

Supplementary Information for

Expert-in-the-loop AI optimization of multicomponent quantum dots in complex synthesis space

First Author^{1,2*}, Second Author^{2,3†} and Third Author^{1,2†}

^{1*}Department, Organization, Street, City, 100190, State, Country.

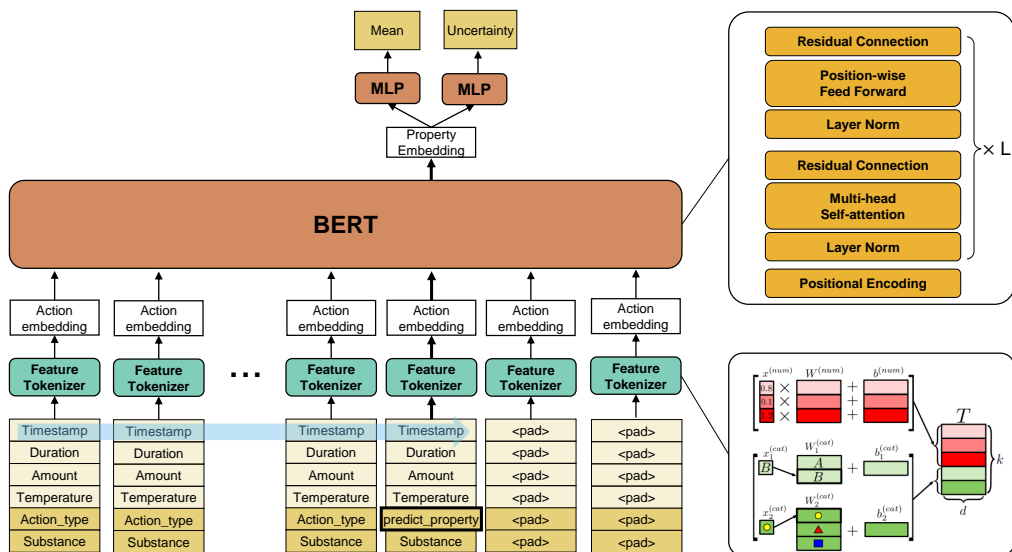
²Department, Organization, Street, City, 10587, State, Country.

³Department, Organization, Street, City, 610101, State, Country.

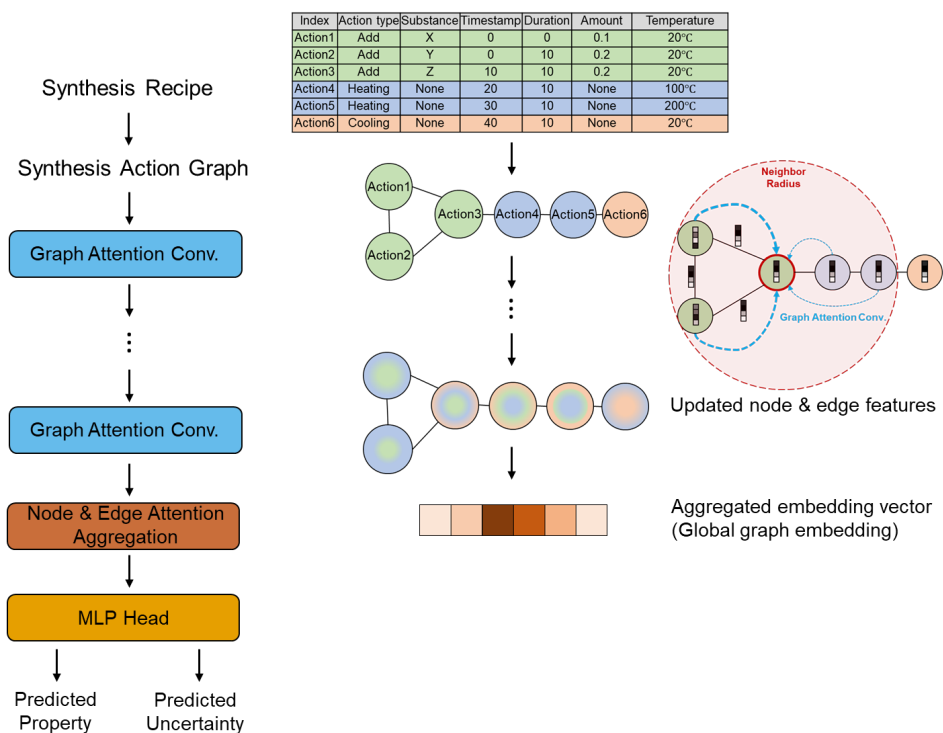
*Corresponding author(s). E-mail(s): iauthor@gmail.com;

Contributing authors: iauthor@gmail.com; iiiauthor@gmail.com;

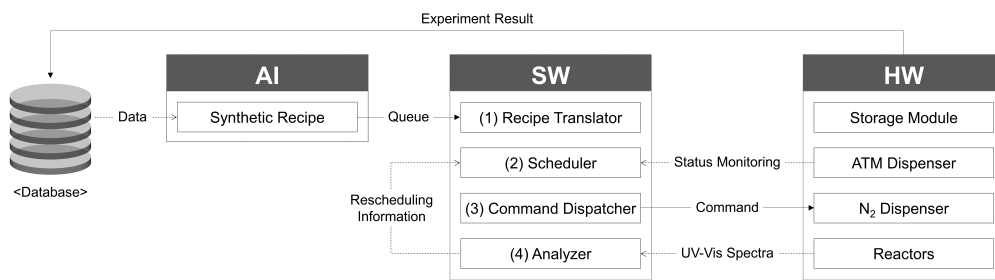
[†]These authors contributed equally to this work.



Supplementary Fig. 1 Transformer-based BERT architecture, which consists of repeated self-attention layers. To incorporate the QD synthesis recipe as an input, a feature tokenizer structure is introduced to embed action tokens. An MLP head is attached to predict the property values and their uncertainty. The configuration of the feature tokenizer is shown in previous literature¹.



Supplementary Fig. 2 The architecture of the GNN-style model. The GNN-style model takes a synthesis action graph represented from a synthesis recipe as input. The graph is encoded via graph attention convolution into an aggregated embedding vector. The resulting vector is then fed into an MLP head to predict the target properties and their uncertainties.



Supplementary Fig. 3 ARS system architecture.

References

1. Gorishniy, Y., Rubachev, I., Khrulkov, V. & Babenko, A. Revisiting deep learning models for tabular data. *Adv. Neural Inf. Process. Syst.* **34**, 18932–18943 (2021).

Supplementary Table 1 Examples of the precursor representation scheme used to enhance model learning. The scheme decomposes precursor information into distinct features, enabling more effective learning of recipe information.

	Subtype1	Subtype2	Subtype3	Solvent	Concentration
Precursor name	Main reagent name	Key element	Counterion, ligand	Solvent used	Molar concentration
0.5M Ag(Oac)/Oam ¹	Ag(Oac)	Ag	Oac	Oam	0.5
0.5M Ag(acac)/Oam ²	Ag(acac)	Ag	Acac	Oam	0.5
0.5M AgCl/TOP ³	AgCl	Ag	Cl	TOP	0.5
1M InCl ₃ /Oam	InCl ₃	In	Cl	Oam	1

¹ Ag(OAc): Silver acetate, Oam: Oleylamine

² Ag(acac): Silver acetylacetonate

³ TOP: Trioctylphosphine