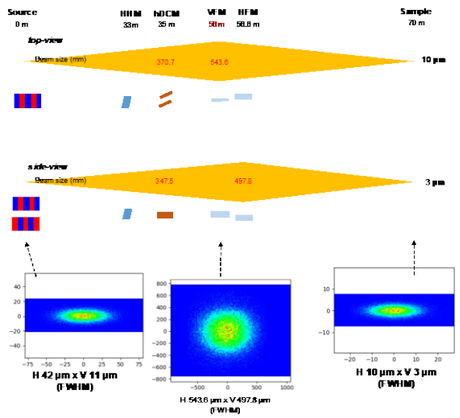
MD3-Up (Arinax)
0.1 μm SoC

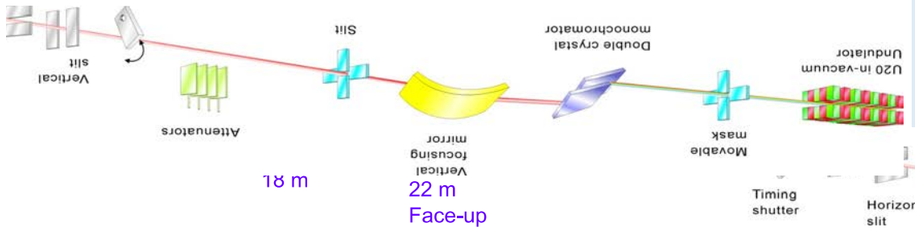


Rastering-Data collection

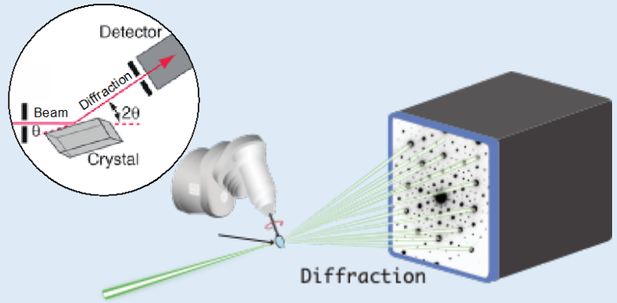
FBDD Program (BL5C)

	Nano MX (ID23) @4GSR	BL-5C @PLS-II
Beam size at sample	3 ~ 10 μm	50 ~ 100 μm
Energy range	6.5 ~ 25 keV	6.5 ~ 16 keV
Photon Flux (ph/s)	> 10E13 (photons/s)	~ 1 ⨉ 10E12 (photons/s)
Data collection Throughput for drug screening (crystals/day)	> 600 crystals/day	~ 300 crystals/day
MAD/SAD Techniqs	available	available
Room Temp. Structure	available	Not available
Time resolved crystallography	available	Not available
In-tray screening	available	Not available
Chemical crystallography	available	Not available

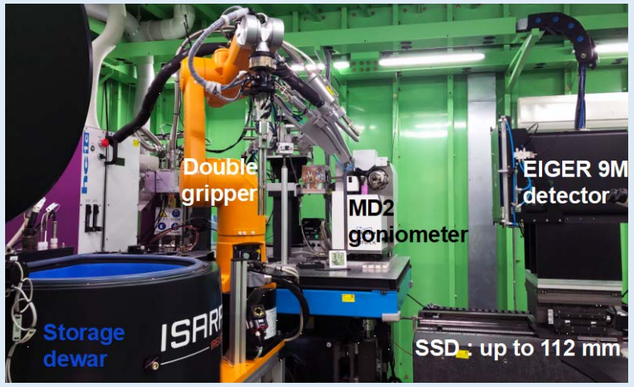




➢ Single Crystal X-ray Diffraction



➢ End-Station Layout

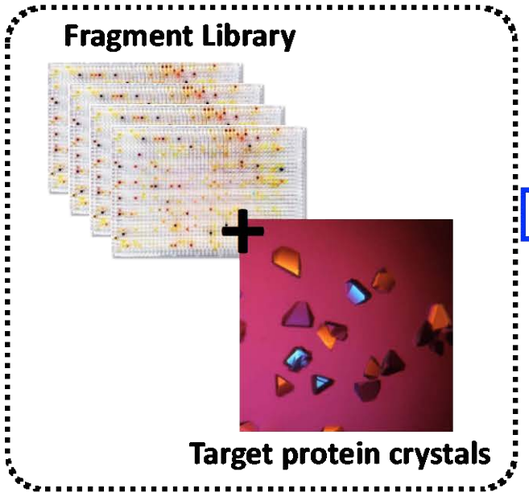


- Diffractions from a protein crystal
- Automatic sample mounting by using a robot
- Automatic sample alignment
- Automatic data collection & processing

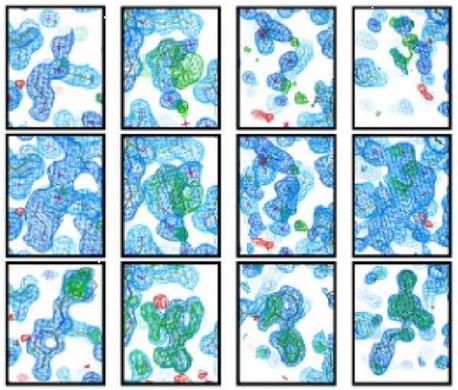
Upgrade Plan of FBDD Program (BL5C)

X-ray Fragment Screening System is established in BL5C for drug discovery

Identification of chemical hits bound to target proteins



400 fragment screening/day



Automatic Hit Identification

To get competitiveness, the throughput should be increased.

To screen more fragments wit hin the given beamtime.

Require more intense beam

- ✓**Replace DCM with Double Multi-layer optics DMM**
  - ✓Two or Three Stripes
  - ✓Ru/B4C(Ruthenium/Boron Carbide): 0.9%, **0.5%, 0.3%** ΔE/E
- ✓**ML will result in Higher flux at a given energy**
  - ✓Current: Si-111 ΔE/E = 0.014 %
  - ✓Upgrade: ML ΔE/E = 0.3 % ,
  - ✓*at least ~20 x Higher flux (Competitive in flux)*

Future Strategy of PLS-II (beamlines)

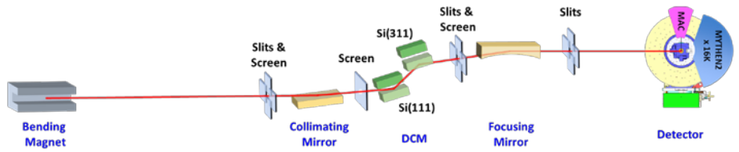
New beamline (2C)*: HEXA
- XRD-XAFS multimodal program
- High-E program (>30keV)
- **5.2M$ /4y** (on-going)

Program change (4B)*: HRPD-II
- Hs-HRPD program
- Old beamline transfer (4B)
- **2.2M$ /4y** (on-going)

(Next presentation)

• Battery & Energy Research

- New Beamline: **Multimodal program**
  : 2C HEXA (on-going)
- Beamline Renovation: **High-throughput**
  : 4B HRPD-II (on-going)



- **Tender X-ray Beamline (planning)**
  : To extend measurable elements
  : Si, P, S, Cl etc
  : New or renovation
- **Detector upgrade Program**
- **Optics upgrade for all beamlines**
  (Next Presentation)

Tender Beamline (plan)
- **2.2~7keV** (upto 15keV)
- **PLS-II Strategy plan**
- All-solid-state batteries and next-gen batteries
- All filed of Energy-related mat.

Detector Upgrade
- **Fast 2D Area detectors**
- XRF detectos

Optics Upgrade
- Optimum optics for PLS-II source + Improve Basic performance
- Overall aging of all beamlines

(Next Presentation)

BL Program change
- Improve Experimental Tech.
- Beamlines older than 20 years
  : Old contract beamlines as well

Red: Corresponding BL to 4GSR

Hs-HRPD-II(4B) Overview (old beamline transfer)

- High-resolution PD experiments (HRPD) are used by various users from academia, research, and industry, and are one of the most in-demand techniques
- Among the PLS-II BLs, 9B HRPD is the only beamline dedicated to PD, and only ab out 50% of the number of days users apply for beam time in the last five years.
- High-speed PD beamline (HRPD-II) required for real-time experimental techniques and various environmental experiments.

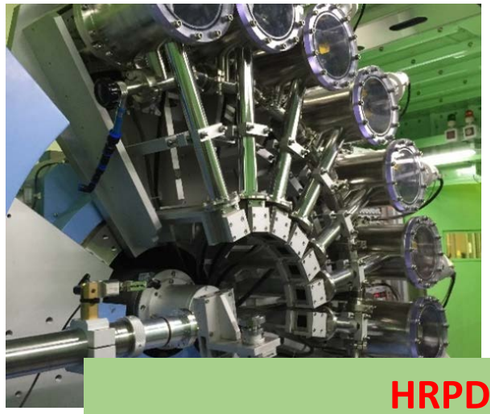
- **Budget: 2.2M$ /4y**
- **Period:** '23~'26

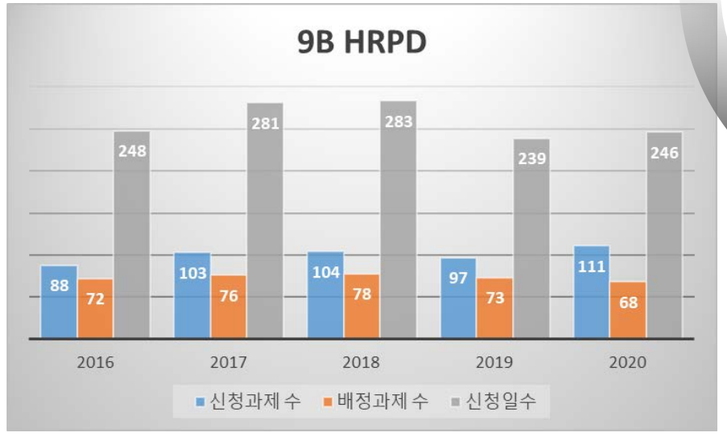
HRPD Gen. I

Multi-detector system with analyzer crystals

: Extremely high angular resolution but slow

- Angular resolution < 0.015° (9B)
- Long measurement time
  ≈ 2h for Rietveld Refinement Analysis
- Bragg-Brentano geometry
- Large amount of samples required





HRPD Gen. II

1D Micro-strip detectors (MYTHEN)

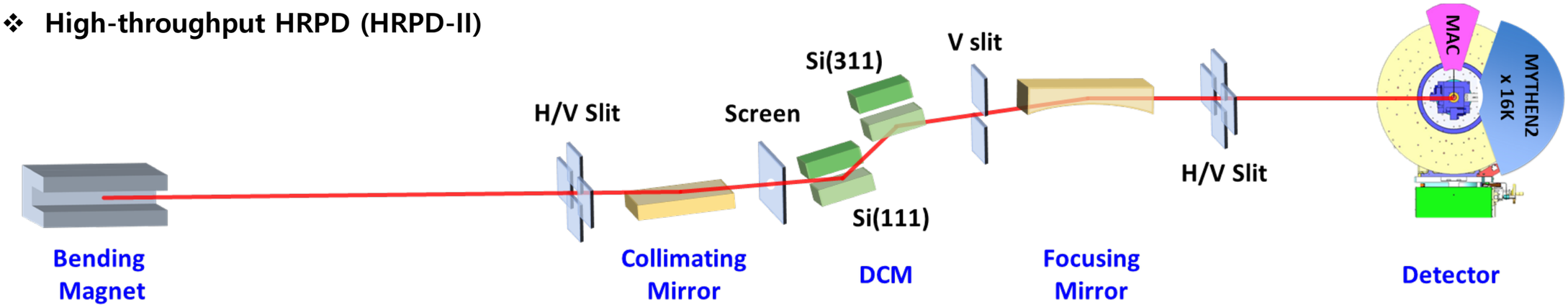
: High angular resolution and fast

- Angular resolution ≈ 0.02~0.03°
- Fast data acquisition < 5 min.
  → High throughput by using robotic arms
- Transmission geometry
- Tiny samples (in a capillary tube) with high S/N ratio

Hs-HRPD-II(4B) Beamline Layout (old beamline transfer)

POHANG ACCELERATOR LABORATORY

❖ **High-throughput HRPD (HRPD-II)**



Source	Bending magnet (PLS-II BL4B port)
Available X-ray Energy	8-30 keV (0.4-1.55Å)
Photon flux (ph/s)	~10^{10} (minimum)
Energy Resolution (ΔE/E)	2 x 10^{-4}
Mirror (M1, M2)	Vertical collimating mirror (M1), Toroidal focusing mirror (M2)
DCM	Si(111) pair/Si(311) pair
Beam size at sample position	100 μm (H) x 100 μm (V)
Angular resolution (LaB_6 @15keV)	<0.015° (Analyzer Crystal), <0.03° (MYTHEN-II)
End station	High resolution position sensitive detector, MYTHEN2 (2θ~80°, 16K modules) + Ge(111) MAC (Multi-Analyzer Crystals) with 3-circle (ω, 2x2θ) diffractometer

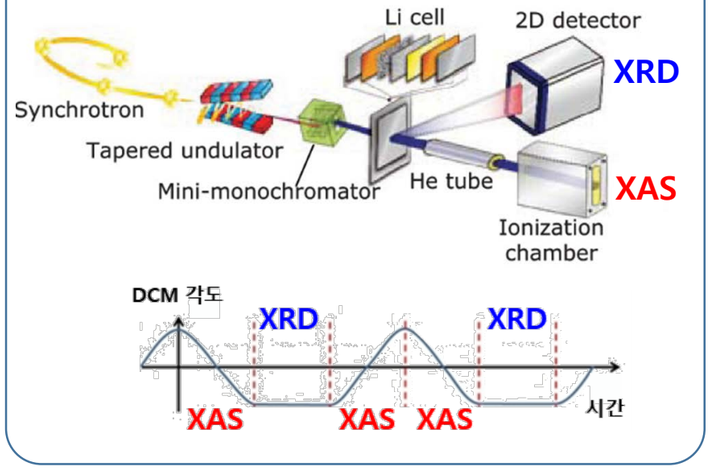
HEXA beamline(2C) Overview (new beamline)

Beamline Overview

Name	• **H**igh **E**nergy **X**-ray combined **A**nalysis (HEXA) Beamline
Scientific Area	• Energy & Eco-friendly Materials Research • Real-time Study on Chemical and Structural Changes of Materials and multimodal Analysis using High Energy X-rays
Techniques	• Multimodal Analysis of hard x-ray XAS and XRD • Real-time and quasi-simultaneous Analysis of XAS and XRD • High Energy X-rays XRD and XAS

- **Budget: 5.2M$ /4y**
- **Period:** '23~'26

Schematic of XAS/XRD analysis



Beamline Requirements

✓Need to introduce **multimodal analysis** techniques that can obtain various analysis data within a limited beam time and support research using **high-energy X-rays**

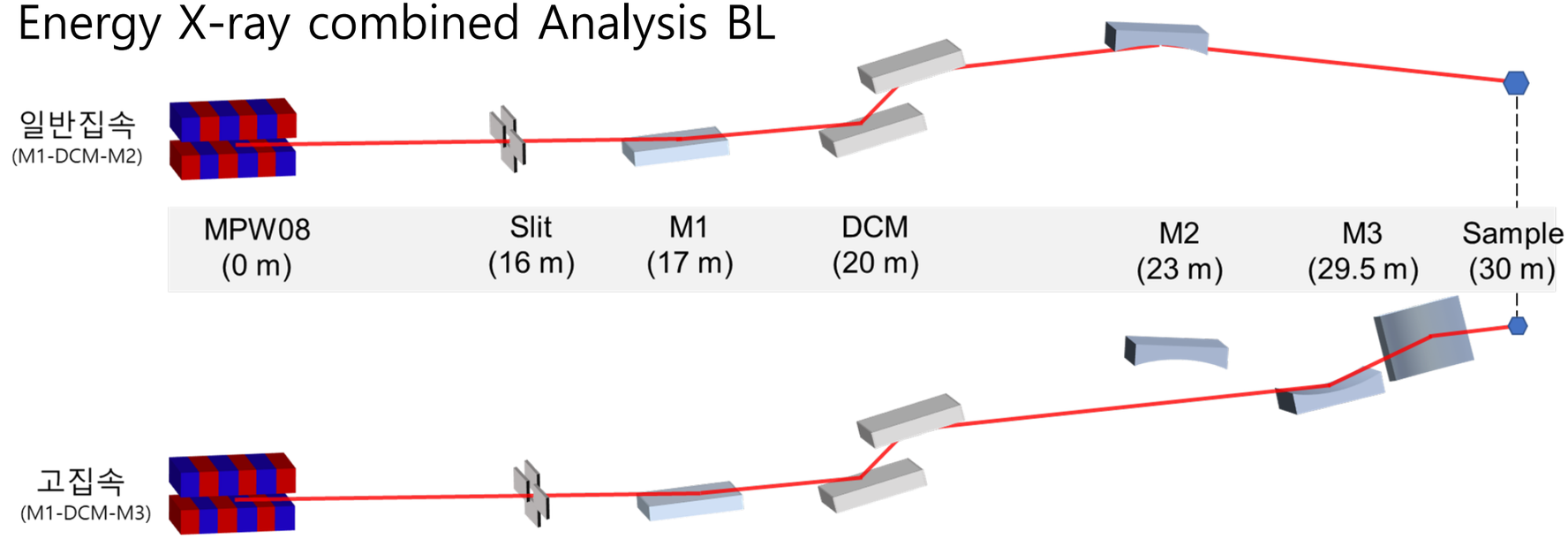
✓**XAS/XRD multimodal Measurements** Improve the Quality of Real-Time Operando

✓Reducing **high Competition Rate** of hard x-ray **XAS** beamtimes (2.5:1)

✓ Real-time material research using high energy X-rays (>**30keV**) in various environments (high-pressure, temperature, electromagnetic field, chemical reaction, and etc)

HEXA beamline(2C) Layout (new beamline)

- High Energy X-ray combined Analysis BL



Source	Multipole wiggler
Available Energy	5-45 keV (1.5 ~ 0.27Å)
Photon flux	> 10^{12} photons/sec
Energy Resolution (ΔE/E)	10^{-4} (@ 5-25 keV) / 10^{-5} (@ 20-45 keV)
Mirror (M1, M2)	Vertical collimating mirror (**M1**), Toroidal focusing mirror (**M2**)
DCM	Si(111), Si(311)
Beam size at sample position	(Normal) : 5mm x 1mm (Focused) : < 5um x 5um
End station	**X-ray focusing optics** : KB mirror (**M3**), Zone plate, capillary lens **Detectors** : Ionization chambers, multielement SDD, Large area 2D detectors

Future Strategy of PLS-II (beamlines)

New Tender beamline (Plan)
- Sharing the future beamline for Energy materials research

EUV Beamline (Industrial Application/Plan)
- Undulator source EUV and beyond-EUV beamline
→ EUV Metrology(Mask & Pellicle etc.) / EUV Lithography
→ Next Gen. photo-resist materials

Upgrade of SX- & HX-imaging beamlines (plan)
- **BL7C** upgrade for **real-time HR Full-field imaging**
- **BL9C** upgrade for (closing CDI program)
: HX-micro beam and ptychography imaging program
- **10A** STXM beamline upgrade
: End-station upgrade for SX-ptychography imaging program

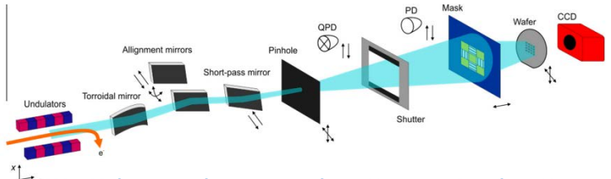
Optics Upgrade
- Optimum optics for PLS-II source+ Improve Basic performance
- Overall aging of all PLS-II beamlines

Red: Corresponding BL to 4GSR

• Chip(semicon.) Research

- **Tender X-ray Beamline: (planning)**
: To cover missing elements and doping elements / Si, P, S etc
: New or renovation (planning)

- **EUV Beamline @ PLS-II: (planning)**
: New or renovation



XIL-II beamline at the Swiss Light Source

- **Upgrade of Imaging beamlines**
: Full-field imaging / BL7C XNI (TXM)
: Ptychography / BL9C CXS (CDI)
: SX- SXTM 및 ptychography / BL10A1

Future Plan

R&D supporting HUB of Bio-, Energy, & Semicon Materials

- **Building Innovative Research Network**
  - Convergence Study of PLS-II+PAL-XFEL
  - Cryo-EM Center (POSTECH)
- **National Research HUB**
  - Converging Nat. Synchrotron Infras
  - POSCO and battery Industries
- **Training Future Researchers**
  - Hyper-disciplinary research
  - PAL-Postech-Rist-POSCO

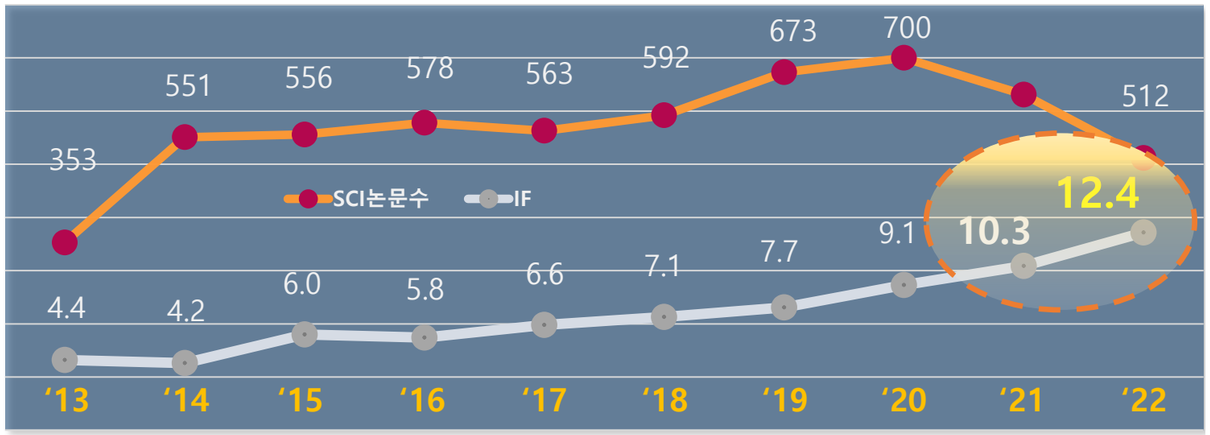
➢ Securing Cutting-edge Research Capability for Next Generation Materials

Thanks to:

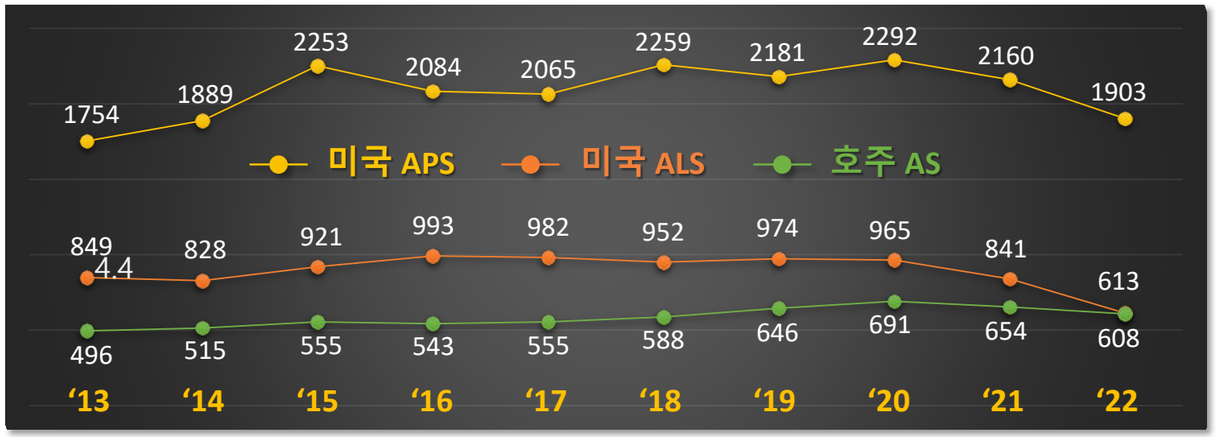
Thank you for your continuous interest and support in Pohang Accelerator Laboratory

Supporting Materials

Supp1) PAL/ SCIE Papers (PLS-II and PAL-XFEL)



SCIE Papers (APS, ALS, AS)



SCIE Papers Count Ranking (South Korea) – Nature Index

#	Institution	Count 2022
1	Seoul National University (SNU), South Korea	566
2	Yonsei University, South Korea	436
3	Sungkyunkwan University (SKKU), South Korea	373
4	Korea Advanced Institute of Science and Technology (KAIST), South Korea	364
5	Institute for Basic Science (IBS), South Korea	333
6	Korea University, South Korea	303
7	Pohang University of Science and Technology (POSTECH), South Korea	260
8	Hanyang University (HYU), South Korea	195
9	Ulsan National Institute of Science and Technology (UNIST), South Korea	187
10	Korea Institute of Science and Technology (KIST), South Korea	185
11	Kyungpook National University (KNU), South Korea	142
12	Pusan National University (PNU), South Korea	140
13	Samsung Group, South Korea	128
14	Kyung Hee University (KHU), South Korea	120
15	Chonnam National University, South Korea	117
16	University of Ulsan (UOU), South Korea	105
17	Chung-Ang University (CAU), South Korea	78
18	Inha University, South Korea	73
19	Ewha Womans University (Ewha), South Korea	65
20	Jeonbuk National University (JBNU), South Korea	65

→ **Nature Index:**

PAL records **International ranking ~90** and **domestic ranking second** in 2022.