

**a**

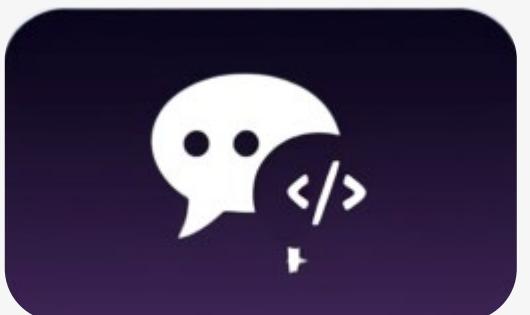
# *AI in science: from Tools to Partners*



Before  
2018



2018-  
2023



2022-  
2024



2024-  
Present

## Computational Tools

Specialised algorithms for analysis, simulation, optimization

## AI for Science

Deep models for structure prediction, materials, simulation

## AI Assistant

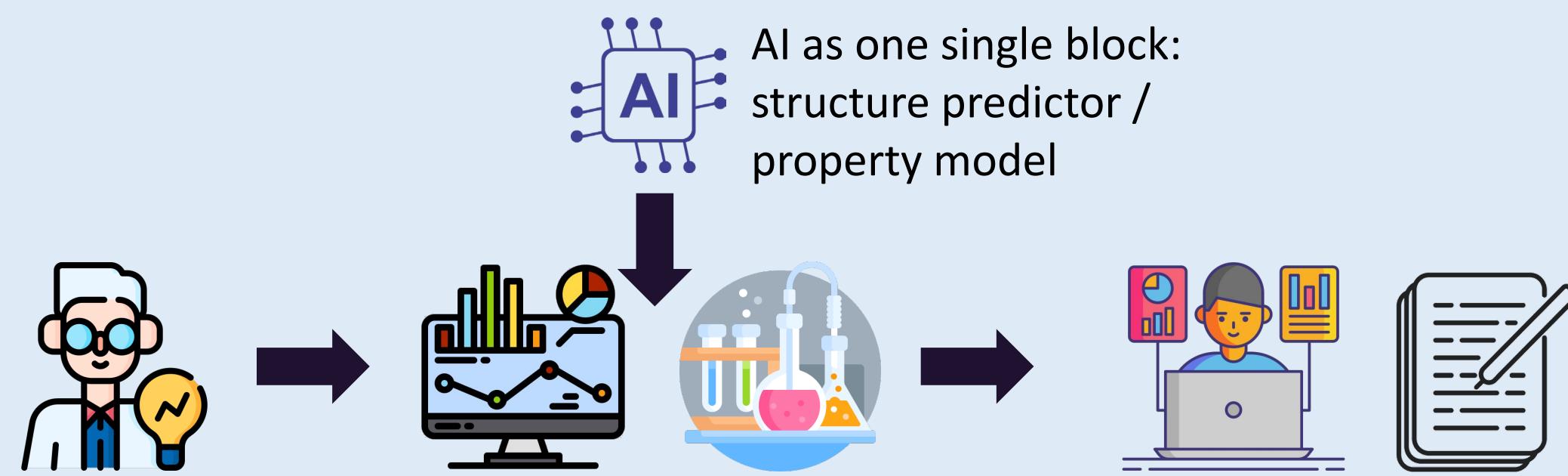
LLM copilots for literature, coding, writing

## AI Scientist

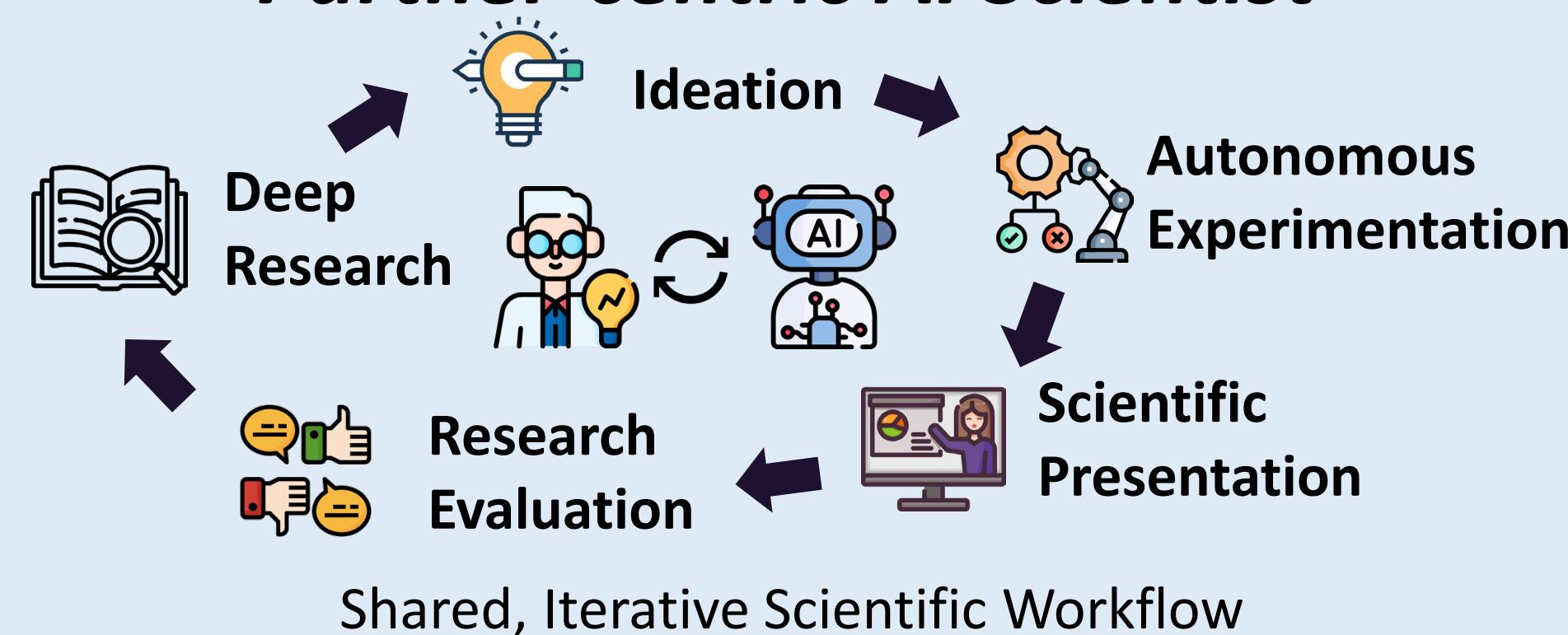
Agentic systems with closed-loop reasoning and multi-step scientific workflows

**b**

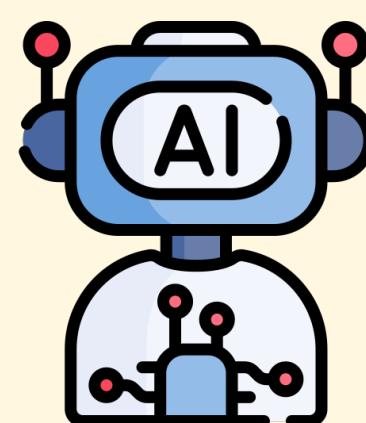
## Tool-centric AI for Science



## Partner-centric AI Scientist

**c**

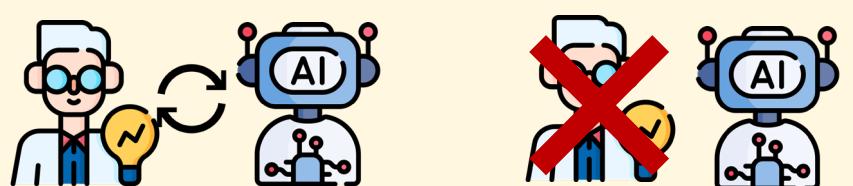
## A Comprehensive Survey of AI Scientists



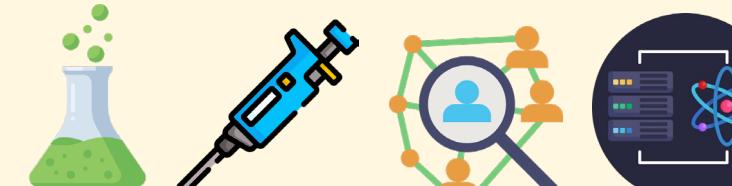
### Section 3: Functional Roles



### Section 4: Human-AI Collaboration



### Section 5: Research Domains



### Section 6: Broader Impacts

