2024 KRICT ChemDX Hackathon

Korea Research Institute of Chemical Technology
Chemical Data-Driven Research Center

Dr. Su-Hyun Yoo

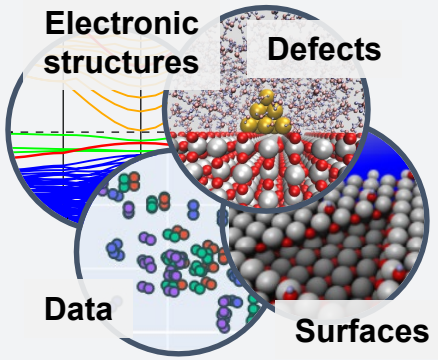
KRICT 한국화학연구원

Self-introduction Research path

2013 — 2015 — 2020 — 2022 — 2023

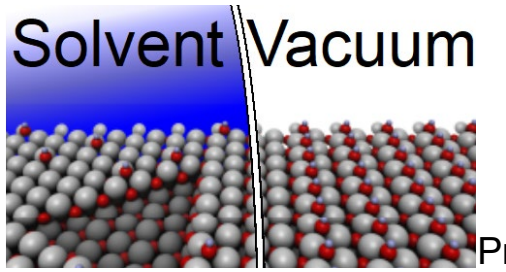
BSc, Master @Yonsei	PhD@MPIE	Postdoc@MPIE	Research fellow @ICL	Senior researcher @KRICT
Materials Theory Group Prof. Soon	Computational Materials Design Prof. Neugebauer		Materials Design Group Prof. Walsh	Chemical Data-Driven Research Center
Nanomorphology	Environment-dependent surface stability	Semiconductor surface/defect	High-throughput @ data-driven research	AI-driven autonomous experimentation

Computational materials science



Self-introduction Research path

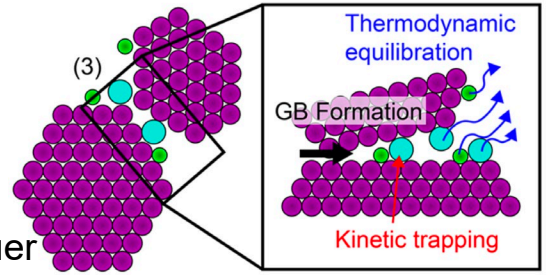
Environment-dependent surface stability



MPIE
Prof. Neugebauer

Phys. Rev. Lett. 120, 066101 (2018)
Editor's suggestion

Impurity incorporation in metal nanostructures

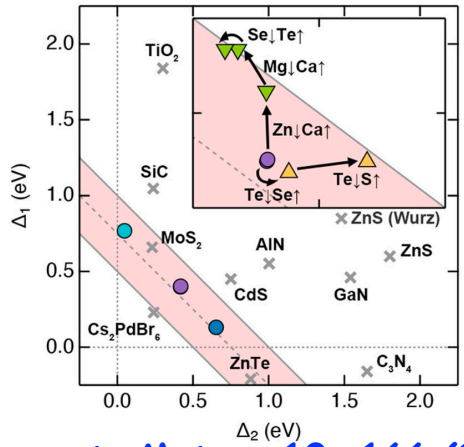


Korea Univ.
Prof. Seho Kim

MPIE
Dr. Gault

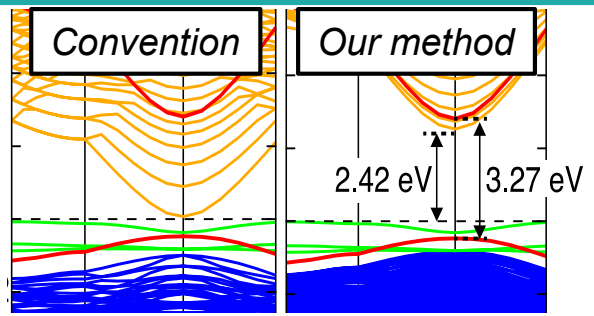
Adv. Mater. 2203030 (2022)
JACS 144, 2, 987 (2022)
New J. Phys. 24, 013008 (2022)

Data-driven research



npj Comput. Mater. 10, 166 (2024)
J. Phys. Chem. Lett. 15, 6451-6457 (2024)

Computational method development

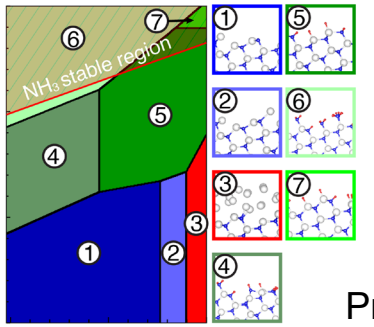


npj Comput. Mater. 7, 58 (2021)
Phys. Rev. Mater. 5, 044605 (20

Finalists in the Gerhard Ertl Award 2022

High-throughput research

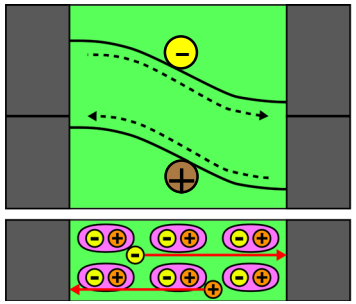
UCSB
Prof. Van de Walle



U. Crete
Prof. Lymperakis

On-going project (2024)

Next-generation photovoltaic materials



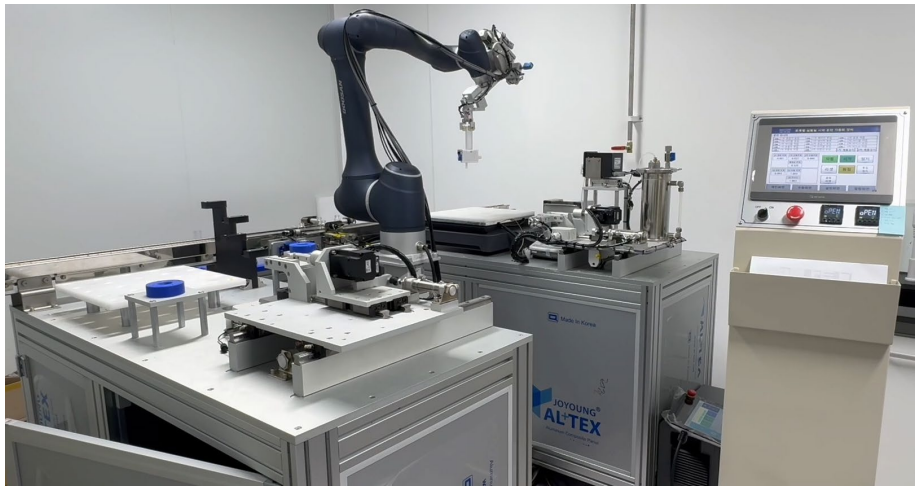
Prof. Walsh

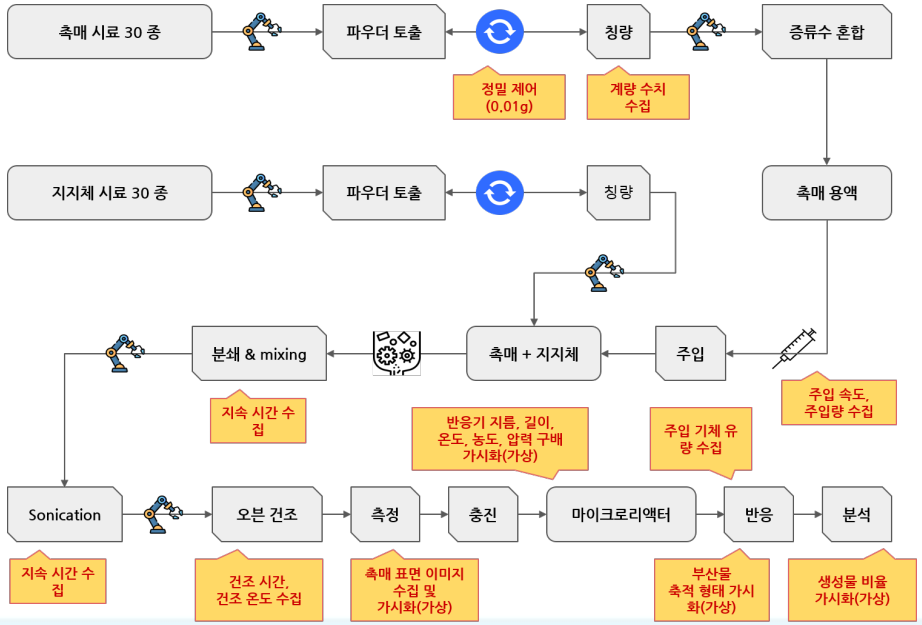
Energy for Future (MSCA co-funded) fellow

KRICT

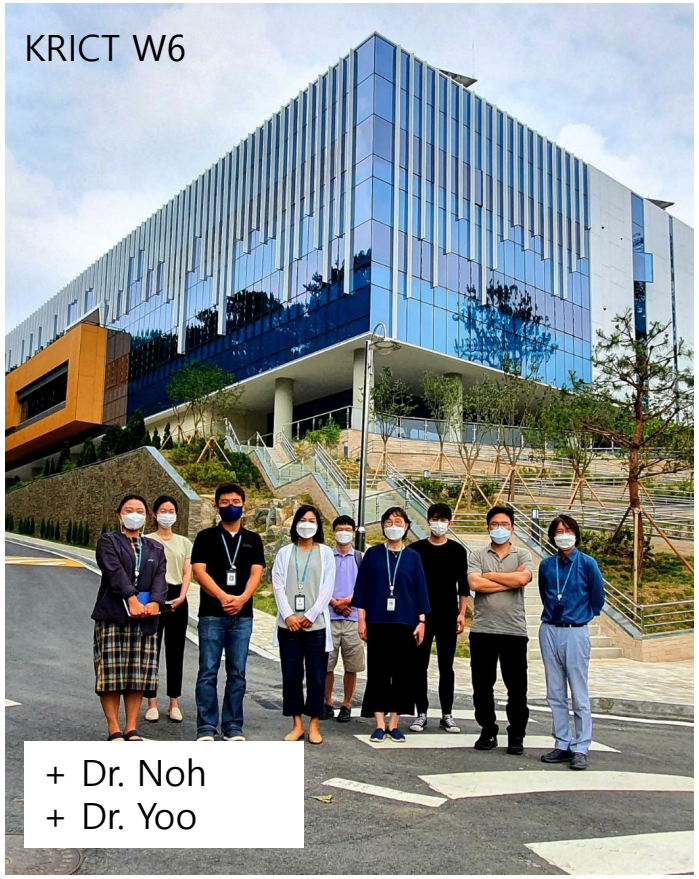
Autonomous lab KRICT K2030 project

- **Design catalysts using AI and intelligent robots**
  - 5 years project
  - Accumulate experimental data and design optimized experiments with AI
  - Tech. for dealing with powders and solutions, constructing database, and machine-learning research





1 Key Research Area

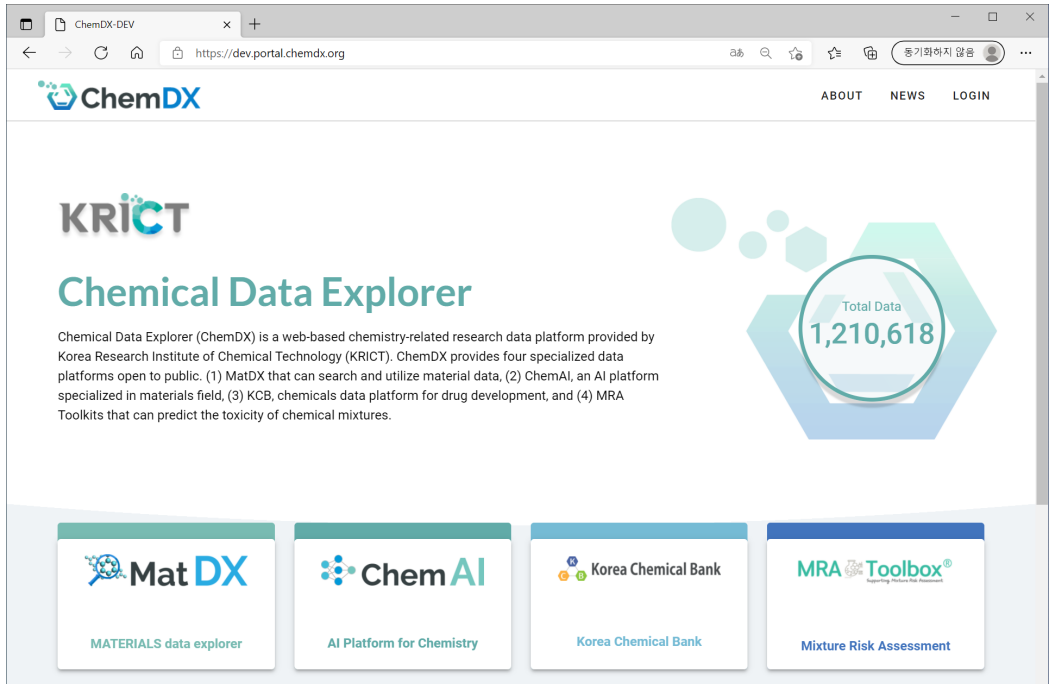


- **Building a Big Data Platform for Chemical Materials**
  - Development of a platform for utilizing chemical materials data
  - Collection and utilization platform for material data
  - Development of a web-based artificial intelligence platform
- **Research on Data-Driven Material Development**
  - Development of material property prediction technology using artificial intelligence
- **Research on Simulation-Based Material Development**
  - Prediction and analysis of material properties using computer simulations

CDDRC Chemical Data-Driven Research Center

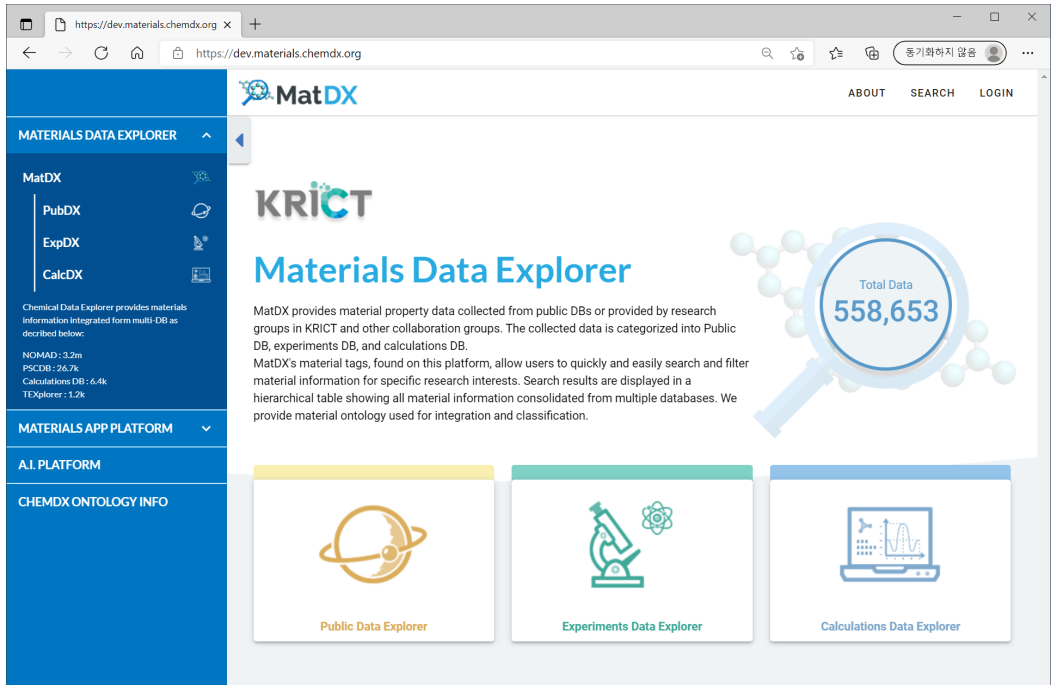
2 ChemDX (Chemical Data Explorer) https://chemdx.org

- Integrated Platform for Chemical Material Data
- Chemical material data search
- Compound library, Web-based machine learning, Compound bank, Compound toxicity data

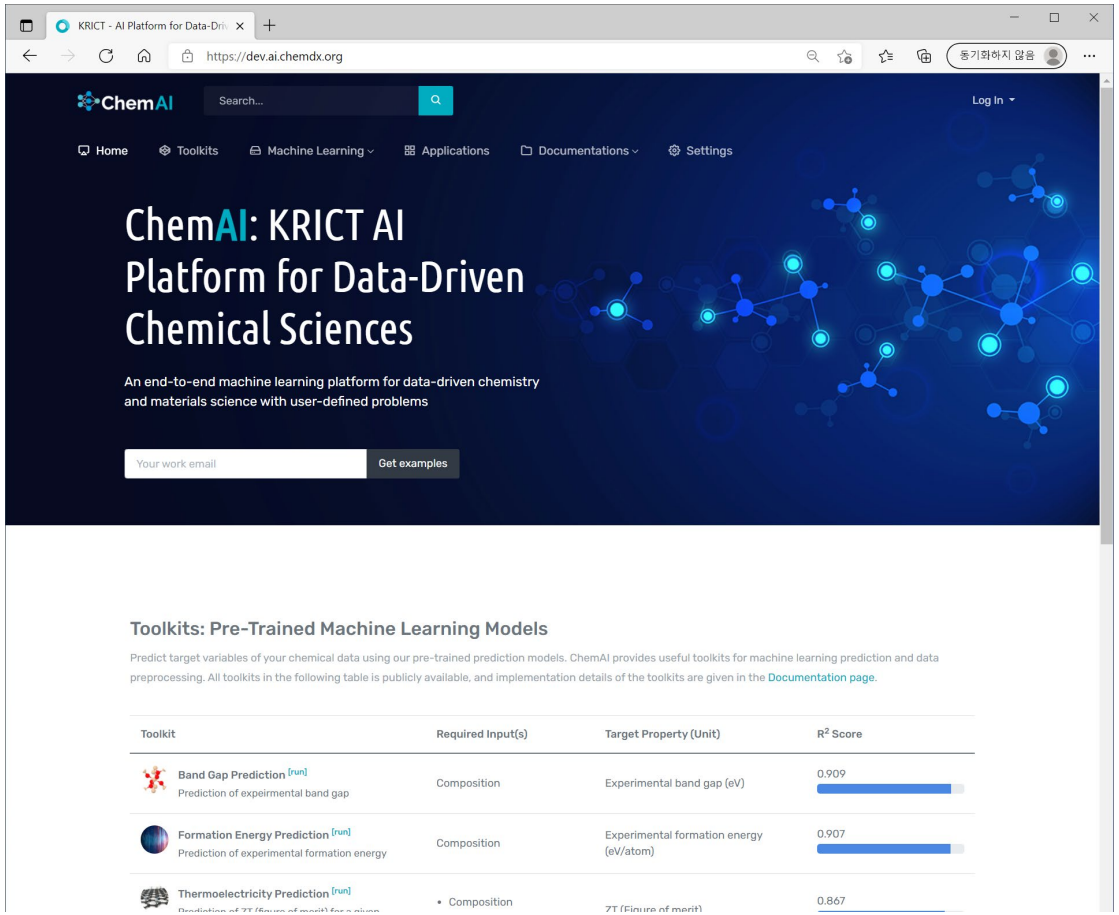


3 MatDX (Materials Data Explorer)

- Public DB: NOMAD, Materials Project, continuously expanding
- ExpDB (to be public): Experimental data on material properties, standard material analysis data, compound toxicity data
- CalcDB: DFT calculation data



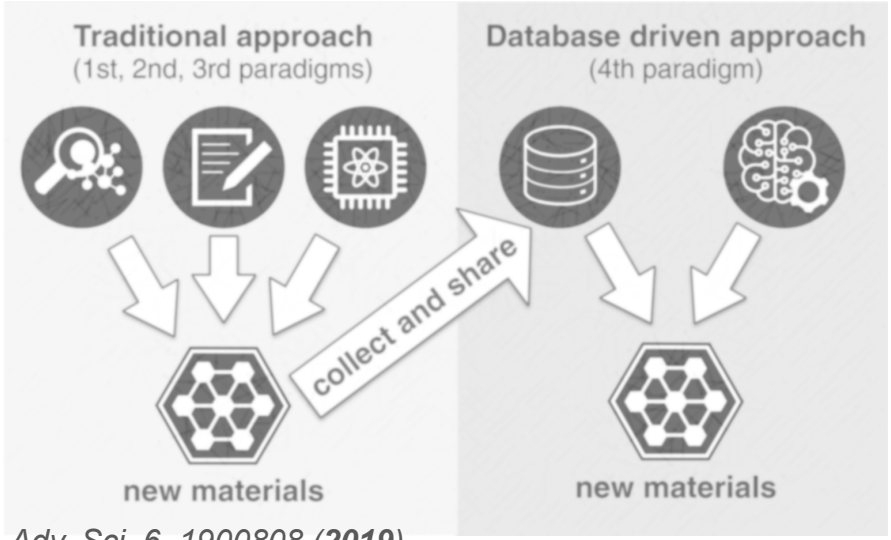
4 ChemAI: AI Platform for Chemistry



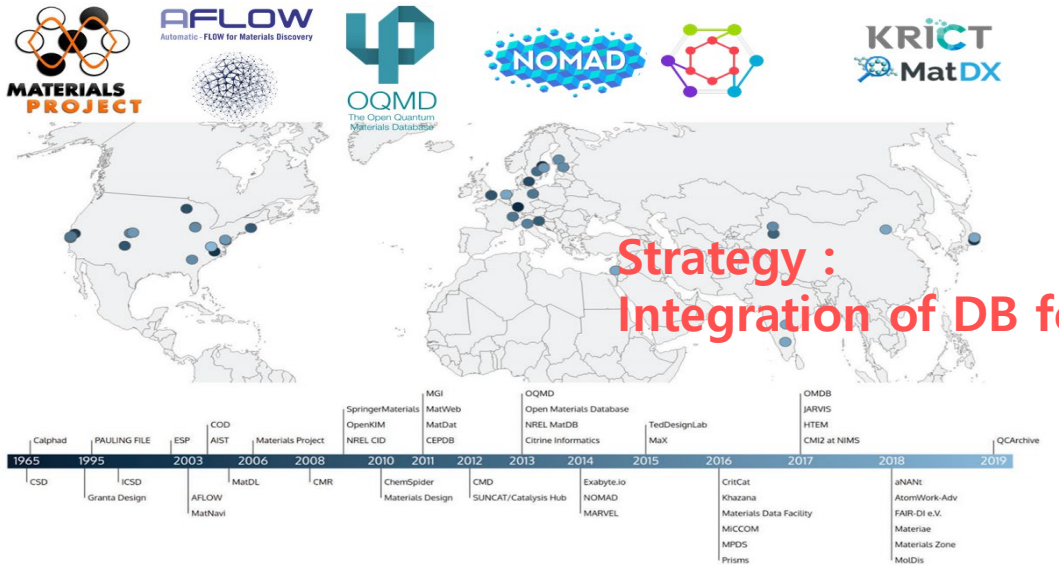
5 Data-driven research

- Machine Learning
  - Provides a platform for generating machine learning prediction models using user data
  - Supports various types of user data (chemical composition, molecular structure, crystal structure)
  - Provides example data
- Toolkits
  - Machine learning prediction tools developed by KRICT are available publicly and continuously expanding

ChemDX & MatDX Purpose and vision



*Adv. Sci. 6, 1900808 (**2019**)*



Strategy :
Integration of DB for Community

The question:

"Why do we need to integrate data repositories?"

which also means,

"What kind of benefits there are if we do integration of data repositories"

"We would like to construct a dataset including all the materials information including properties, applications, input data in the materials science field"

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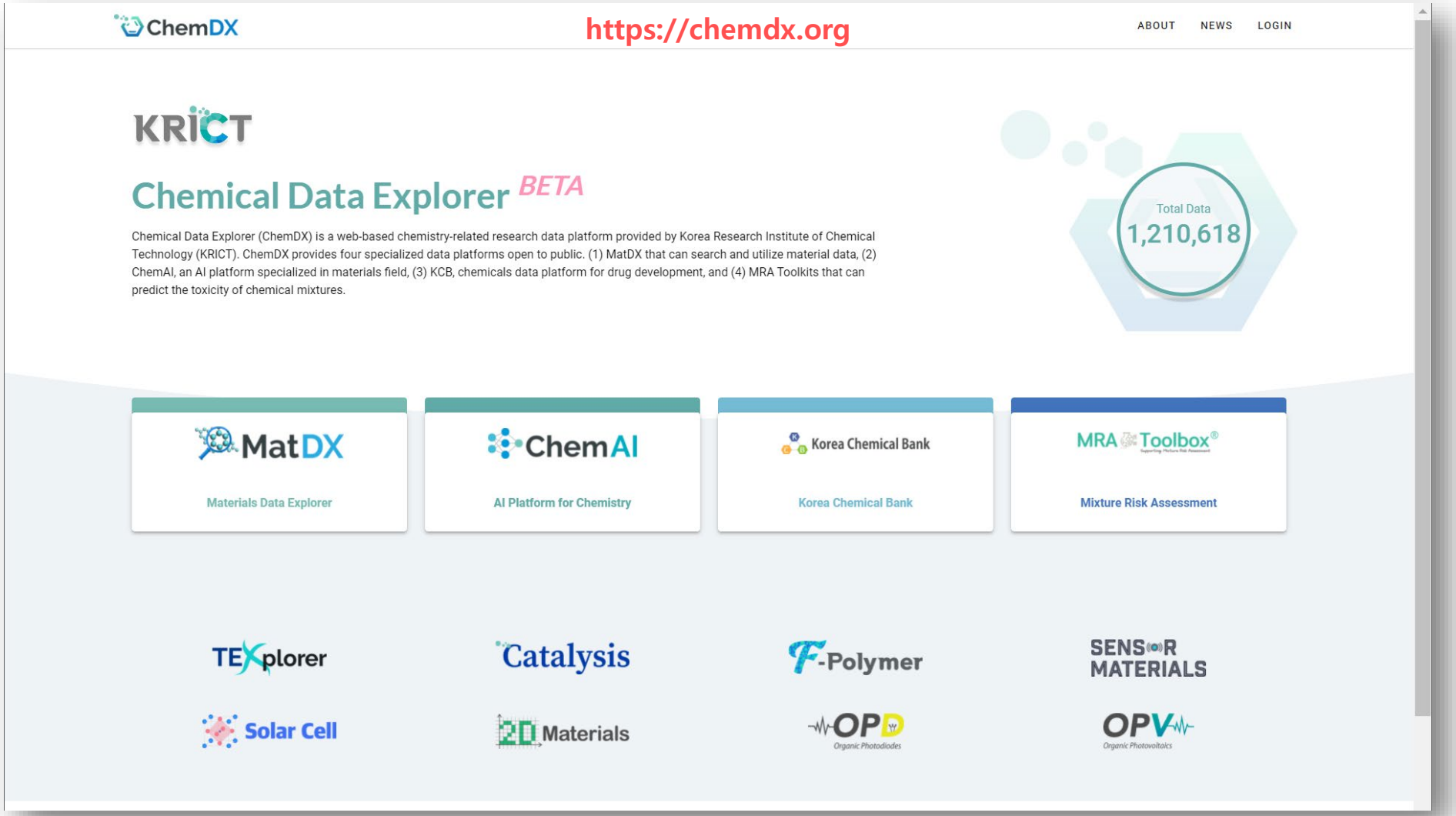
ChemDX & MatDX



ChemDX & MatDX Structure

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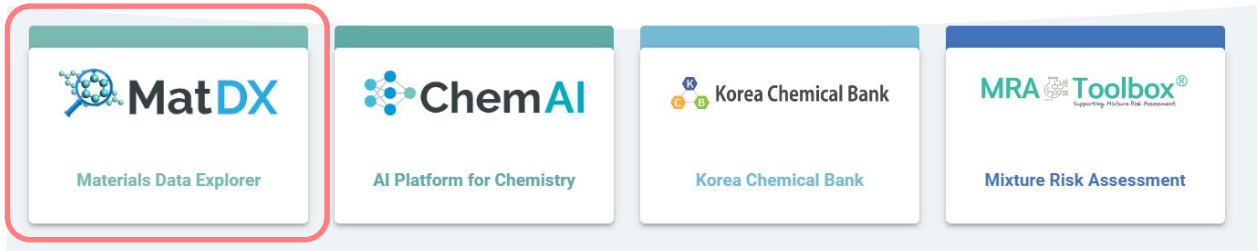
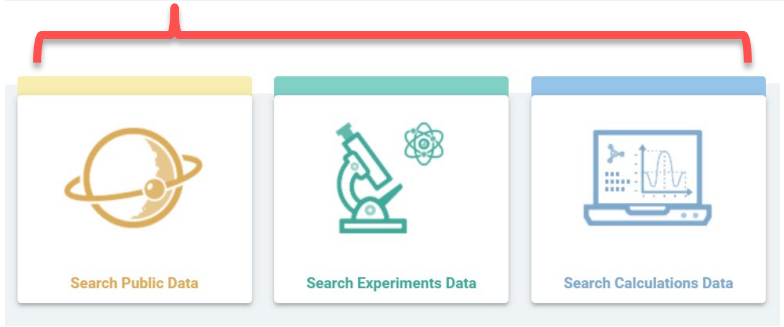
Chemical Data Explorer *BETA*

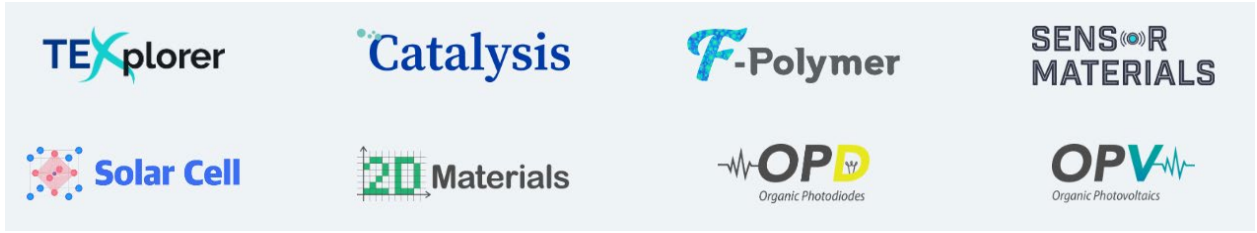


Materials Data Explorer *BETA*



Experimental Data Explorer ExpDX *BETA*

Materials Applications



KRICT

ChemDX Hackathon Purpose and vision

- ChemDX in beta version: aiming to gather professional feedbacks to move closer to a public release.

- The main goal of this hackathon is to receive expert/general opinions:
  - Development of general ML models using ChemDX-MatDX data
  - Creative features for data visualization (API) to enhance data interaction
  - UI/UX improvement suggestions to refine user experience
  - Feedback on database usage (particularly for MatDX, SolarCell, and 2D Materials data)
- Freely share your ideas while using DBs and developing your ideas
- Task examples will also be provided to guide discussions.
- We plan to use the outcomes from this hackathon to make meaningful improvements to KRICT's database

Day 1	Day 2	Day 3
• Morning: Fresh talk & Team formation • Lunch • Afternoon: Development • Dinner: (한우천국: 0507-1349-1140) walk within 10min	• Morning: Development • Lunch • Afternoon: Development • Dinner: (더함뜰: 0507-1402-9294) walk within 15min	• Morning: Presentation & Evaluation • Lunch • Afternoon (~3-4PM): Award ceremony • Dinner: (더함뜰: 0507-1402-9294) walk within 15min

Hackathon Guidelines

- Team Composition
  - ➢ Teams of 2-3 members, formed through 1-2 minute introductions
- Project Topics
  - ➢ Choose freely after exploring ChemDX or select from the example sets
  - ➢ Apply your skill for machine learning, data visualization, or UI/UX enhancements to ChemDX datasets
- ChatGPT account
  - Free to use only for the hackathon (https://chatgpt.com/)
  - ID: syoo.gpt@gmail.com
  - PW: gpt.syoo123
  - Available only during the hackathon
- Communication
  - ➢ Use GitLab issue tracker for questions or support

Project examples

Modeling Tasks

MatDX: ML model to predict formation energy of materials

LitDX - TE: ML model to predict properties of thermoelectric materials (e.g., seebeck coefficient)

Solar cell: ML model to predict fill factor, efficiency, V_oc, and J_sc

LitDX - IPO: Build ML model to predict properties of inorganic phosphoroptical properties (e.g., Emission max.)

Visualization Tasks

Develop functions for graphing and representing data, such as MatDX, SolarCell and LitDX

Develop Raman spectrum fitting fun ctions using data from Sensor Mater ials

UI/UX Improvement Tasks

Enhance visualization, improve webpage layout, add statistical analysis and Raman spectrum fitting for Sensor Materials

General Tasks

Identify and suggest specific improvements for user experience

Project Evaluation and Awards

Evaluation

Submit materials (syoo@krict.re.kr)

10-min presentation on the final day

PPT: explain your idea, work flow, data utilization, and how it works, etc

Source code: e.g., jupyter notebook, python file, etc

- Evaluation committe
  - KRICT: Dr. Jungho Shin
  - Yonsei University: Prof. Woosun Jang
  - Fordham University: Prof. Joshua Scrier

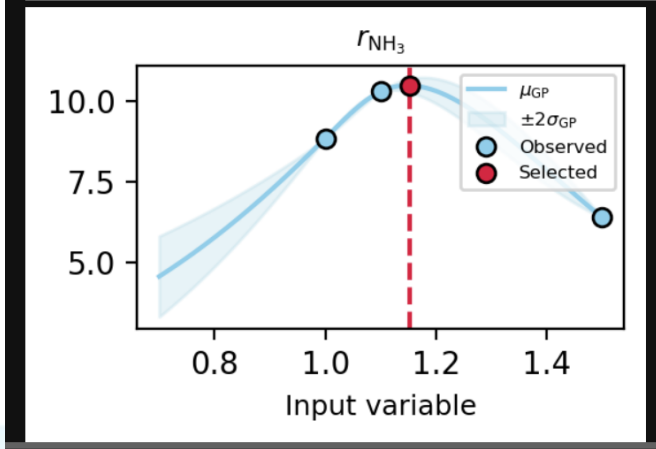
Bayesian Optimization for Composition Space Exploration

Guiding experimental catalyst design under the scheme of one-at-a-time of materials design

- Find next composition based on the Bayesian optimization
- Gaussian process (GP) regression implemented in scikit-learn with Matern(nu=1.5) kernel
- Kernel parameter is fixed, and therefore will not be optimized during training of GP model
- In current implementation, only one variable is used as input of GP

```
import numpy as np
import pickle
import pandas as pd

from scipy.optimize import minimize
from scipy.stats import norm

from sklearn.gaussian_process import GaussianProcessRegressor
from sklearn.gaussian_process.kernels import *

import matplotlib.pyplot as plt
```

```
plt.subplot(2,1,2)
plt.plot(x_grid,EI_grid,'-',c='skyblue',label='EI')
plt.plot(x,EI_train,'o',c='skyblue',mec='k',label='Observed')
plt.axvline(x_grid[np.argmax(EI_grid)],c='crimson',ls='--')
plt.plot(x_grid[np.argmax(EI_grid)],np.max(EI_grid),'o',c='crimson',mec='k',label='Selected')
plt.title('Expected Improvement',fontsize=9)
plt.xlabel('Input variable',fontsize=9)
plt.legend(loc='upper right',fontsize=6)
plt.tight_layout()

# Save figure
plt.savefig(filename_figure,dpi=200)
```



KRICT

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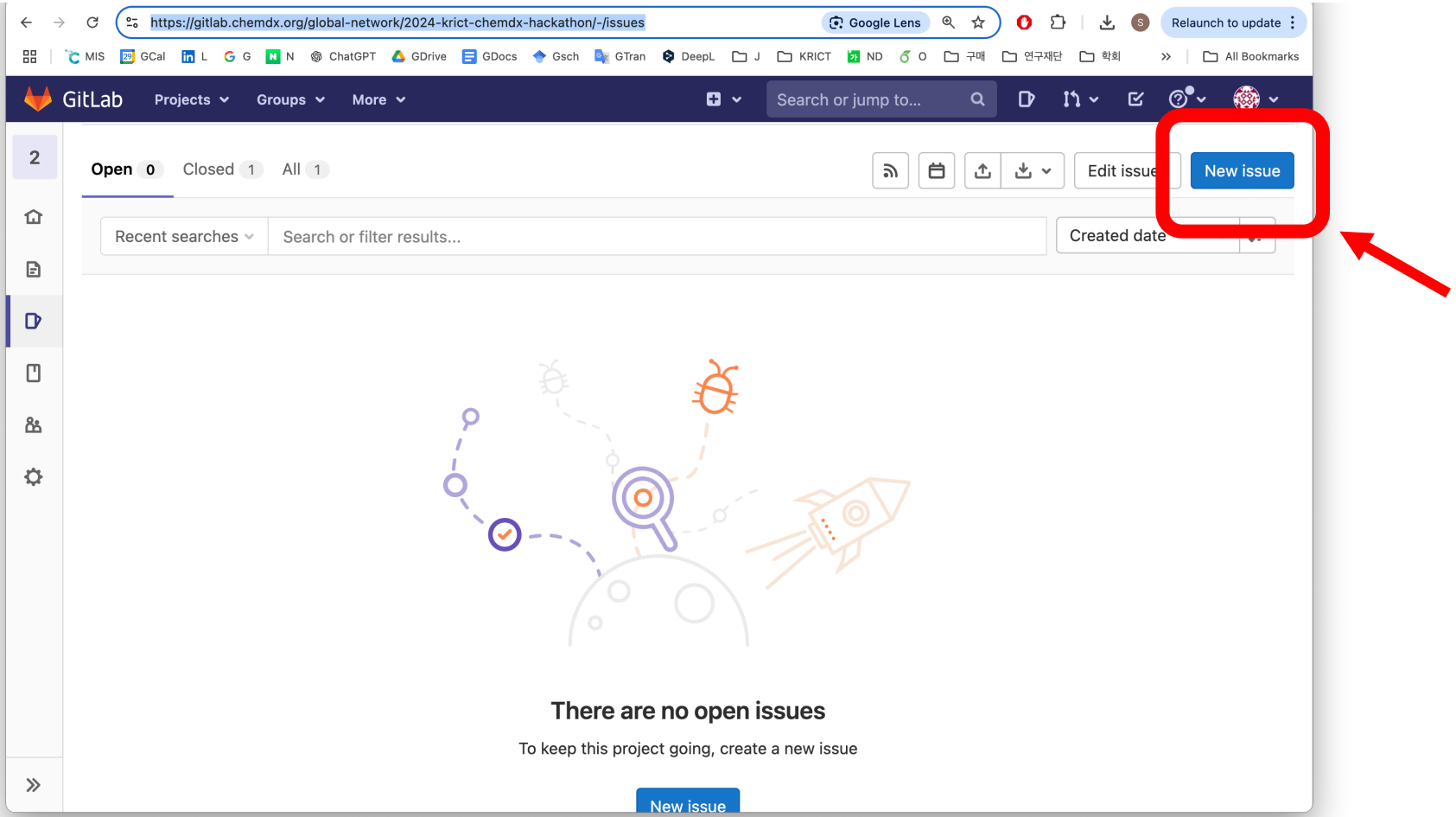
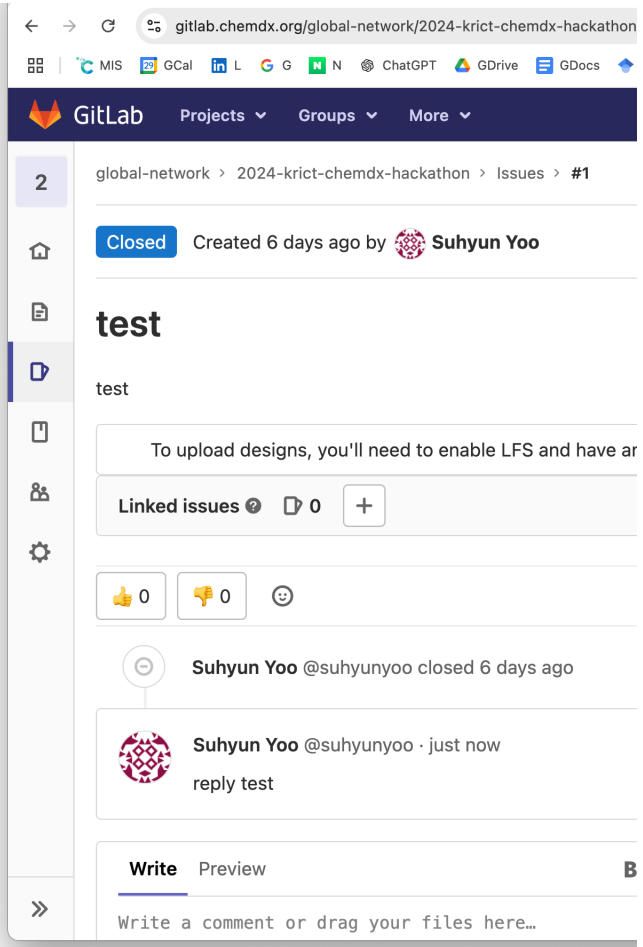
- Evaluation criteria

1. Data Utilization and completeness (30%):
   - ➢ How effectively did the team utilize the provided chemical and material property data?
   - ➢ How complete is the solution or prototype in addressing the problem within the given time?
2. Creativity and Innovation (40%):
   - ➢ How original and innovative is the proposed solution?
   - ➢ Did they present new perspectives and creative solutions for problem-solving?
3. Technical Feasibility (15%):
   - ➢ How well did the team overcome technical challenges and limitations?
4. Teamwork and Presentation (15%):
   - ➢ How effectively did the team collaborate with each other?

Q&A

- Use the GITLAB issue board
- https://gitlab.chemdx.org/global-network/2024-krict-chemdx-hackathon/-/issues





Project examples

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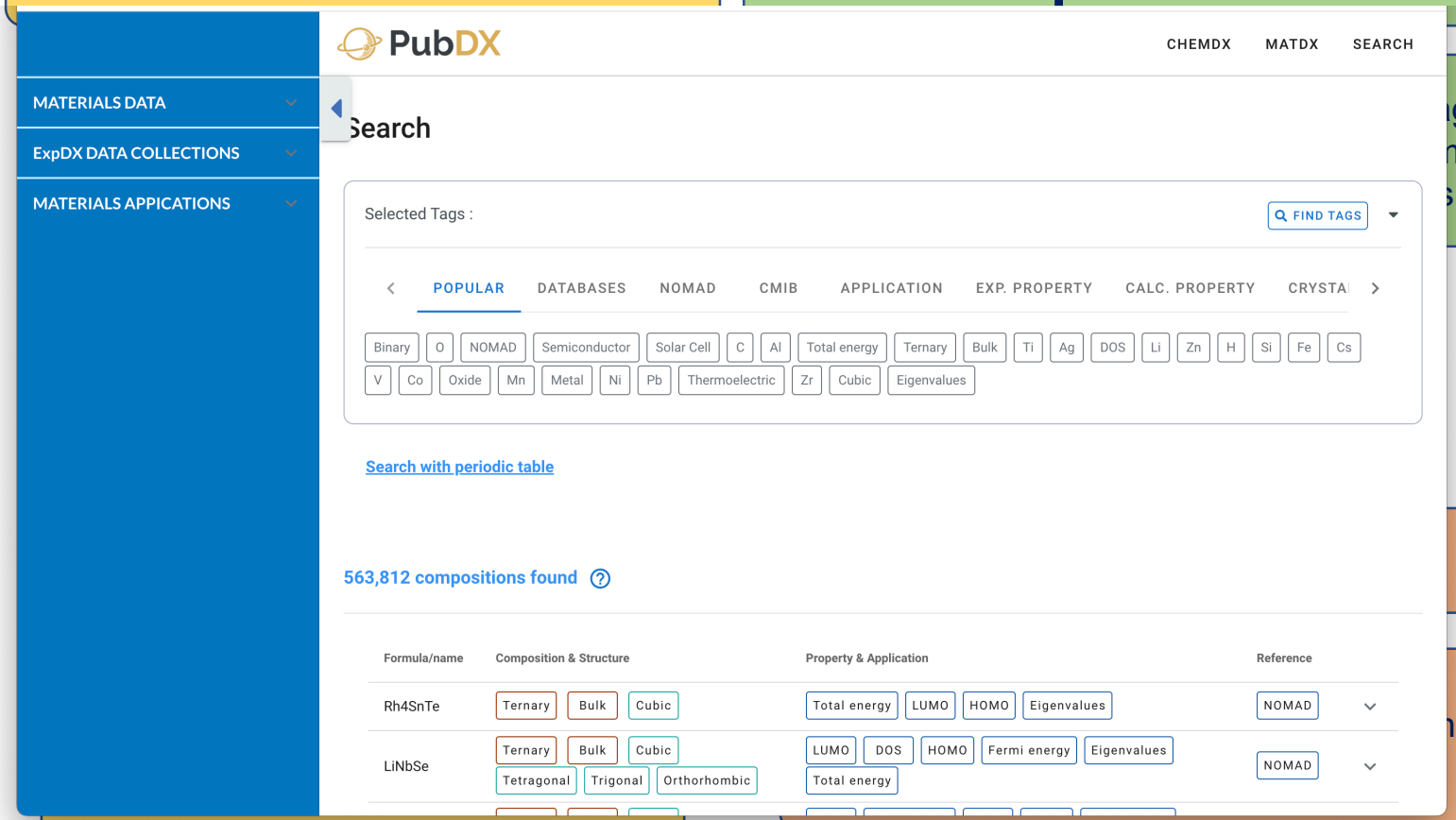
Visualization Tasks



UI/UX Improvement Tasks

Project examples

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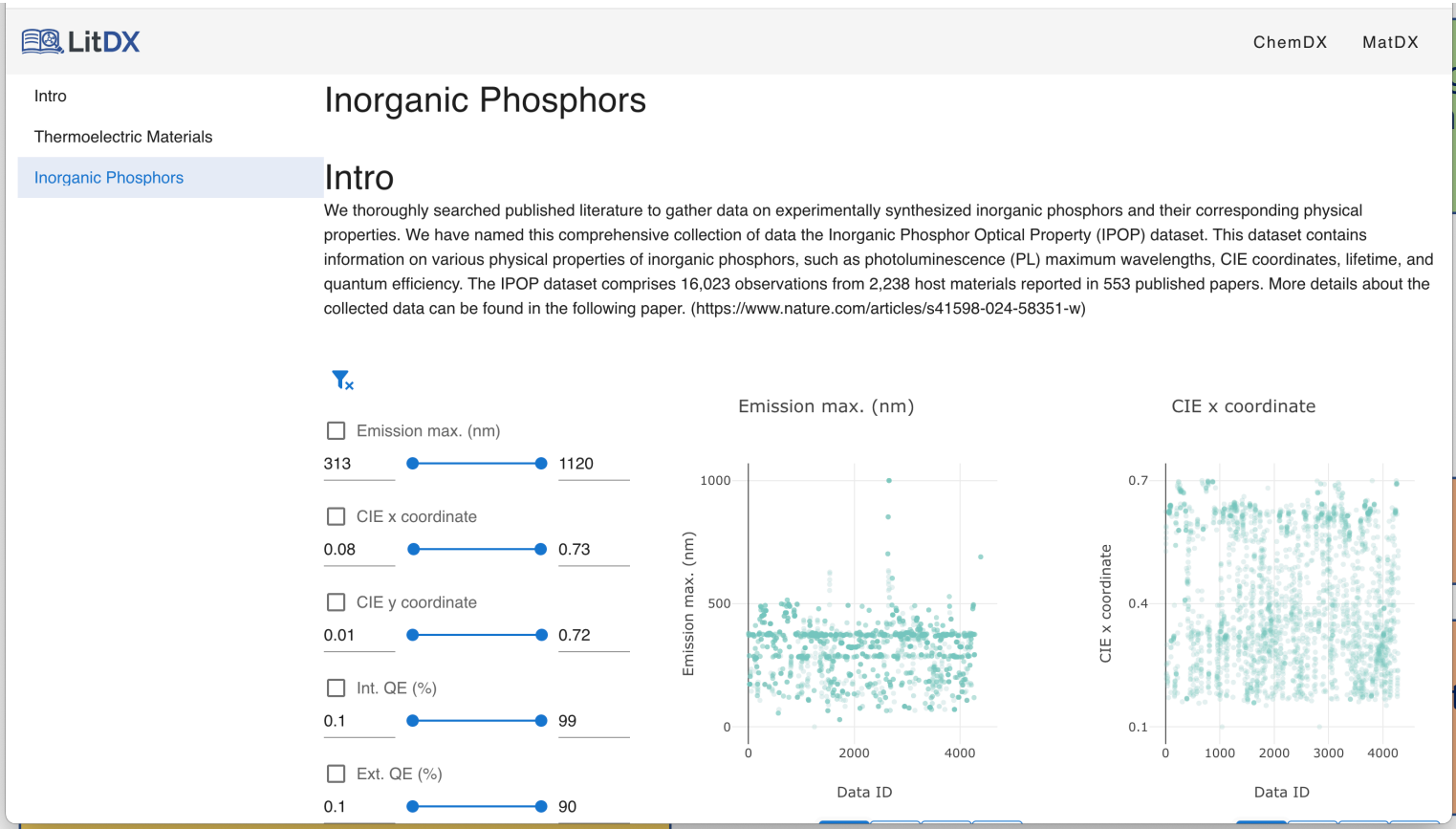

UI/UX Improvement Tasks

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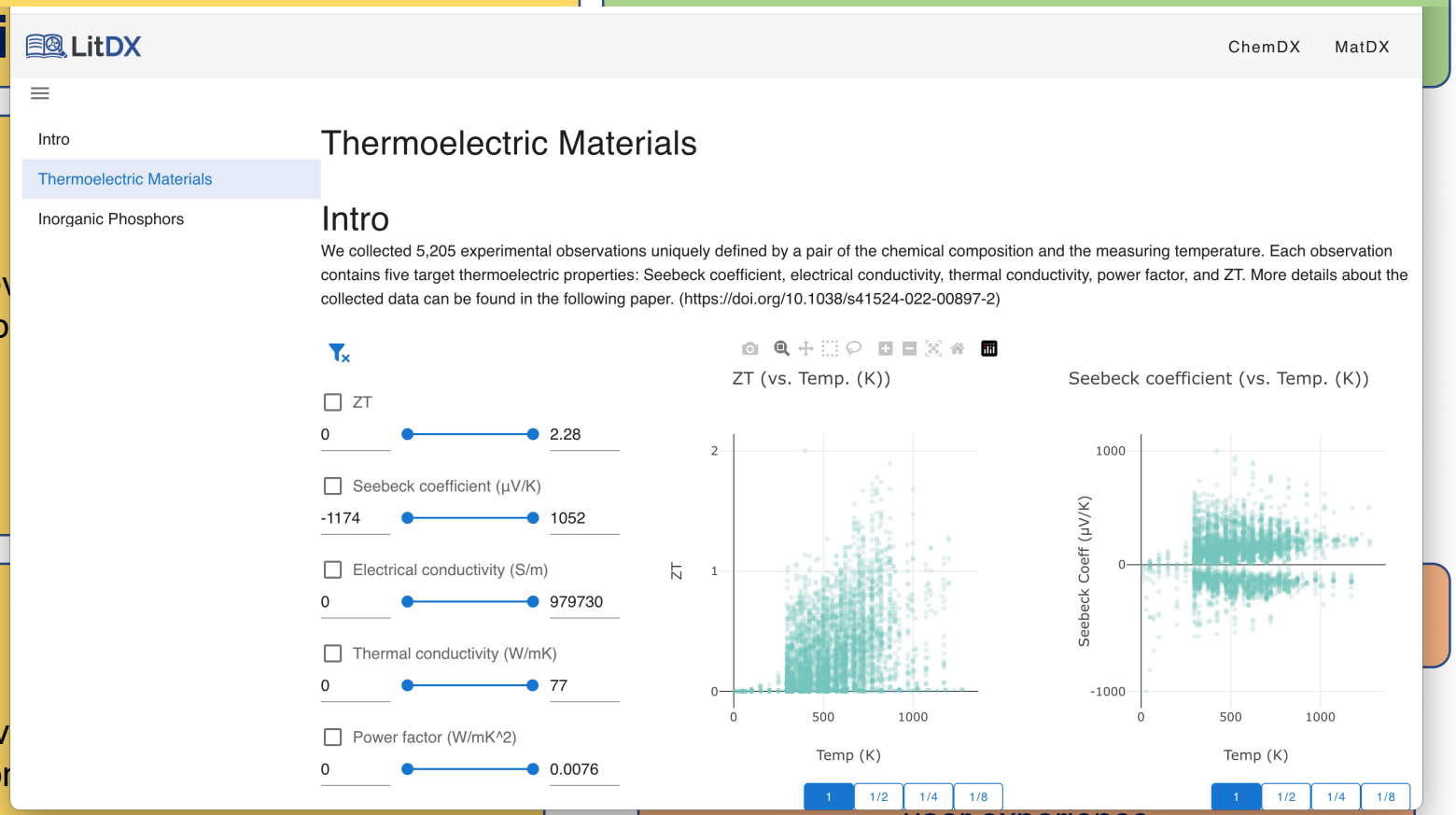

user experience

KRICT

Project examples

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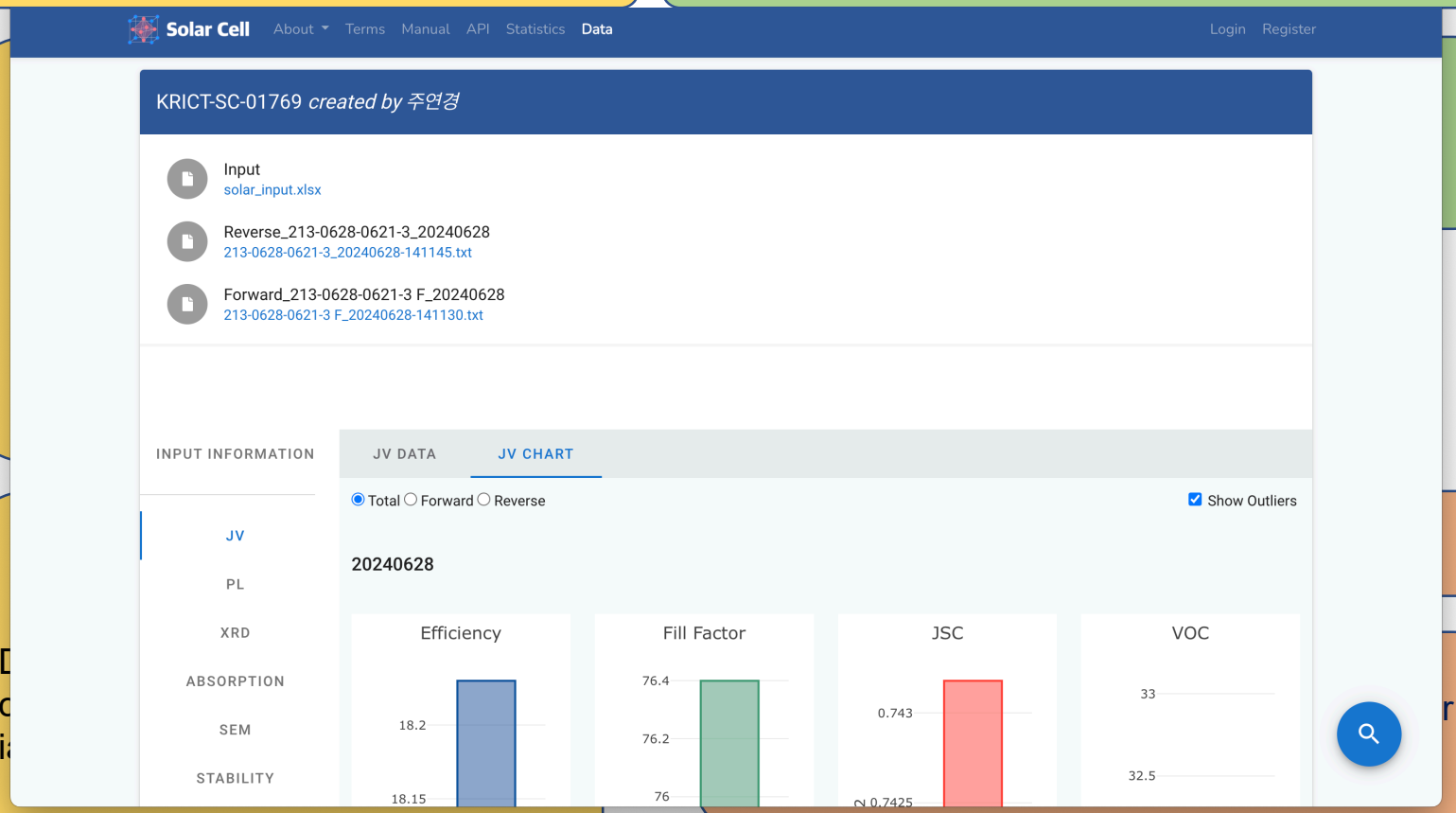


KRICT

Thank you
for your attention

KRICT

포럼

- 장소: 디딤돌플라자 강당
- 아침 이동: 온천교 704번
- 스트리밍 준비: 더에쓰시브이
- 다과: 케이터링 50인분
- 오전 세션 (장우선 교수 좌장)
- 점심: 성심당 도시락 40개 (교육장 48석)
- 오후 세션1 (손알로이시우스 교수 좌장)
- 오후 세션2 (김병현 교수 좌장)
- 저녁: 식당 추천?

- 5일 포럼 오후 행사 진행 서폿
- 포럼 점심 – 도시락 (40명 이상 참가시 구내식당 식권)
- 포럼 저녁 – 외부식당
- 포럼/해커톤 개회사 (원장님?)

- 클라우드 크레딧
- CPU서버

- 3명 한팀

해커톤

- 장소: S8-110 국립한밭대학교
- 아침 이동: 셔틀버스 8:28분 유성온천역 6번출구
- 행사장 준비: 더비엠씨 (박찬식)
- 다과: 유수현
- 개회사: 원장? 과기부?
- 오전
    - Fresh talk (인당 2분)
    - Project Intro (유수현 – 20분)
    - Teaming (30-60분)
- 점심: 도시락 (더비엠씨)
- 오후
    - Development
- 저녁: 한밭대 주변 한식당 (한우천국: 0507-1349-1140)
- 저녁 이동: 셔틀버스 18:10분 한밭대 주차장

- 장소: S8-110 국립한밭대학교
- 아침 이동: 셔틀버스 8:28분 유성온천역 6번출구
- 행사장 준비: 더비엠씨 (박찬식)
- 다과: 유수현
- 오전
    - Development
- 점심: 도시락 (더비엠씨)
- 오후
    - Development
- 저녁: 한밭대 주변 한식당 (더함뜰: 0507-1402-9294)
- 저녁 이동: 셔틀버스 18:10분 한밭대 주차장

- 장소: 디딤돌플라자 강당
- 아침 이동: 온천교 704번
- 행사장 준비: 더비엠씨 (박찬식)
- 다과: 케이터링
- 오전
    - Presentation & Evaluation
- Eval. Committee: Dr. Shin, Prof. Jang, Prof. Schrier
- 점심: 도시락 (더비엠씨), 3층 교육장
- 오후
    - 시상 (최우수: 아이패드 3개, 상장 / 우수 2팀: 에어팟프로 3개씩, 상장)
- 저녁 이동: 704번 한국화학연구원 정류장

Code

```
[33]: import numpy as np
from scipy.optimize import curve_fit
import matplotlib.pyplot as plt
import pandas as pd

# Function to calculate the Gaussian with constants a, b, and c
def gaussian(x, a, b, c,d):
    return a*np.exp(-np.power(x - b, 2)/(2*np.power(c, 2)))+d

# ref: https://mathworld.wolfram.com/LorentzianFunction.html
def lorentzian(x,a,b,c,d):
    return 0.5*c*a/np.pi/(np.power(x - b,2)+np.power(0.5*c,2)) + d

rawdata=pd.read_csv('./화학연구원 과제_데이터 형식/cvd ws2 pl mapping data_pl-pos.txt', sep='\s+')

range_cutting_start=400
range_cutting_end=1200

raw_numpy=rawdata.to_numpy()
x=list(raw_numpy[:,0])

height=list()
center=list()
fullwidth=list()


pl_center_input1=630.0  # read from xls file
pl_center_input2=640.0
pl_cutoff_count_input=1000.0  # read from xls file

for i in range(1,rawdata.shape[1]):
    y=list(raw_numpy[:,i])


    pars, cov = curve_fit(f=lorentzian, xdata=x, \
                          ydata=y, \
                          p0=[10000, pl_center_input1, 10, pl_cutoff_count_input], \
                          bounds=(-np.inf, np.inf))

    height.append(2.0/np.pi/pars[2]*pars[0]+pars[3])
    center.append(pars[1])
    fullwidth.append(pars[2])

    #print(pars)
    #print(cov)
    #print(_2lorentzian(x[range_cutting_start:range_cutting_end],1000.0, pl_center_input1, 30.0, pl_cutoff

    plt.plot(x[range_cutting_start:range_cutting_end],y[range_cutting_start:range_cutting_end],'bo')
```

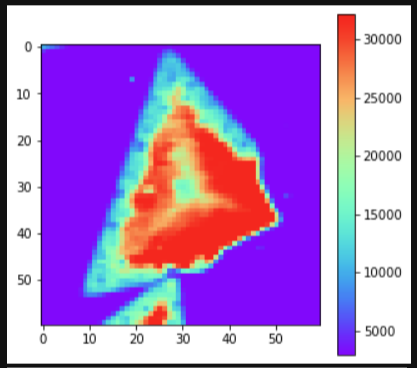
Code

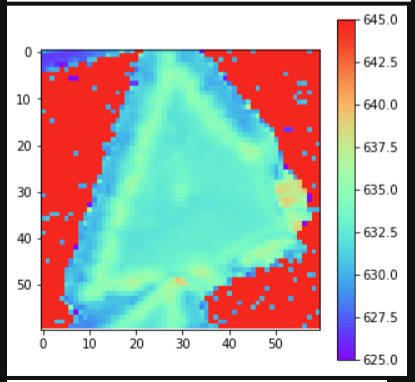
```
fig.show()



fig=px.imshow(center_matrix, zmin=center_min, zmax=center_max, color_continuous_scale='rainbow')
fig.update_layout(autosize=False, width=350, height=350)
fig.update_xaxes(showticklabels=False)
fig.update_yaxes(showticklabels=False)
fig.show()

fig=px.imshow(width_matrix, zmin=0, zmax=30, color_continuous_scale='rainbow')
fig.update_layout(autosize=False, width=350, height=350)
fig.update_xaxes(showticklabels=False)
fig.update_yaxes(showticklabels=False)
fig.show()
```





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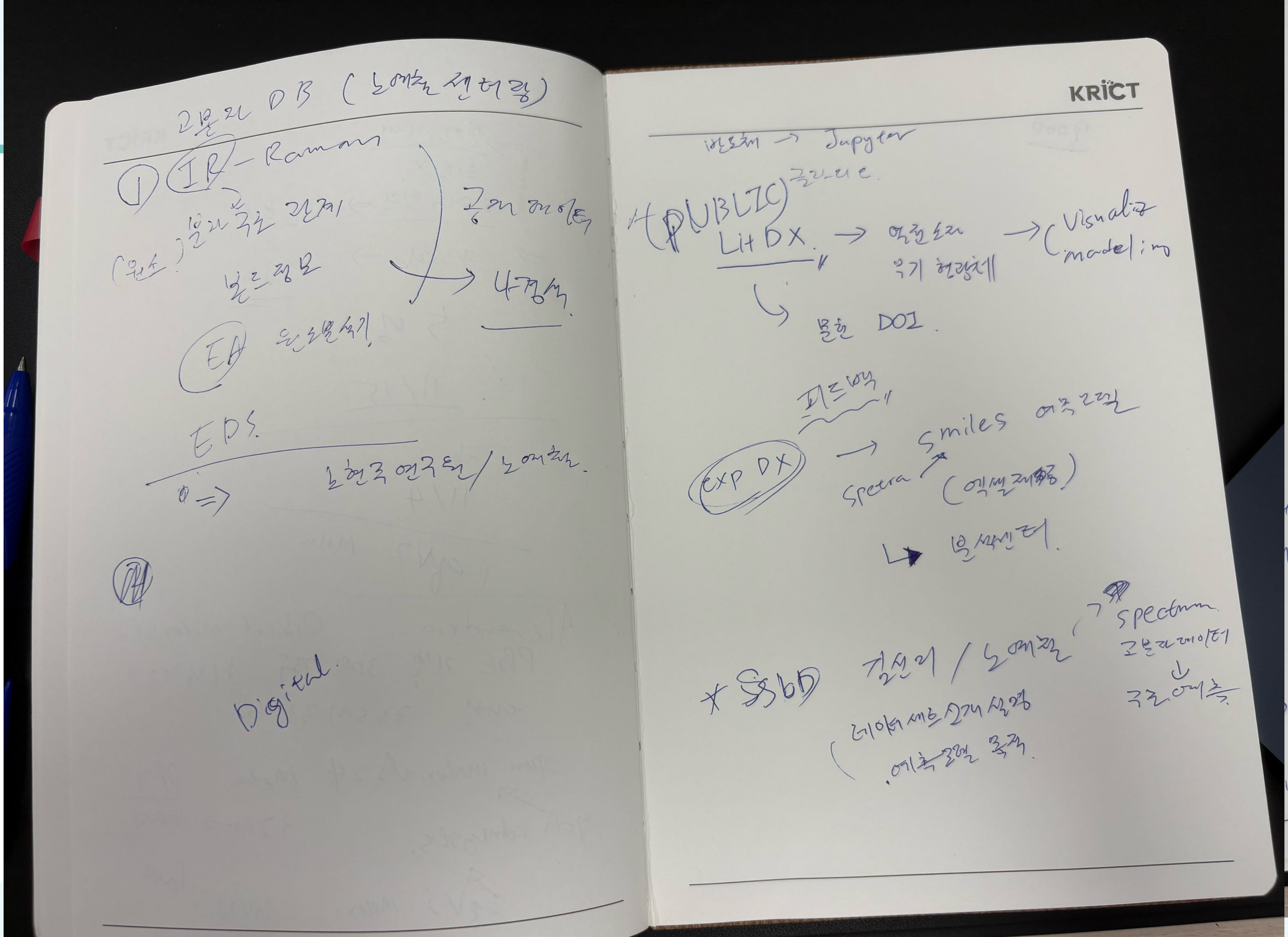

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