



Experimental Data Infrastructure with BENTEN for Fuel Cell Project at SPring-8



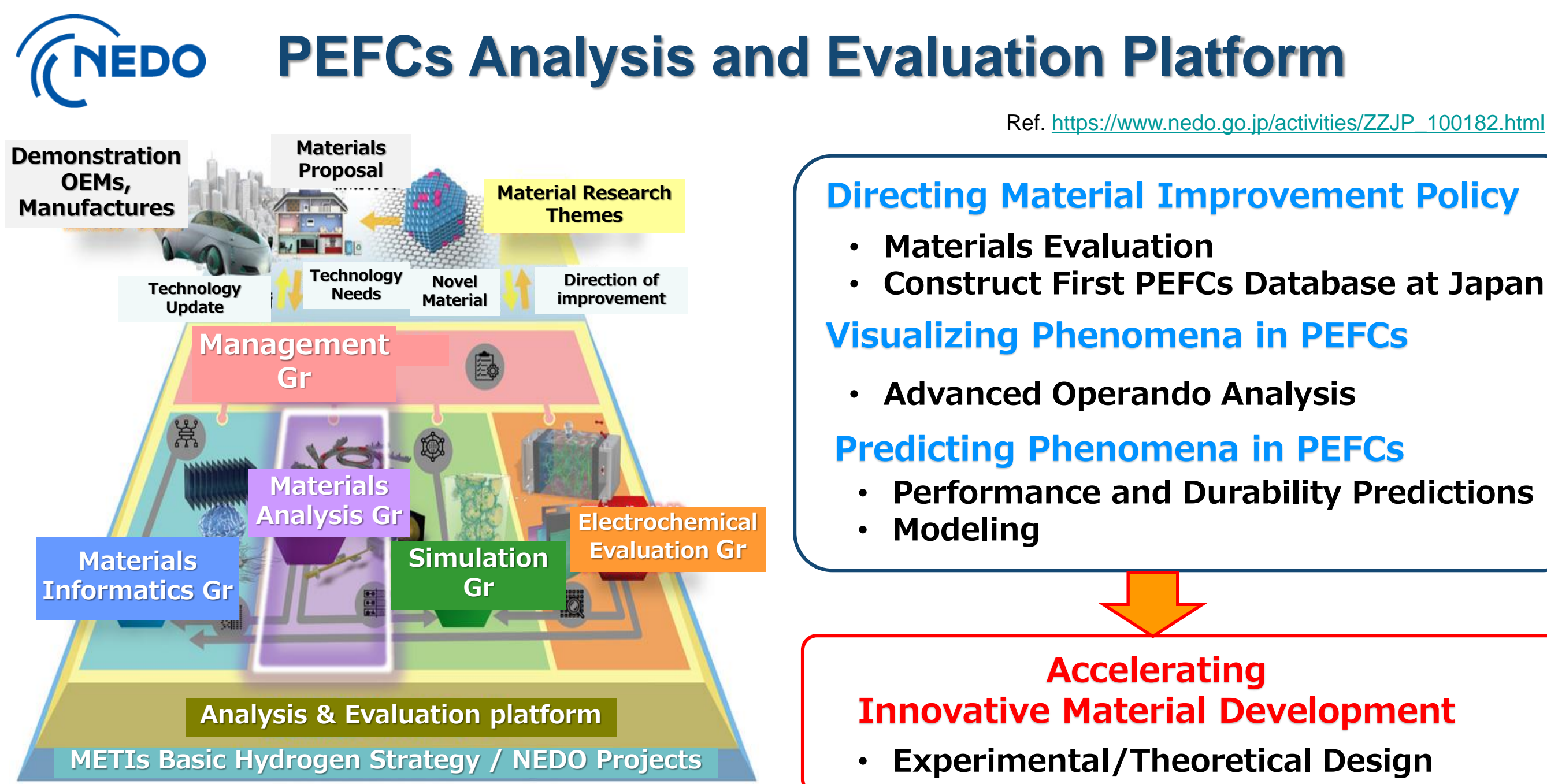
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Abstract

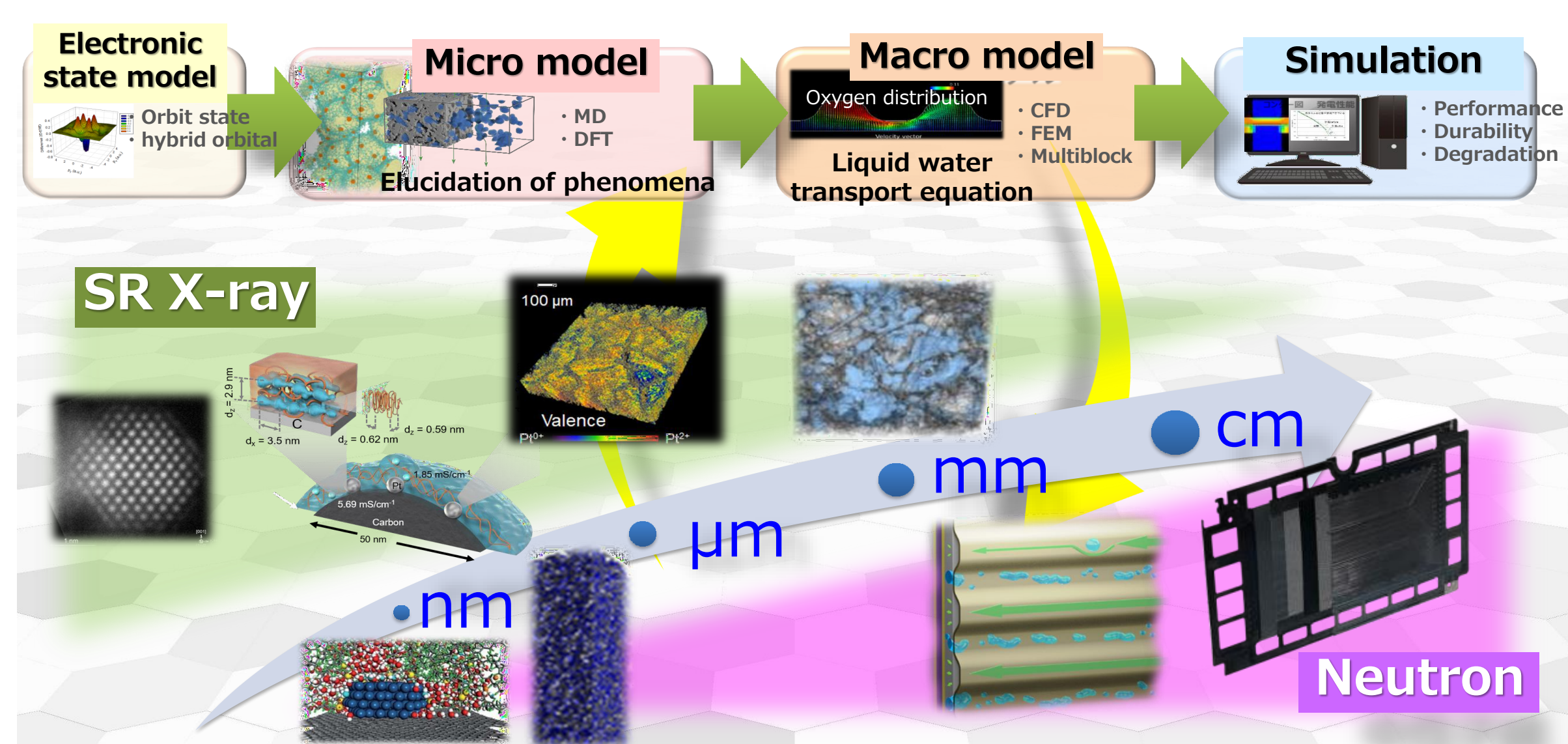
Analysis platforms of Polymer Electrolyte Fuel Cells (PEFCs) were organized in the PEFCs development Project by the New Energy and Industrial Technology Development Organization (NEDO), to accelerate R&D of PEFCs since FY2020.

We present Data infrastructure used for the Fuel Cell project at SPring-8 for the NEDO project. We utilized Beamline Experiment stations oriented data transfer system (BENTEN), and developed database for various X-ray analysis methods. To realize reliable database, we promoted standardization of the procedure, and common data format by reducing the costs in generation. We plan to transfer the data catalogues into National Institute for Material Science (NIMS) for Material Informatics (MI) Platform.

Introduction to PEFCs development Project at Japan

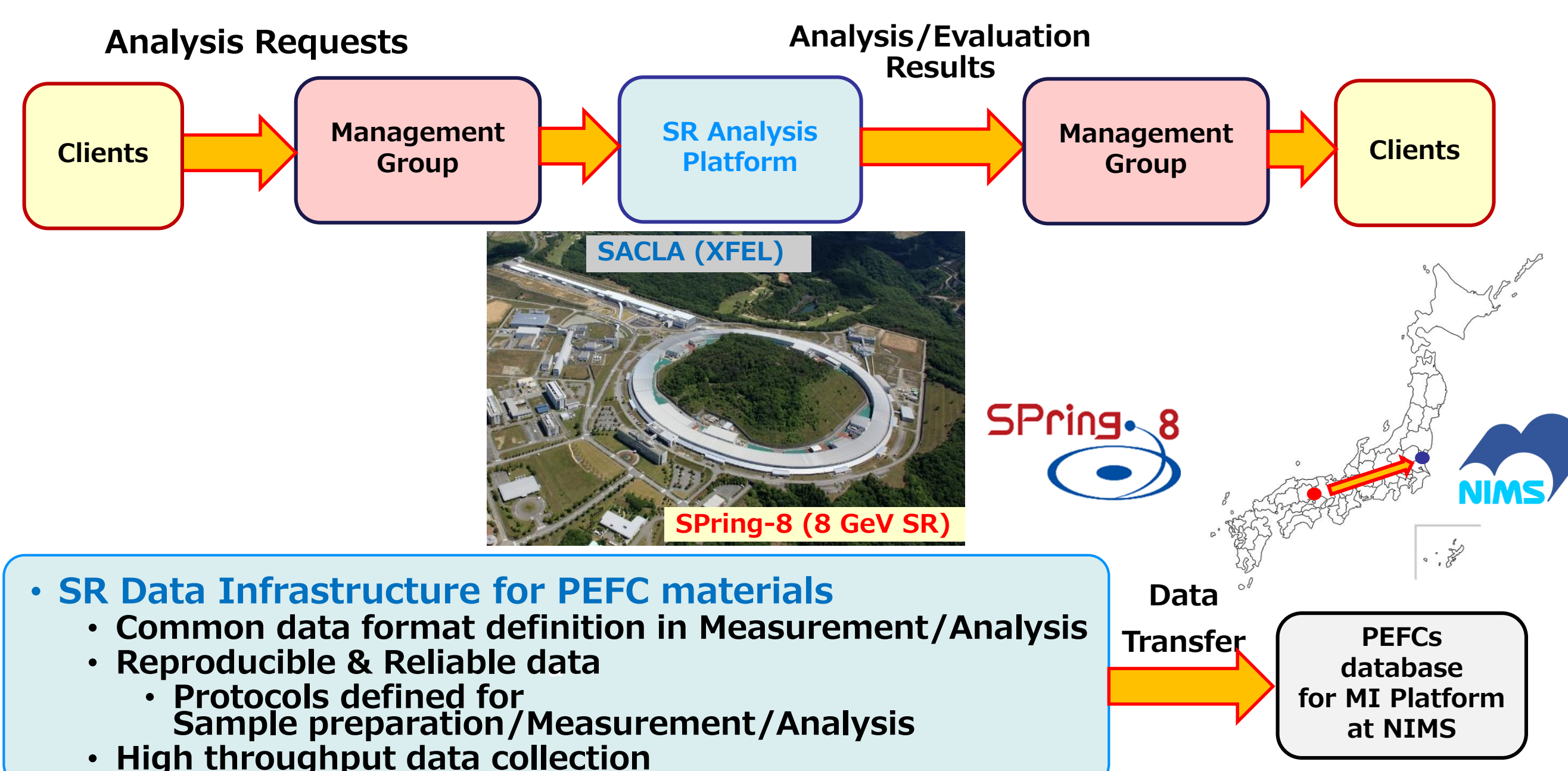


PEFCs Platform "Simulation ↔ Visualization"

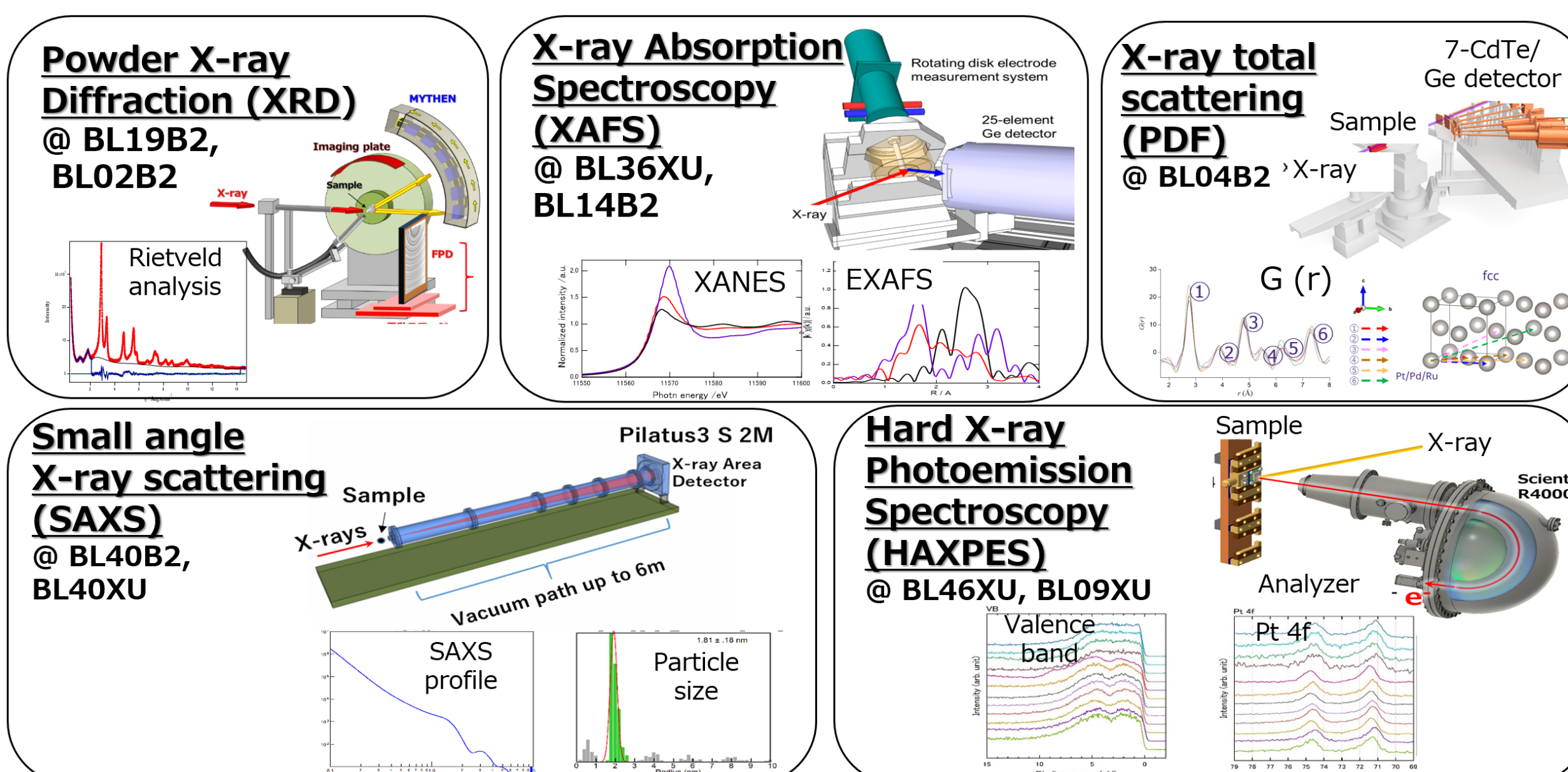


SR Analysis Platform at SPring-8

Work Flow



Standardized SR X-ray Analysis Methods



Catalyst

Techniques	Material Information
XRD	Crystal Structure, Degree of Alloying
XAFS	Local Structure, Valence State, Degree of Alloying
SAXS	Average Particle Size, Particle Size Distribution
PDF	Non-crystalline Structure, Average Particle Size
HAXPES	Electron State, d-band Center

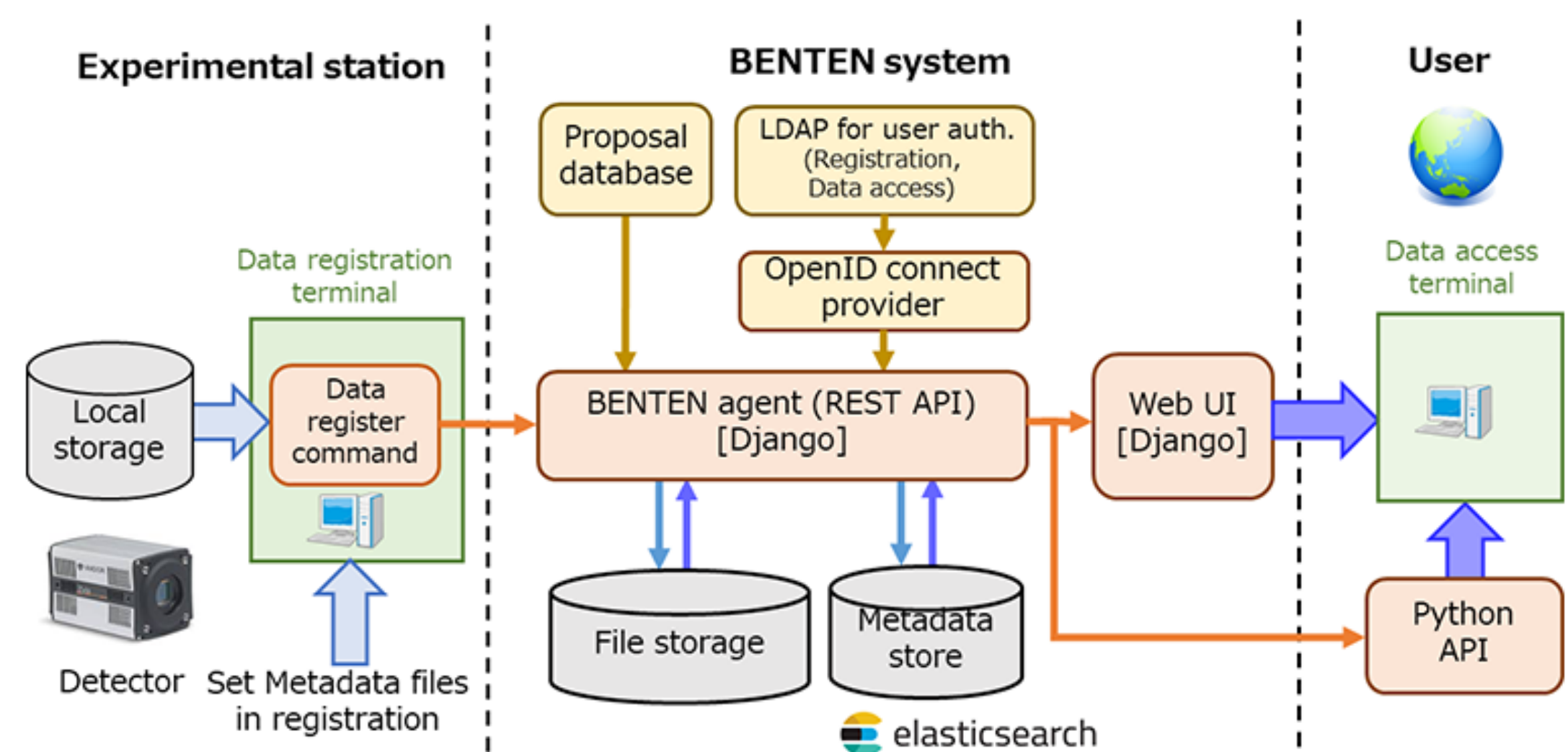
Electrolyte Membrane

Techniques	Material Information
SAXS, WAXS	Higher Order Structure, Crystal Structure, Degree of Orientation
XAFS (Soft X-ray)	Functional Group

SR Data Infrastructure for PEFCs Project with BENTEN

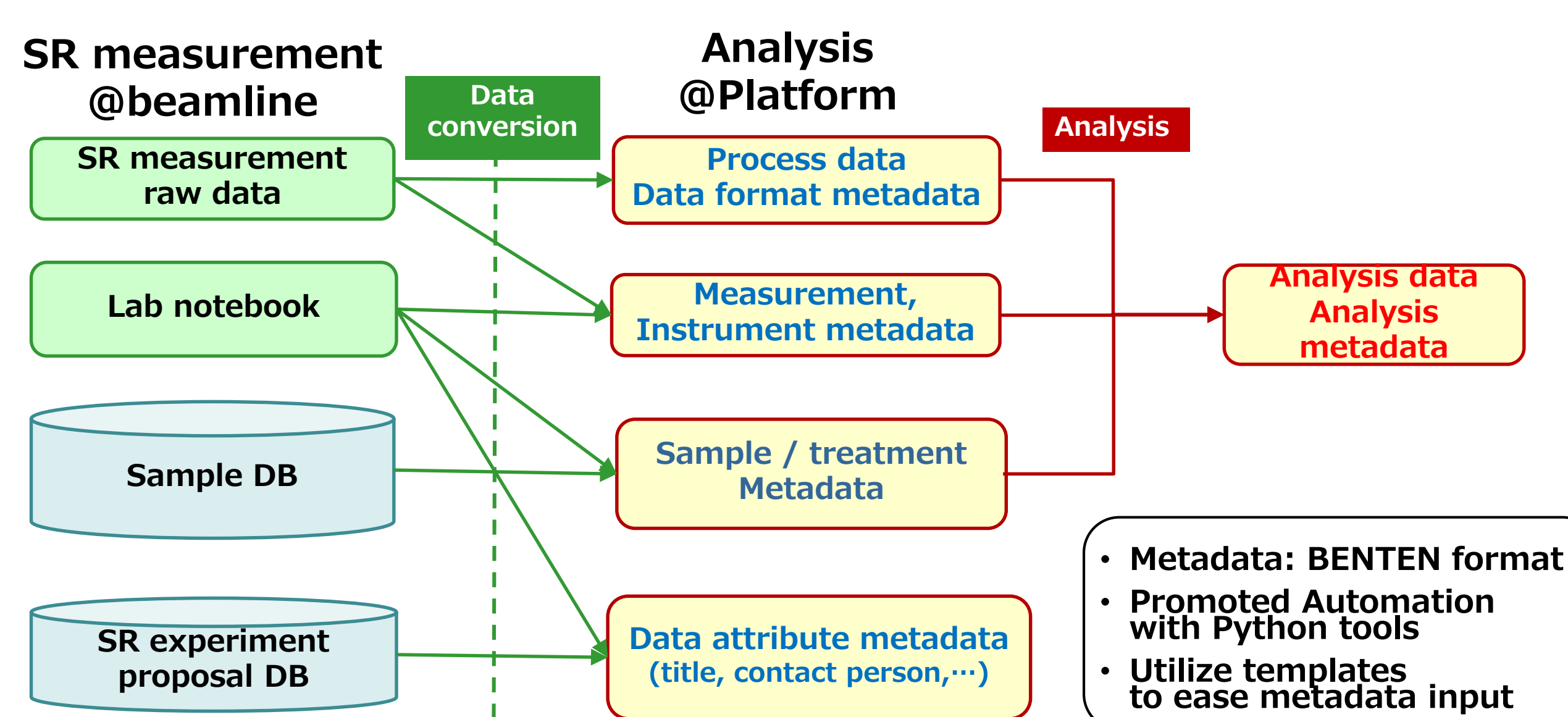
BENTEN for Experimental data transfer system

T. Matsumoto et al., AIP Conf. Proc. 2054, 060076 (2019). Proceedings of ICALPECS 2019, p.702-706



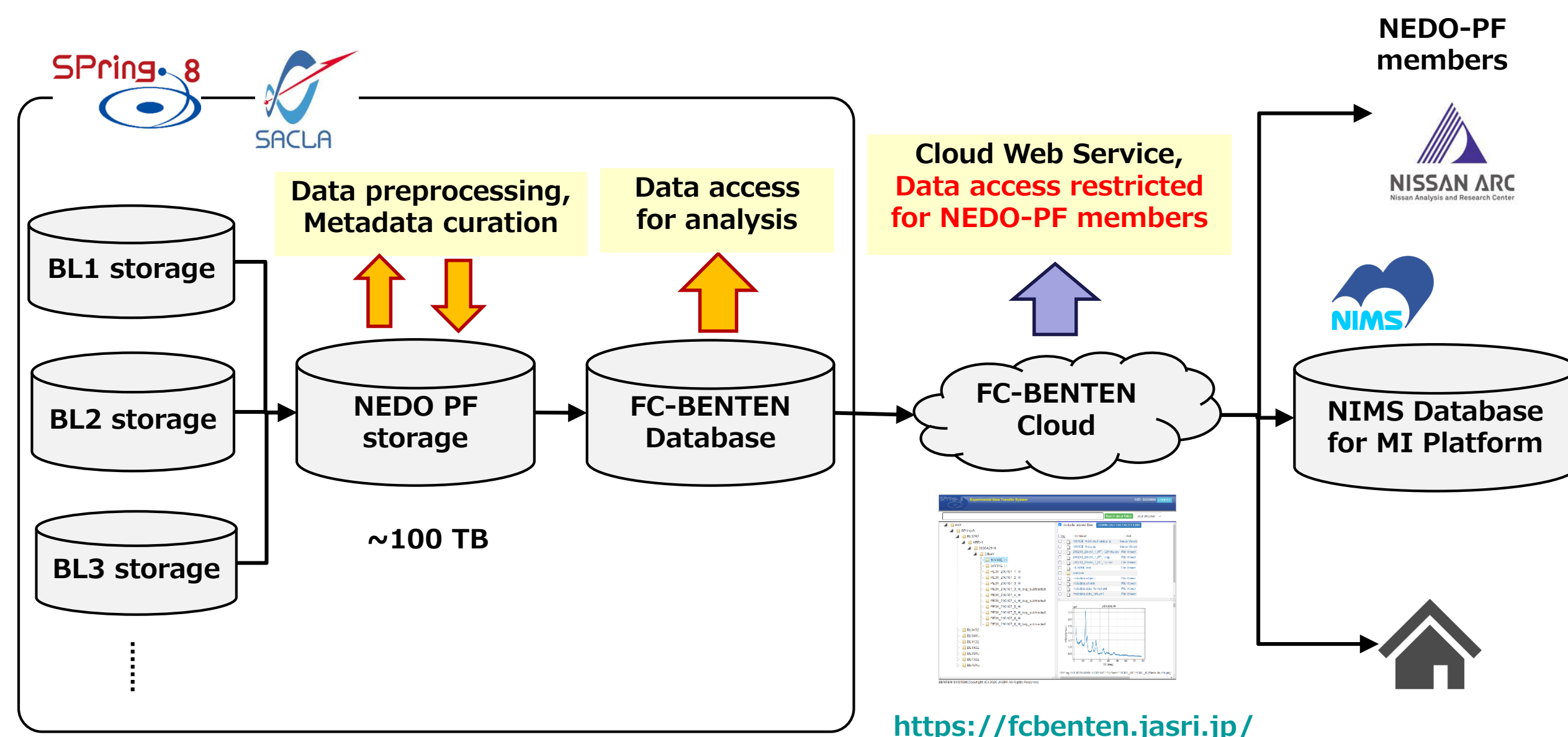
- Data sharing for users with Authentication (SPring-8 ID) and Authorization
- 2 factor auth. with e-mail address confirmation to ensure security
- Applied for Open access of XAFS/HAXPES standard sample
- URL: <https://benten.spring8.or.jp/>
- Data is also registered to NIMS MDR <https://mdr.nims.go.jp/> with DOI

Generation Flow of Metadata & Analysis data



FC-BENTEN for Data infrastructure of PEFCs Project

- Adopted BENTEN by using Cloud, access is limited among NEDO-PF members



Example in HAXPES data

README.md to describe dataset overview

DL	FILENAME	LINK
	10V.thumb.png	Image Viewer
	C1s_10V_0001.csv	File Viewer
	README.md	File Viewer
	analysis	
	metadata.all.json	File Viewer
	metadata.all.yaml	File Viewer
	metadata.schema.csv	File Viewer

Measurement Metadata

```

1 measurement:
2 methods:
3 category: spectroscopy
4 sub_category: HAXPES
5 detection: Transmission
6 incident_photon:
7 angle: 10
8 angle_unit: deg
9 photoelectron:
10 take_off_angle: 80.0
11 take_off_angle_unit: deg
12 spectral_line:
13 name: C 1s
14 energy_scale: Kinetic
15 date:
16 start_time: "2021-04-13 20:57:54"

```

Sample Metadata

```

27 sample:
28 name:
29 id:
30 structure:
31 form: powder
32 catalyst:
33 pretreatment_id: H
34 pretreatment: 水素ガス還元処理
35 form: "2. 合金"
36 carrying_rate: "45"
37 composition: Pt 40.4at% Co 4.6at%
38 uniformity: 合金触媒 Ptスキャン層
39 particle_size: "3.4"
40 particle_size_unit: nm

```

Process Data (NIMS CSV)

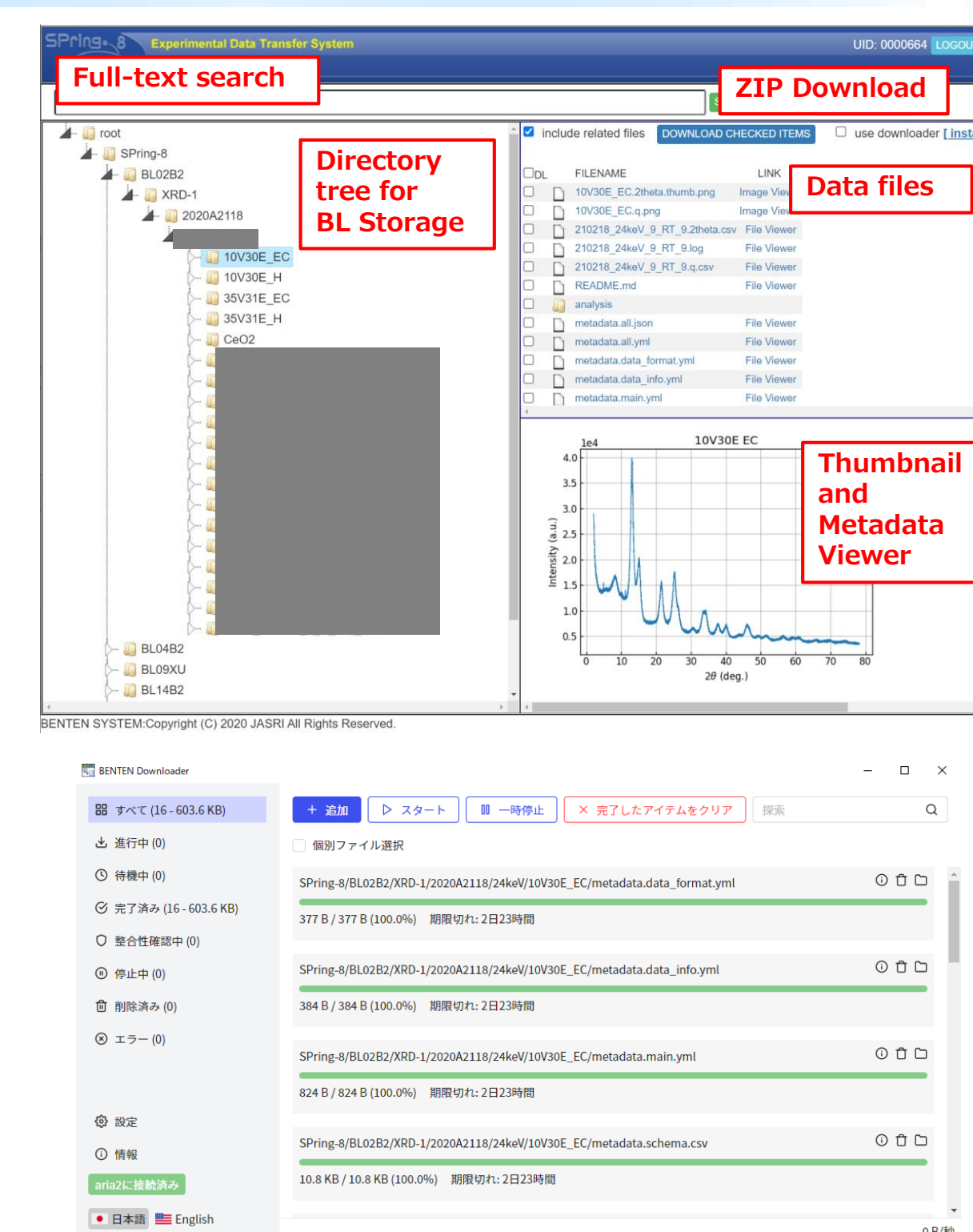
	A	B	C	D
1	#title	10V30E H		
2	#dimension	x	y	
3	#x	Binding ereV	reverse	
4	#y	Intensity	a.u.	
5	#legend	10V30E		
6				
7	298.188	828.84		
8	298.138	805.243		
9	298.088	771.676		

Analysis Metadata

```

109 entry:
110 analysis:
111 hapes:
112 spectral_peak:
113 binding_energy: 298.8
114 binding_energy_FWHM: 0.94
115 binding_energy_unit: eV
116 signal: doniach-janjic
117 background: Shirley
118 energy_uncertainty: 0.25
119 energy_uncertainty_unit: eV
120 dataset:
121 hapes:
122 processed_file: 4_0001_region19_4_2_C1s.csv
123 raw_file: raw_data/4_0001_region19_4_2_C1s.txt
124

```



- Large data download with Electron UI
- utilize metalink file, aria2

Future Prospective

To complete Project by FY2024, Under Developed for:

- Data transfer to NIMS PEFCs database to accelerate PEFCs dev. with MI
- Data retriever to ease understanding of datasets in FC- BENTEN (ex. via Summary table)