



# AI-driven design of new materials

INSTITUTE OF NANOMATERIALS ADVANCED TECHNOLOGIES AND INNOVATIONS

CXI TUL

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# Research Directions @ TUL CXI



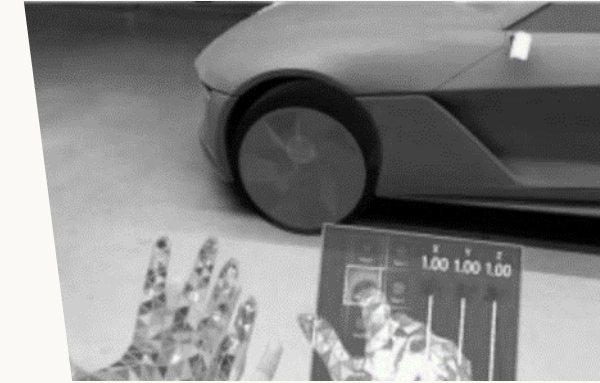
## Nanomaterials in the natural sciences

study and application of **advanced materials**, especially **nanomaterials**, mostly in the field of environmental protection, biotechnology and life sciences, including hi-tech analytic techniques.



## Competitive engineering

research, development and use of **advanced engineering technologies** and structures, mechatronic systems, power units and other components of machines and vehicles, **advanced methods for processing new materials**.



## System integration

development of **state-of-the-art SW solutions**, data processing and Integration, **robotics, including the use of collaborative and sensitive robots**, design and development of appropriate control software.

# Digitalization, Automation and AI: The New Research Foundation

1

## AI Transformation

Rapidly changing how we understand our world

2

## Data-Driven Shift

Moving from experimental to model-guided research

3

## Predictive Science

We can use the predictive analytics and autonomous discovery







# From Lab to Algorithm: How AI Transforms Materials Development



## Property Prediction

Forecasting mechanical, electrical, thermal properties before synthesis, guiding targeted material design



## Structure Discovery

Revealing novel crystal structures using machine learning. Speed up of molecular design and synthesis, making innovation more efficient and accessible



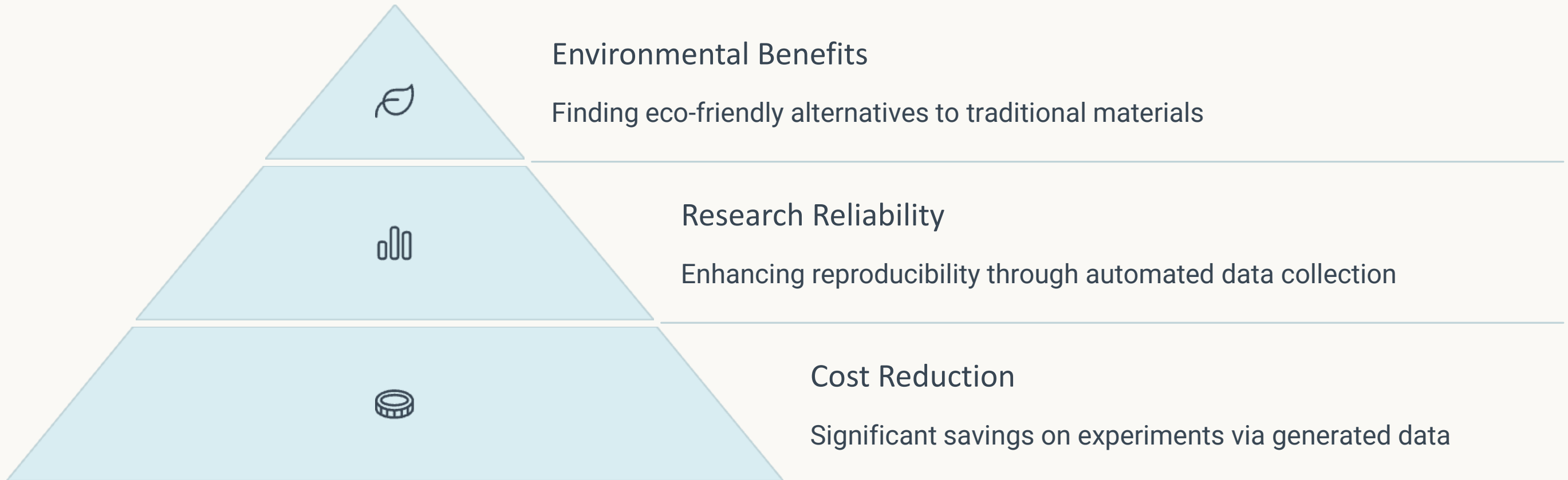
## Extreme Conditions

Material simulation under diverse conditions with high accuracy, enabling versatile material design

# Large Language Models as Research Assistants



# Digitization Saves Time, Money and the Planet



# Digital Tools for More Open and Efficient Science



## FAIR Data Management

Findable, Accessible, Interoperable, Reusable research data



## Automated Documentation

Standardized metadata and workflows for better reproducibility



## Open Science Practices

Publishing data, protocols, code for transparency and collaboration







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Resources: CXI TUL and AI generated by <https://gamma.app>

