

a

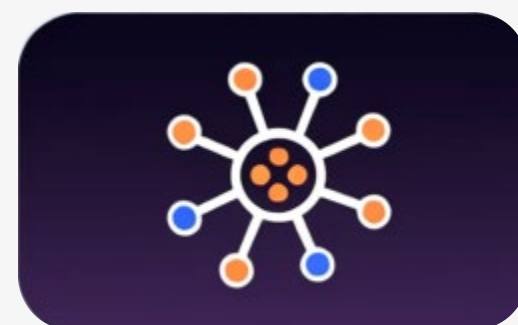
## AI in science: from Tools to Partners



Before  
2018

### Computational Tools

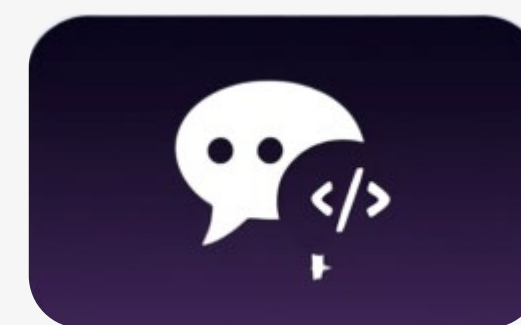
Specialised algorithms for analysis, simulation, optimization



2018-  
2023

### AI for Science

Deep models for structure prediction, materials, simulation



2022-  
2024

### AI Assistant

LLM copilots for literature, coding, writing



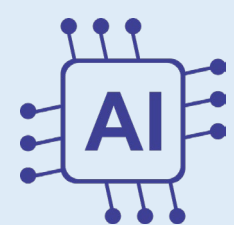
2024-  
Present

### AI Scientist

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

b

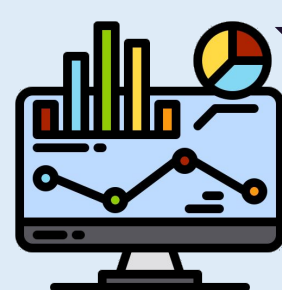
## Tool-centric AI for Science



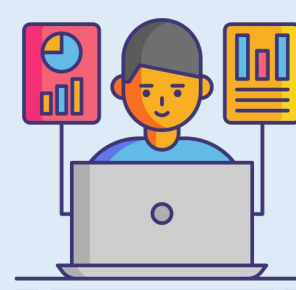
AI as one single block:  
structure predictor /  
property model



Human Scientist



Data / Experiment



Human Analysis and Writing



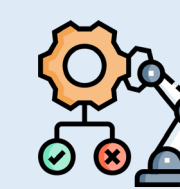
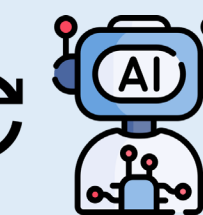
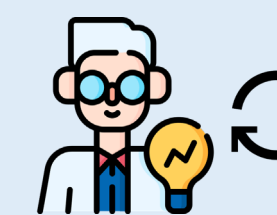
## Partner-centric AI Scientist



Deep  
Research



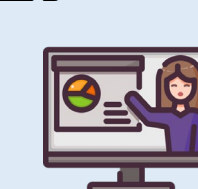
Ideation



Autonomous  
Experimentation



Research  
Evaluation

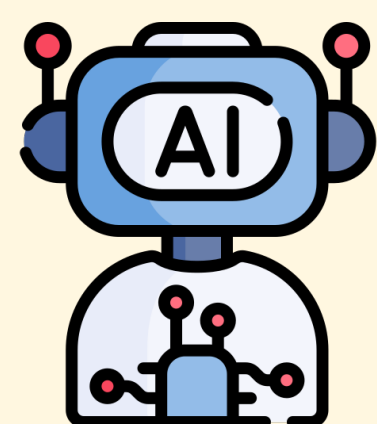


Scientific  
Presentation

Shared, Iterative Scientific Workflow

c

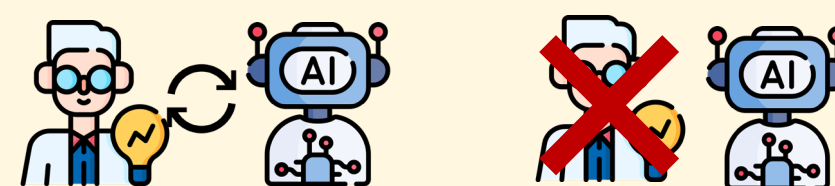
## A Comprehensive Survey of AI Scientists



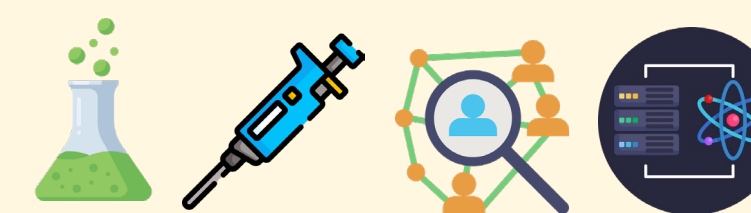
### Section 3: Functional Roles



### Section 4: Human-AI Collaboration



### Section 5: Research Domains



### Section 6: Broader Impacts

