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Challenges & Opportunities of Adopting AI in Materials Design:
Current applications & future directions

Challenges

Industry
- Understanding of applicability
- Conservative Validation
- Providers / education
- Digitalisation
- Priority, integration

Data
- Availability
- Sparse and noisy
- New experiments & simulations
- Security
- Storage aggregation

Budget & Investment
- Waste time & effort
- Grant funding
- Innovation
- Invest time and money but fails or do not invest and fall behind
- Intellectual property

Opportunities

Batteries
Improve chemistry, processing, and geometry by targeting properties such as charge capacity, charging time and weight.

Lubricants
Optimise alkane properties for lubricants by combining sparse experimental data with molecular dynamics simulations to predict physical properties of alkanes to design optimal lubricant base oils.

3D Printing Alloy
Design better alloys for additive manufacturing technologies such as direct laser deposition by using historical data about other similar techniques such as welding to guide a predictive model.

Drug Design
Design optimal drugs with target properties including activity, toxicity, and side effects.

Real-World Solutions

Our collaborations have used **data** to deliver:

Maximised formula performance for multiple target properties
Reduced prototype costs - reduction in experiments
Reduced material costs - minimisation of expensive properties
Reduced environmental impact
Standardised design process across a company

Concrete for Construction

Challenge: Deliver best mix based on project conditions
380 factors: Local sand, local aggregate, cement, environmental conditions, project type, travel time, target strength, admixtures
Current approach: Industry experts, pick from historic mixes and similar projects
Solution: Tool to suggest optimal "mixes" taking into account cost, location, and time of year. Knowledge from previous projects shared and adding future value

Chromium in Steel

Advantages: Chromium makes steel corrosion resistant and hard
Disadvantages: Chromium is toxic, environmentally unfriendly, and expensive
Challenge: Design a new steel with the same physical properties but with less Chromium
Current heuristic approach: Industry experts, duplicate historic mixes
Solution: Tool to run "virtual experiments" to simulate low-chromium steels, whilst maintaining physical targets

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