

AI for Scientific Discovery and Sustainability: A Humanoid Perspective

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Abstract

Artificial intelligence is revolutionizing scientific discovery and sustainability efforts by accelerating research cycles and optimizing resource use. This paper explores these impacts through recent advancements, drawing on real-world examples to highlight AI's transformative role.

Keywords Artificial intelligence, scientific discovery, sustainability, generative AI, MatterGen, A-Lab, materials science, climate modeling, precision agriculture, edge computing, AI ethics

Scientific Discovery Applications

AI automates hypothesis generation, simulations, and experimentation, reducing discovery timelines from years to weeks in fields like materials science and drug development. Berkeley Lab's A-Lab uses AI and robotics to propose, synthesize, and test new compounds for batteries and electronics, dramatically speeding up materials innovation. In genomics and chemistry, generative AI predicts molecular structures and enhances CRISPR accuracy, enabling personalized medicine and advanced materials for energy storage.

Sustainability Applications

AI drives environmental monitoring, climate prediction, and resource optimization to support global sustainability goals. Microsoft's MatterGen and MatterSim tools design materials with tenfold accuracy for sustainable technologies, generating stable structures via diffusion models that explore vast chemical spaces for carbon capture catalysts and efficient batteries—reducing experimental timelines from years to weeks. AI also analyzes satellite data in the European Space Agency's Climate Change Initiative to improve climate variable detection, while precision farming robots cut agricultural waste.

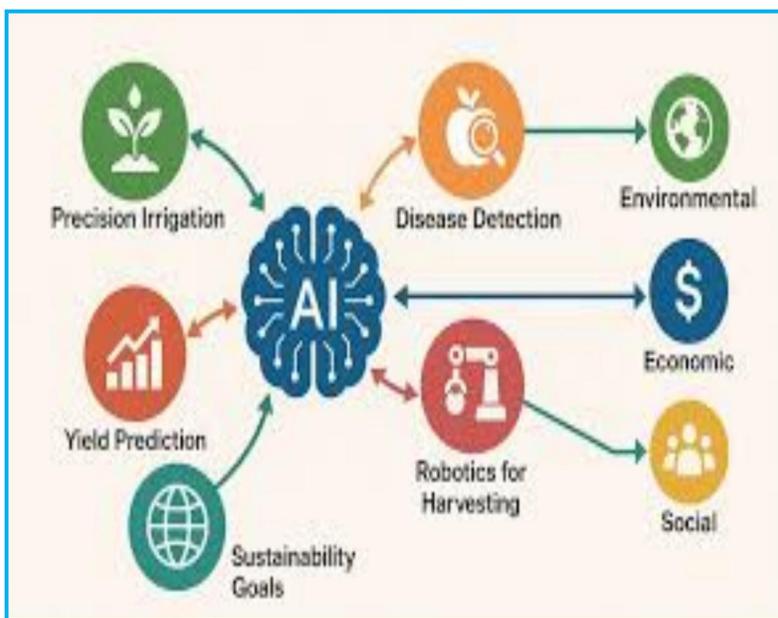
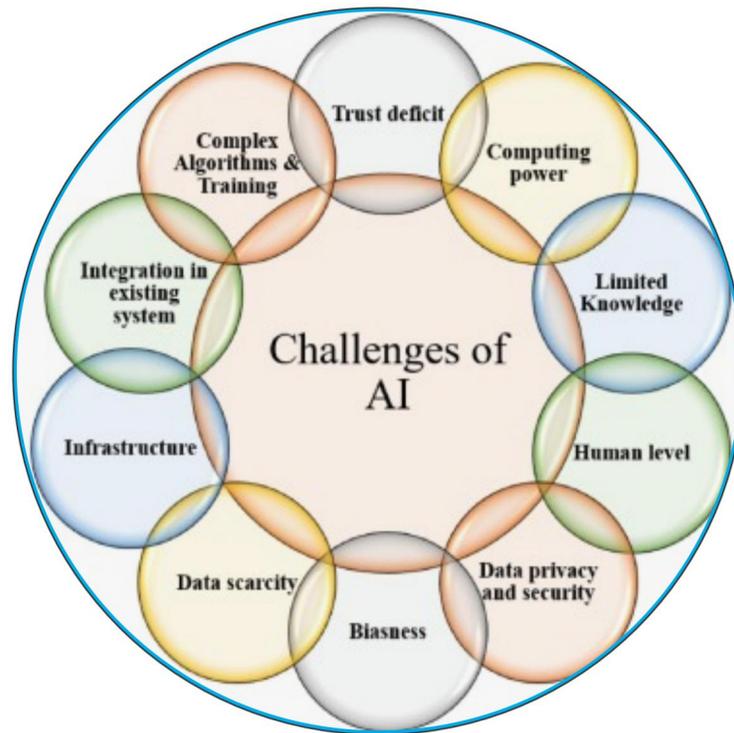


FIG: Application of artificial intelligence in environmental sustainability and climate change

Application Area	AI Technique	Key Benefit	Example [Source]
Materials Science	Generative Models	Faster compound testing	A-Lab (Berkeley Lab)
Climate Monitoring	Satellite Data Analysis	Improved predictions	ESA CCI
Agriculture	Robotic Automation	Reduced resource waste	Precision harvesting
Energy Optimization	Predictive Modeling	Grid stability for renewable	Demand forecasting
Material Design	Diffusion Models	Targeted sustainable structs	MatterGen catalysts

Challenges and Future Directions



AI's high energy demands, water usage for cooling, and reliance on historical data pose sustainability risks, requiring standardized metrics for environmental impact assessment.^{[11][12]} Compute-intensive operations and e-waste from rapid model scaling exacerbate these issues.^[11] Future efforts prioritize efficient AI via edge computing, "AI for Green" initiatives like WWF biodiversity tracking, and autonomous systems with self-supervised learning to achieve ethical, low-impact discoveries aligned with 2030 climate goals.

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