# Executive Summary

# Knowledge-integrated machine learning for materials: lessons from gameplaying and robotics

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## Introduction *Pg. 242*

Machine learning (ML), techniques where computers learn from experience, is an area of great potential for materials research. However, bridging the gap between using ML to solve extensive engineering problems and the single-scope applications of today is a multi-faceted problem. Tasks such as materials selection and synthesis have seen improvements through ML assistance, but the self-sustainment required to handle problems independent from human involvement is yet to be realized. In this review, ML advances from robotics and gameplaying are used as examples for methods applicable to materials science. Three levels of implementation are identified:

1. Toolset integration, where ML is used to bolster experimental and simulation toolsets.
2. Workflow integration, where ML is expanded to several steps for a larger workflow.
3. Knowledge integration, where ML studies are shared and pooled into databases.

The following section gives commentary on these levels in materials research. After which, transferable ML implementations from robotics and gameplaying are presented and discussed.

## Machine learning levels in materials research *Pg. 242-247*

Well-established ML algorithms have been introduced into materials research with techniques such as weighting and interpolation to account for sparse and biased data. Despite this, ML toolsets have often required significant human involvement to handle and process data, leaving the general laboratory workflow mostly unaltered. This can be remedied by constructing an interface between algorithms and instrumentation, possibly providing secondary benefits as well. Take, for example, a single ML tool which accelerates X-ray spectra classification in a novel way. Researchers can now focus on streamlining the hardware tool design to lower costs.

After single tool optimizations are complete, workflows can be developed to address different steps of the scientific process. For example, a suite of ML algorithms could search for new, stable materials for solar cells by funneling down possibilities based on desired properties and then rapidly characterizing the remaining materials. This could grow materials databases through autonomous surveying. Picture an imaging lab which performs rapid optical measurements on its own, increasing throughput of simple characterization. However, adaptability to new tasks remains in need of improvement for artificial intelligence (AI) like this.

Fully realizing the potential of ML workflows requires dissemination of knowledge from one study to the next. This ensures that the efficiency and power of algorithms is maximized. Studies have been conducted to identify promising energy materials through ML by scanning millions of manuscript abstracts and finding patterns in desired properties. Collaboration, both direct and indirect like the above, is integral to increasing ML presence in materials research.

## Machine learning in gameplaying and robotics *Pg. 247-248*

The first implementations of AI in gaming involved creating full solutions for every outcome, or hand-crafted rulesets to govern an AI's search for optimized techniques. However, as the scope of the game in question increases, solutions and rulesets must follow, either becoming too restrictive or unreasonably complex to develop. Machine learning provided a remedy to this. For example, reinforcement ML allows AI to undergo training sessions rewarding desirable behavior. Training capabilities can be bolstered through manually demonstrating expert techniques. Now, the AI can adapt to new rulesets on its own, such as a varying board size in the game Go. Over time, hybrid models that combine the strengths of both model and learning-based systems have been introduced, offering a balance between adaptability and computational time.

Robotics have been a prime area to apply AI and ML. Abilities such as perception, sensory interpretation, and autonomous reasoning are enabled by ML. Multiple AI agents may be combined on a problem to interface both with the environment and each other, improving the learning process through cross-referencing and task breakdown. Allowing agents to interact with one another ensures each agent works with up-to-date information on the task, but incurs serious costs in operation complexity. Costs can be decreased when agents are set to ignore one another, but this may undermine the agreement among the agents' solutions.

## Integration of lessons from gameplaying and robotics *Pg. 248-256*

Within toolset integration, materials research can work to implement the capabilities of robots to produce output without copying human workflows. Research laboratories can either fully automate themselves for high throughput and consistency, or identify key points in the workflow that can be automated for maximum cost/benefit. Robotics can also assist in the transition from lab to a robot-abundant manufacturing scene, a common end goal of materials research.

Within workflow integration, well-defined targets can help communities focus on improving databases. Compared to the robotics and gameplaying scenes, materials databases are plagued with bias and lacking in numbers. Open-source instrumental design, inspired from robotics, can assist in standardizing data for better interoperability. Gameplaying demonstrated the strengths of hybrid models for utilizing this data, a technique materials research should press into given the current successes. For example, solar cell manufacturing was improved through constraining search spaces with prior observations of materials quality and tool capabilities.

Knowledge integration, the most difficult level, is characterized by three challenges:

1. Connecting ML algorithms and knowledge pools, allowing both input and output.
2. Making the knowledge bases more accessible among different studies.
3. Developing ML algorithms that can effectively reuse pooled knowledge.

Gameplaying demonstrates knowledge integration with algorithms that transfer knowledge from one game instance to another without forgetting. To this date, materials research has primarily built specialized models for niche studies, providing high accuracy but low generalizability. An effort should be made to increase generalizability, facilitating AI to be inventive.

## Conclusion and outlook *Pg. 256-257*

The promise of more efficient, higher throughput research should encourage the implementation of ML into materials science, as exemplified by gameplaying and robotics. Some important lessons are the benefits of combining human knowledge with learning algorithms, and the importance of developing community based goals. So far, materials research has shown progress in both toolset and workflow integration. Going forward, this field should strive to lead the development of knowledge integration, since a network of standardized databases can help make breakthroughs in device performance. Areas of creativity once thought exclusive to humans can be unlocked with knowledge-based ML. Now, it falls on humans to conduct extensive research into the legal and ethical use of this AI, ensuring product safety for humans and the environment.

**Supporting information:** Hippalgaonkar, K., Li, Q., Wang, X. et al. Knowledge-integrated machine learning for materials: lessons from gameplaying and robotics. Nat Rev Mater 8, 241–260 (2023). https://doi.org/10.1038/s41578-022-00513-1

Summary of changes made

- I cut down on quite a bit of wordier sentences, and took out a few as well. This made room for a better, larger title to the document, larger headings, and a citation at the end for the original paper.
- I changed my indentation to try to match a more scientific style. I added in page numbers by the headings for reference to the original paper.
- I added in bullet points to break up the monotony of my text, also trying to make it easier to read, and emphasizing important points.
- I reworded some sentences to be less clumsy, like the first sentence of the conclusion. I addressed some grammatical mistakes highlighted by the peer feedback.
- I added an extra toolset integration example at the end of the first paragraph in the section "Machine learning levels in materials research".
- I tried to set up the following sections after the introduction with a few added sentences.
- I rephrased the heading "Lessons from Gameplaying and Robotics" to "Integration of lessons from gameplaying and robotics".
- I did get a few comments telling me I should include figures or several citations. I decided not to do this because we discussed in class that executive summaries do not typically include figures or specific references.