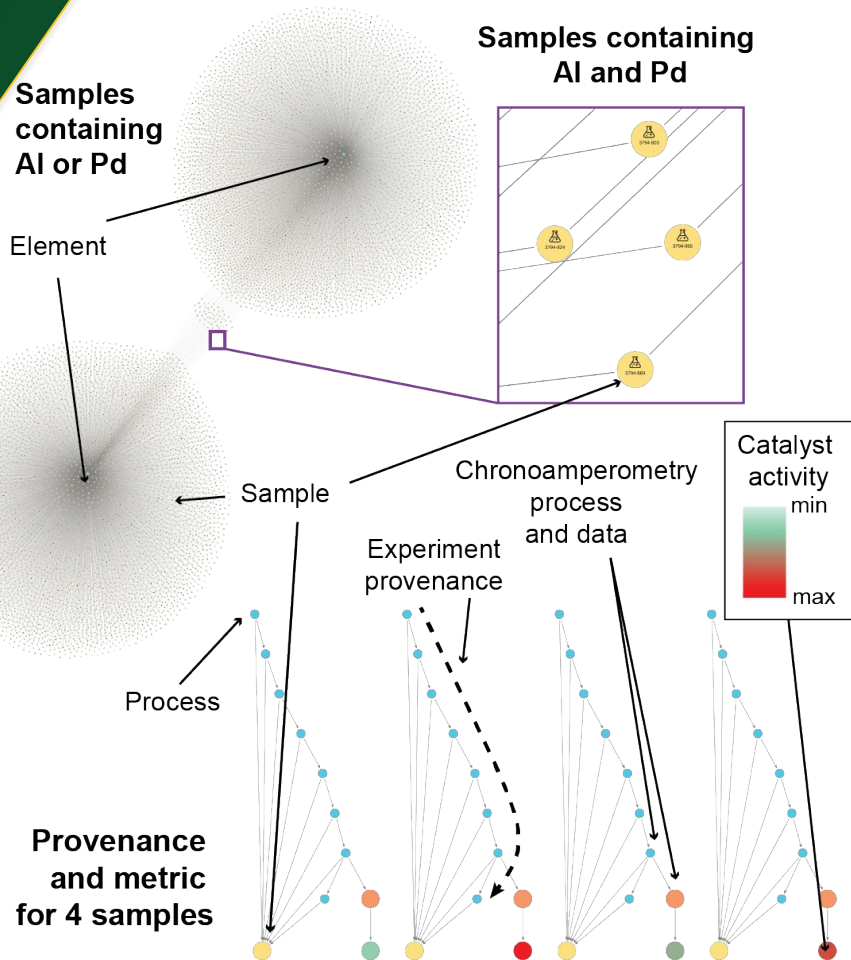


Elevating data management to knowledge representation



Scientific Achievement:

We have established the Materials Provenance Store (MPS), a materials and chemistry database focused on management of experiment provenance and metadata, which provides the basis for establishing the largest knowledge graph for experimental data, the Materials Experiment Knowledge Graph (MekG).

Significance and Impact:

As the materials and chemistry communities seek to capitalize on recent advancements in artificial intelligence, we must establish the appropriate representations of data, metadata, and ultimately scientific knowledge. The challenges are most apparent in experimental materials chemistry where observables depend on the full experiment provenance, which we addressed through the establishment of a database schema for provenance management and its translation into a knowledge graph that can scale to include billions of experiments.

Research Details:

- The MPS is based on high throughput experiments and contains 11 million materials and 2.5 million electrochemical experiments.
 - The knowledge graphs contains nodes for samples, processes applied to them, performance metrics, etc., with relationships enabling exploration by humans and computers.
- Rohr, B.; Guevarra, D.; Breeden, J.; Suram, S.; Gregoire, J. The Materials Experiment Knowledge Graph. ChemRxiv April 19, **2023**. <https://doi.org/10.26434/chemrxiv-2023-md55t>.
Statt, M. J.; Rohr, B. A.; Guevarra, D.; Suram, S. K.; Morrell, T. E.; Gregoire, J. M. The Materials Provenance Store. *Sci Data* **2023**, 10 (1), 184. <https://doi.org/10.1038/s41597-023-02107-0>.

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