

# Integrating AI into nanoHUB: Toward Intelligent and Connected Scientific Workflows

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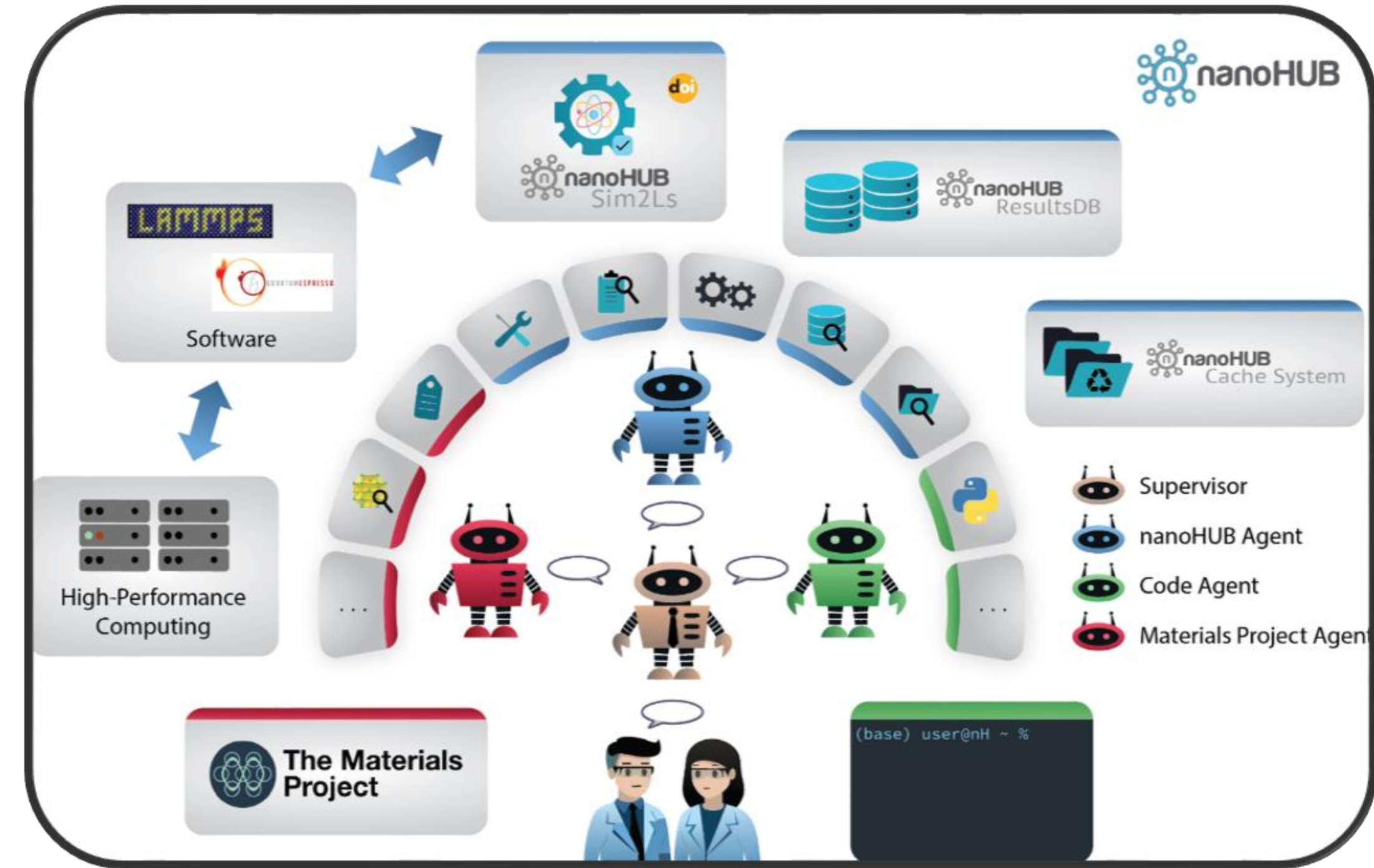
## MOTIVATION

AI is reshaping scientific collaboration by integrating distributed knowledge, automating reasoning, and guiding experimentation<sup>1,2,3</sup>.

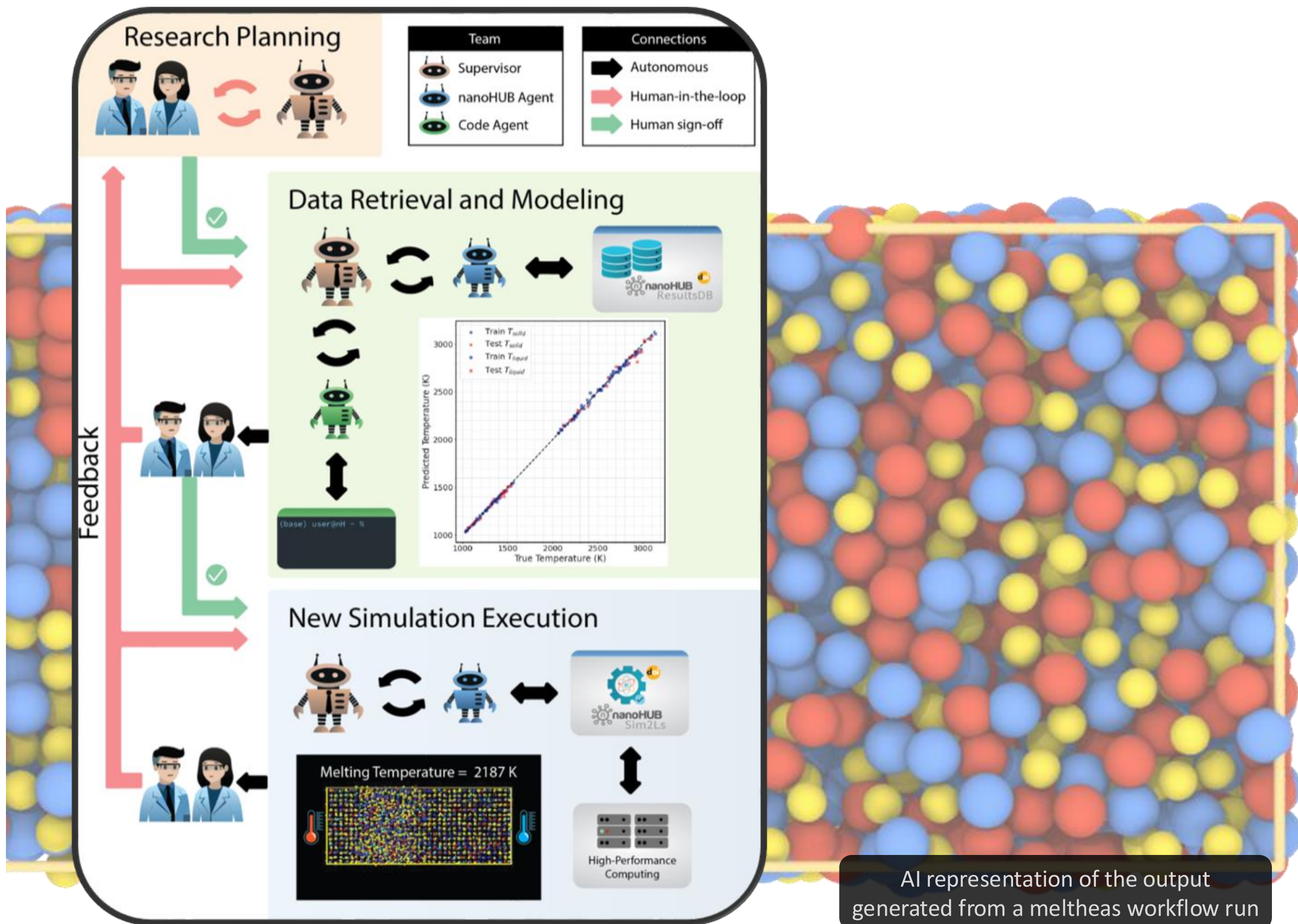
Integrating these technologies into nanoHUB<sup>4</sup> expands the platform’s role from hosting simulations, to enabling intelligent, data-driven workflows.

## AI-Driven Scientific Workflows

NanoRA is an agentic AI system that leverages a team of independent agents powered by LLMs to solve scientific endeavors.



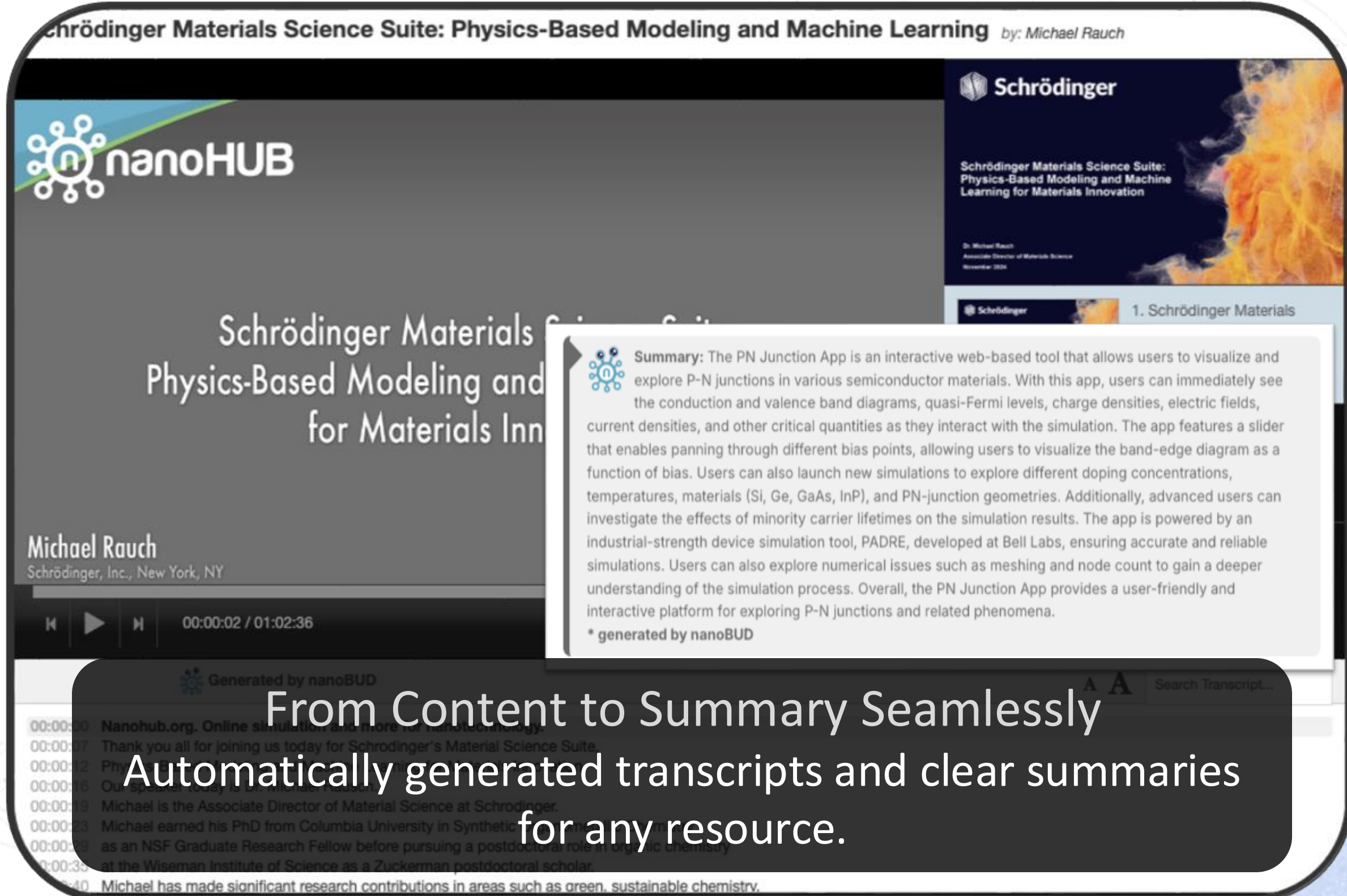
Each agent has its own tools to plan, select, and run scientific workflows. Powered by nanoHUB tools and the resultsDB, It uses standardized end-to-end simulation workflows with validated metadata and more than **1,500,000** stored simulation records.



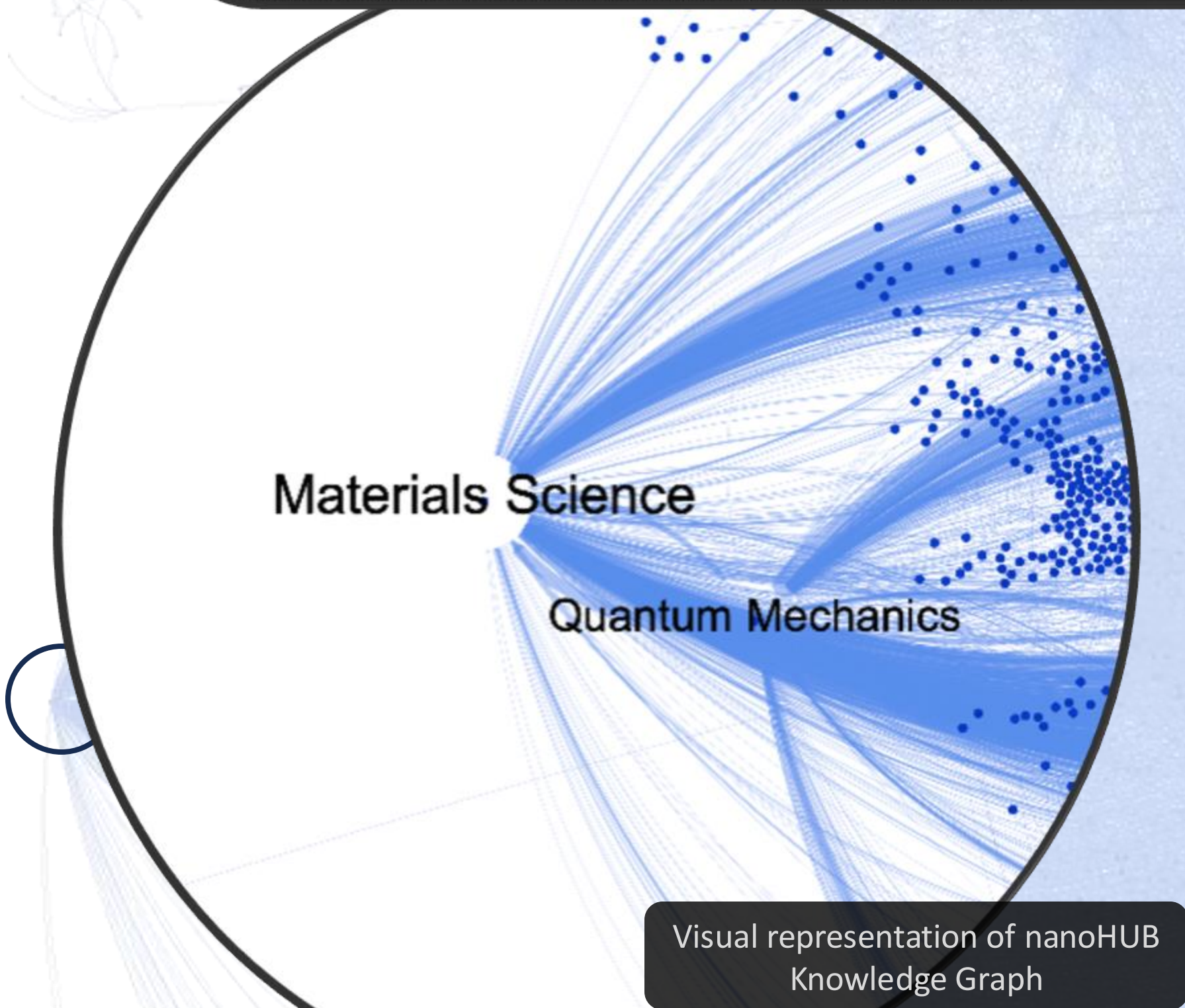
AI representation of the output generated from a meltheas workflow run

## AI-Enhanced Content Discovery

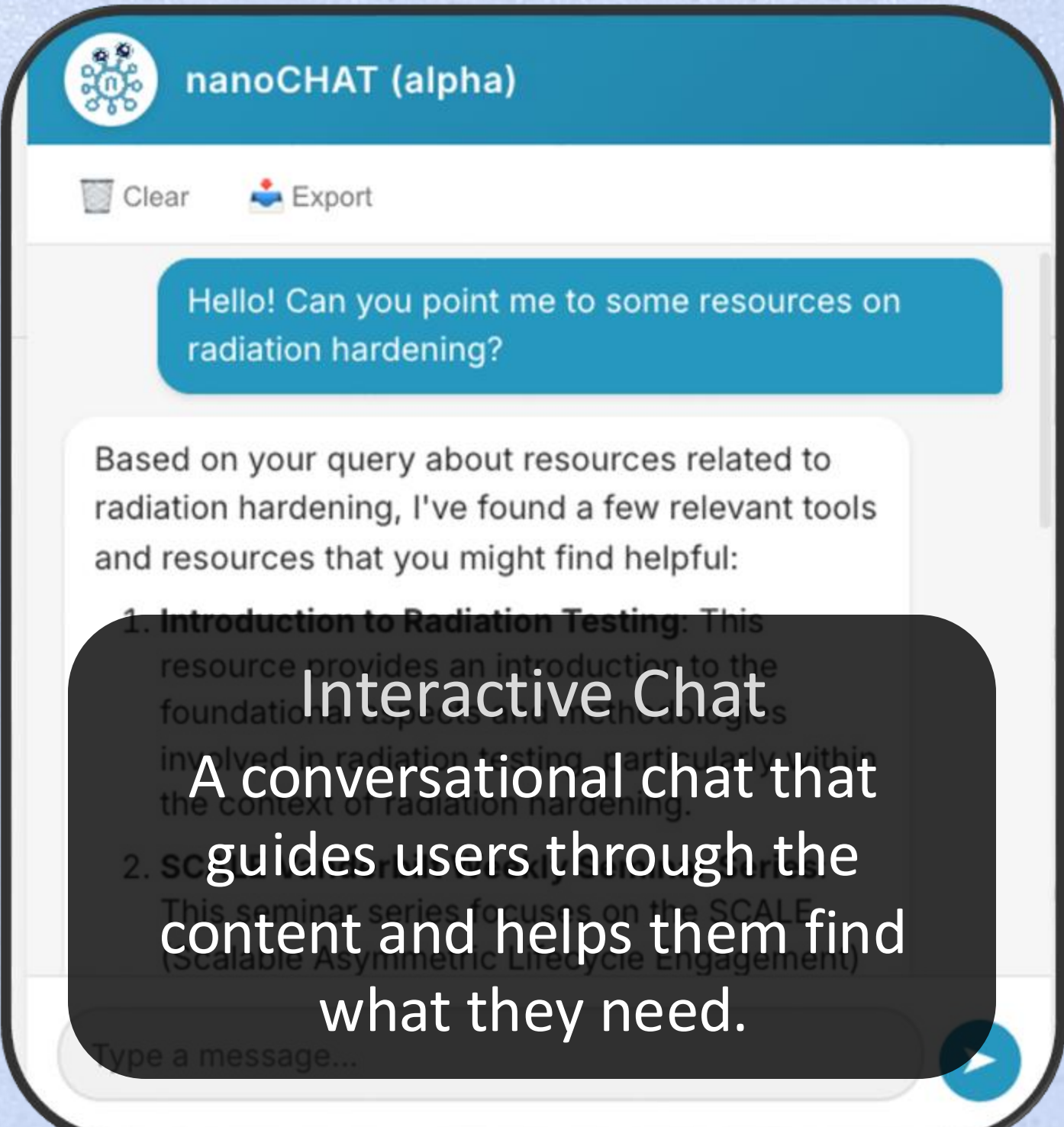
NanoBUD integrated AI-assisted features that processed more than **8,500** curated resources made up of videos, documents, and tools. It extracted transcripts, abstracts, and tags from content and built a knowledge graph with over **150,000** relations.



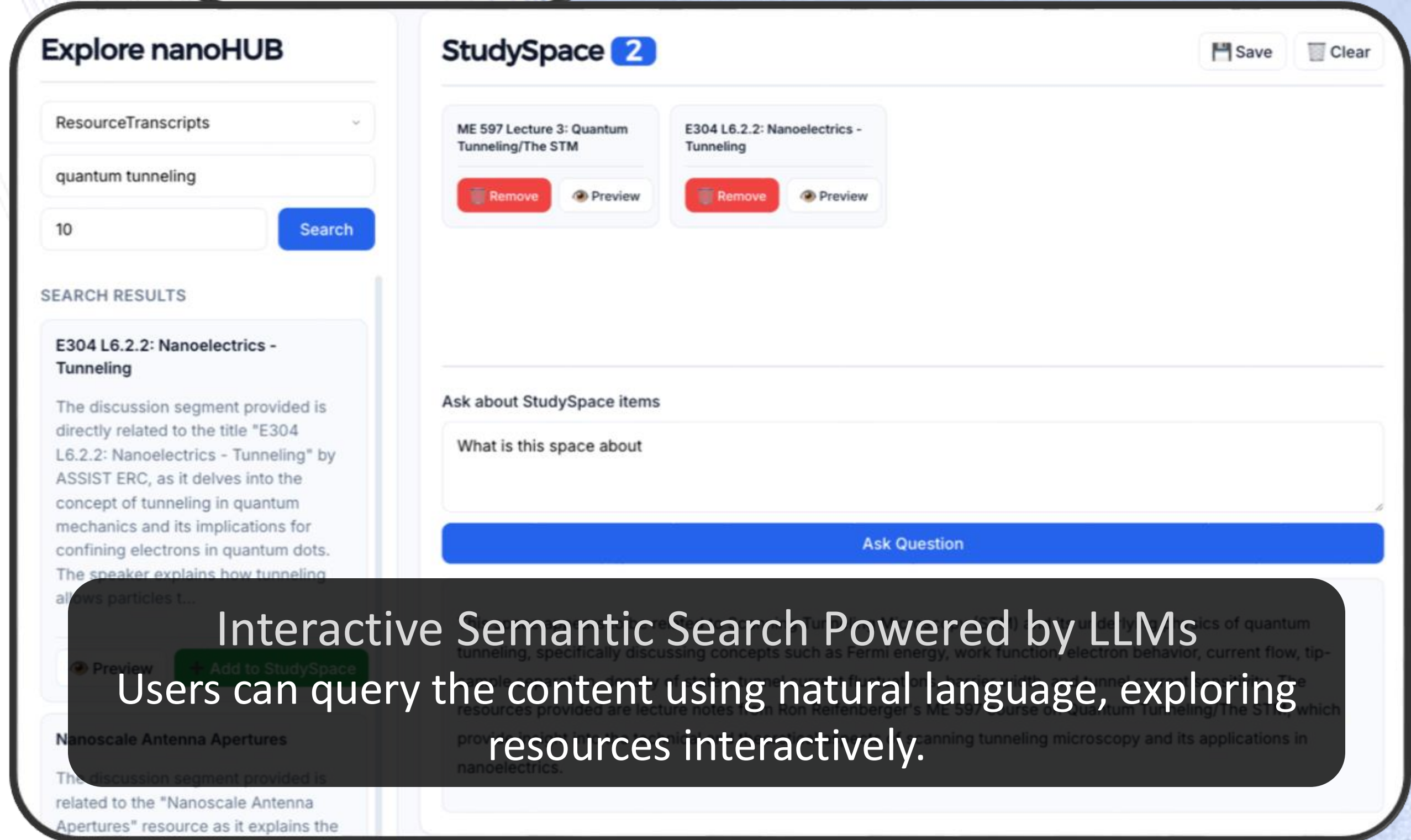
From Content to Summary Seamlessly  
Automatically generated transcripts and clear summaries for any resource.



Visual representation of nanoHUB Knowledge Graph

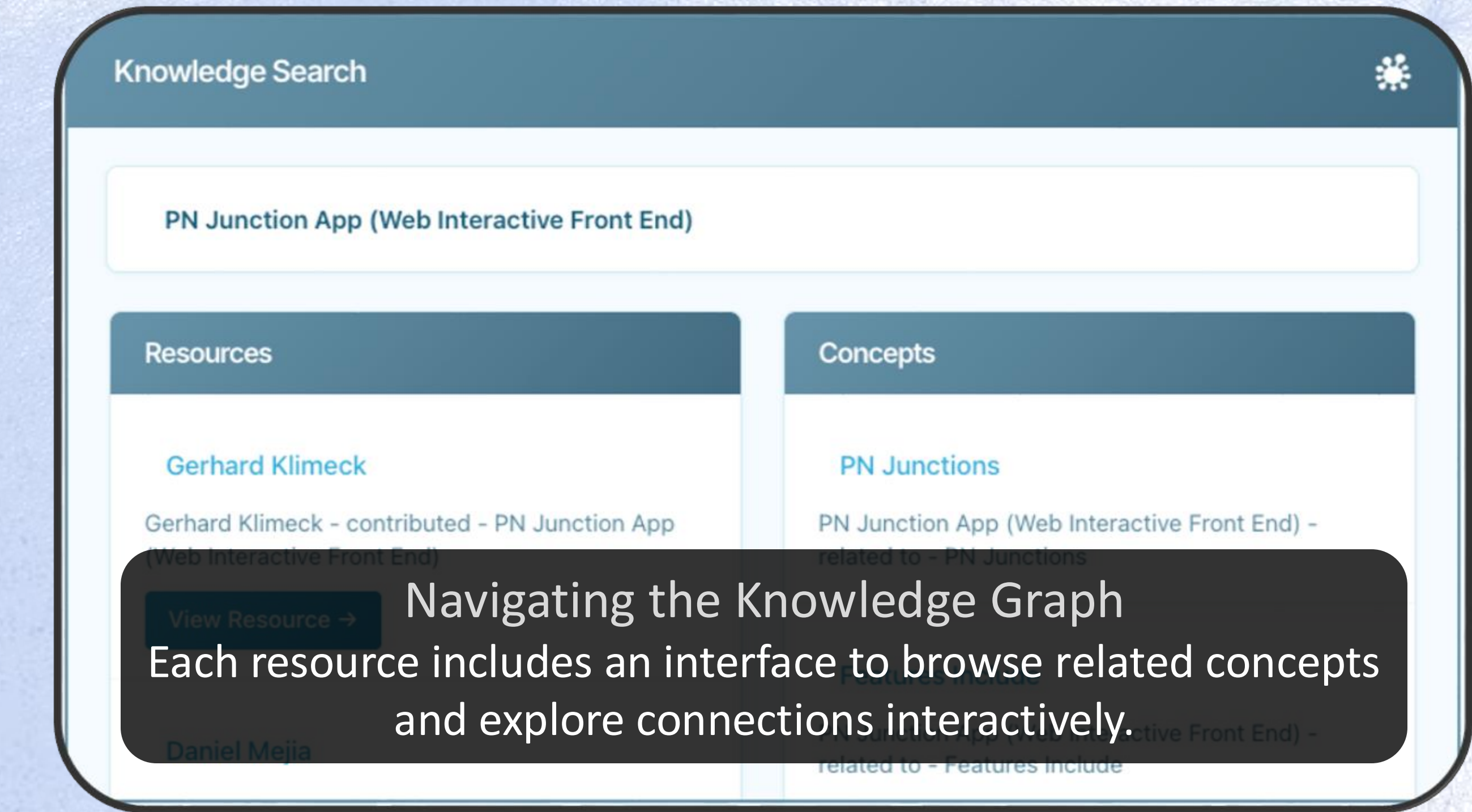
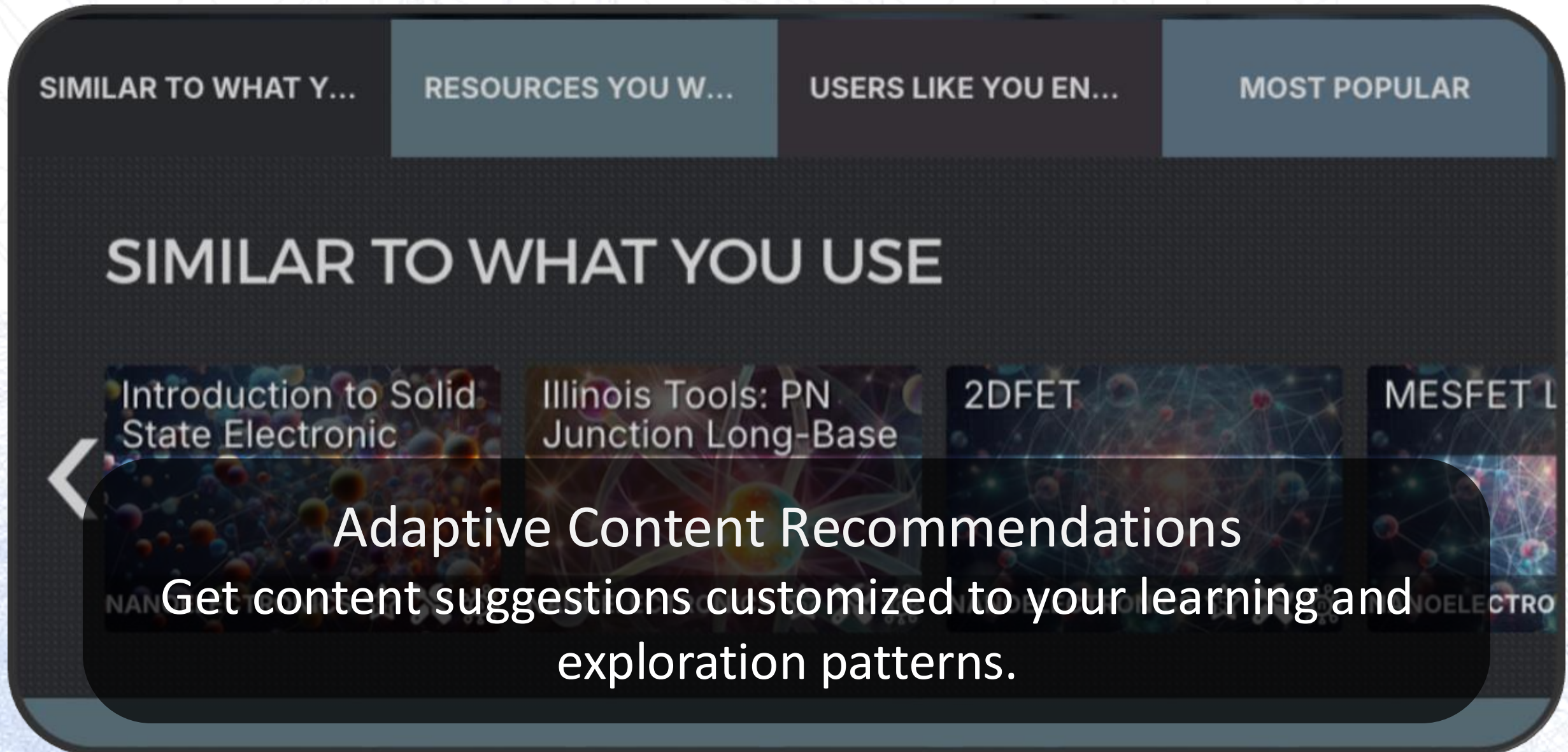


Interactive Chat  
A conversational chat that guides users through the content and helps them find what they need.



Interactive Semantic Search Powered by LLMs  
Users can query the content using natural language, exploring resources interactively.

An interactive agentic AI assistant that enables users to discover and explore scientific resources conversationally. It exposes the content as queryable records, storing more than **500,000** semantically searchable data entries.



## CONCLUSIONS

By integrating AI, nanoHUB reshapes the way users explore scientific content, simplifying access to complex tools and enabling understanding through natural, intuitive conversations.

Together, these systems create a seamless experience: nanoCHAT guides users through dialogue, nanoRA runs and interprets simulations, and the platform’s AI connects data, tools, and results into one unified environment.

## REFERENCES

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