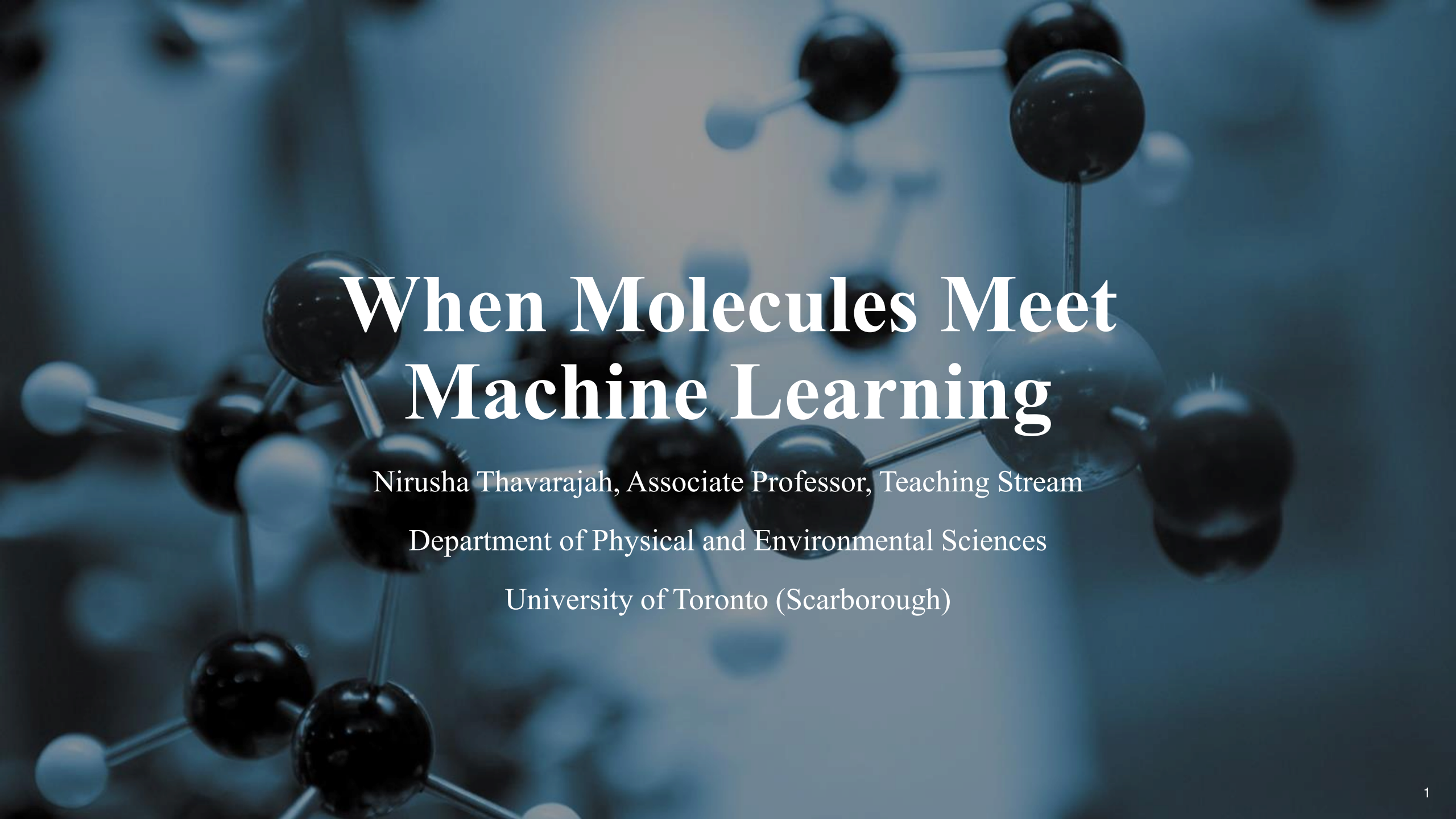

When Molecules Meet Machine Learning

Nirusha Thavarajah, Associate Professor, Teaching Stream

Department of Physical and Environmental Sciences

University of Toronto (Scarborough)

Artificial Intelligence and Machine Learning in Chemistry Education

Personalized Learning: ML algorithms adapt content to individual student needs and pace.

Intelligent Tutoring Systems: AI-powered platforms offer real-time feedback and guidance.

Virtual Labs & Simulations: Enable interactive, safe, and scalable experimentation.

Accessibility: AI tools improve access to learning materials and support diverse learners.

Iyamuremye, A., Niyonzima, F.N., Mukiza, J. *et al.* Utilization of artificial intelligence and machine learning in chemistry education: a critical review. *Discov Educ* **3**, 95 (2024). https://doi.org/10.1007/s44217-024-00197-5

Adaptive Learning Mastering Chemistry

- **AI-Guided Practice**: Targeted feedback and remediation.
- **Dynamic Study Modules**: Adapt to student performance in real time, reinforcing key concepts based on individual progress.
- **Chemistry Diagnostic Tools**: Use AI to assess math and chemistry readiness, then generate personalized learning plans.

Berber, S.; Bruckner, M.; Maurer, N.; Huwer, J. Artificial Intelligence in Chemistry Research—Implications for Teaching and Learning. J. Chem. Educ. 2025, 102 (3), 456–472. https://doi.org/10.1021/acs.jchemed.4c01033
Gligorea, I.; Cioca, M.; Oancea, R.; Gorski, A.-T.; Gorski, H.; Tudorache, P. Adaptive Learning Using Artificial Intelligence in e-Learning: A Literature Review. Educ. Sci. 2023, 13 (12), 1216. https://doi.org/10.3390/educsci13121216

Mastering Chemistry: Is it True Machine Learning?

- Mastering Chemistry uses rule-based adaptive algorithms, which are a form of basic AI, but not full ML.
- These systems don’t train on large datasets or improve autonomously over time like ML models do.
- Instead, they follow pre-programmed logic to personalize learning experiences.

AI in Chemistry Education — Tools Compared

Feature	Mastering Chemistry	ML-Powered Platforms (e.g., Chemprop, IBM RXN)
AI Type	Rule-based adaptive algorithms	Data-driven machine learning & deep learning models
Learning Focus	Personalized instruction, feedback & pacing	Predictive analytics, molecular modeling, retrosynthesis
Main Tools/Modules	Dynamic Study Modules, Skill Builder, Diagnostics	Chemprop, AiZynthFinder, IBM RXN for Chemistry
Student Interaction	Structured learning paths with adaptive quizzes	Exploratory tools with predictive simulations
Chemistry Applications	Concept review, formula mastery, foundational understanding	Reaction prediction, property estimation, synthesis design
Customization	Based on learner responses and confidence	Based on chemical structure, training data, algorithms
Educator Use Case	Homework assistance, concept reinforcement	Research-grade analysis, curriculum enrichment
Limitations	No real-time learning from new data	Requires clean datasets and computing power

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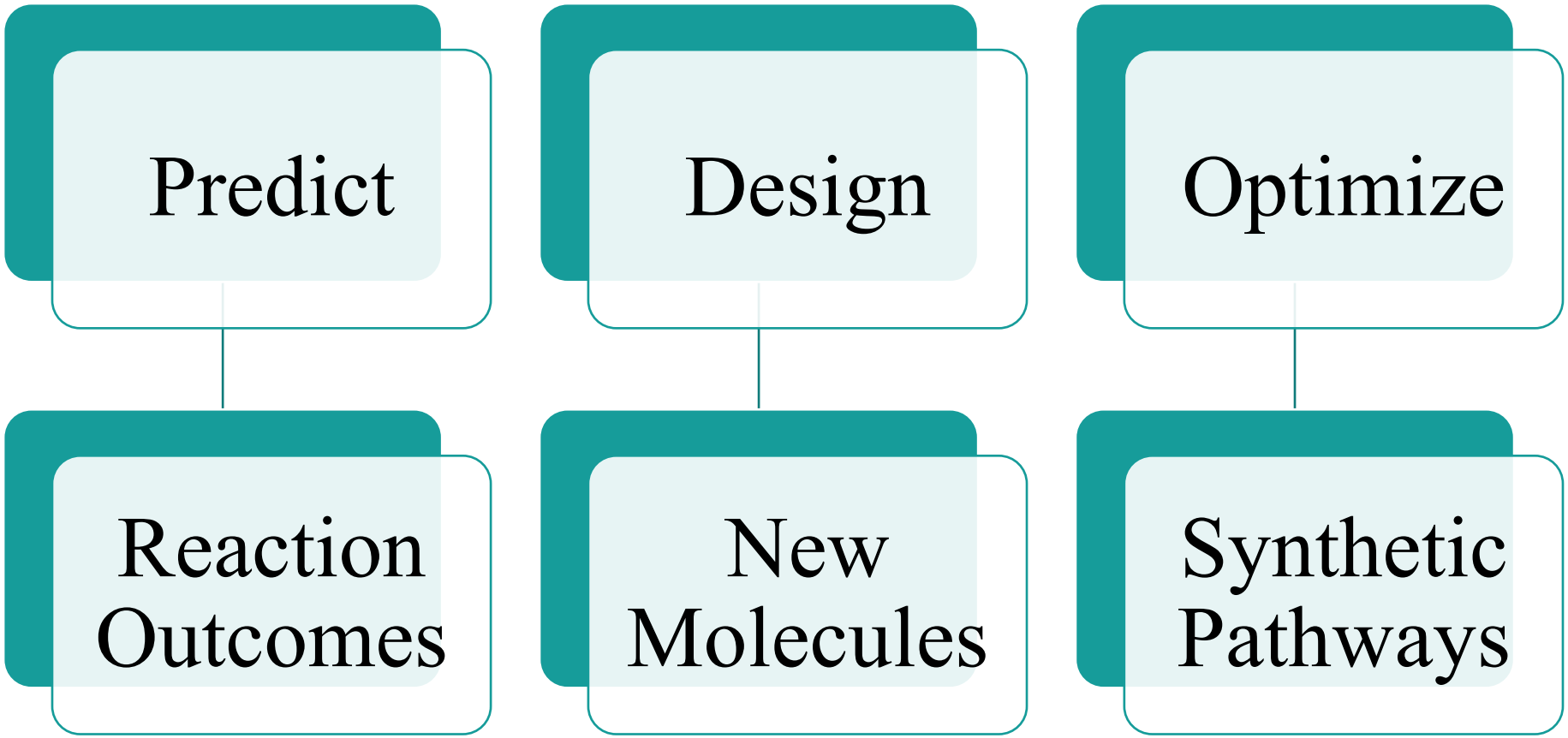
Exploring the Intersection of Machine Learning (ML) and Chemistry



Pedagogical Implications of Machine Learning in Chemistry Education

Pedagogical Theme	Implication	Example from the Study
Curriculum Enrichment	ML bridges theoretical chemistry with applied scientific practice and interdisciplinary learning	Using ***AiZynthFinder*** to teach retrosynthesis in organic chemistry
Technological Content Knowledge (TCK)	Teachers must understand core AI/ML concepts to integrate tools meaningfully	Demonstrating ***Chemprop*** to model structure–property relationships
Teacher Training	Structured professional development enhances educators' AI confidence and readiness	Workshops showing ML tools in pharmacology and materials chemistry
Student Engagement	ML tools boost interest, inquiry, and awareness of emerging scientific careers	Using ***AlphaFold*** to explore protein folding and molecular structure
Ethical Awareness	Lessons should include discussion of bias, transparency, and privacy in AI systems	Debating the fairness of ML in drug discovery models and real-world applications

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Key Challenges in Using ML in Chemistry

Challenge	Description
Limited Educator Training	Many teachers lack the technical background to confidently use or explain ML tools in chemistry.
Curriculum Misalignment	ML concepts often don't fit neatly into traditional chemistry syllabi, especially at the K–12 level.
Data Privacy & Ethics	Concerns about student data collection, algorithmic bias, and transparency in AI systems.
Dependence on Preexisting Data	ML models require large, high-quality datasets—often unavailable or inaccessible in schools.
Tool Complexity	Research-grade ML platforms (e.g., Chemprop, IBM RXN) can be too advanced for classroom use without simplification.
Infrastructure Gaps	Schools may lack the computing resources or internet bandwidth needed to run ML simulations.
Assessment Difficulties	Evaluating student understanding of ML-enhanced chemistry concepts can be tricky without standardized metrics.

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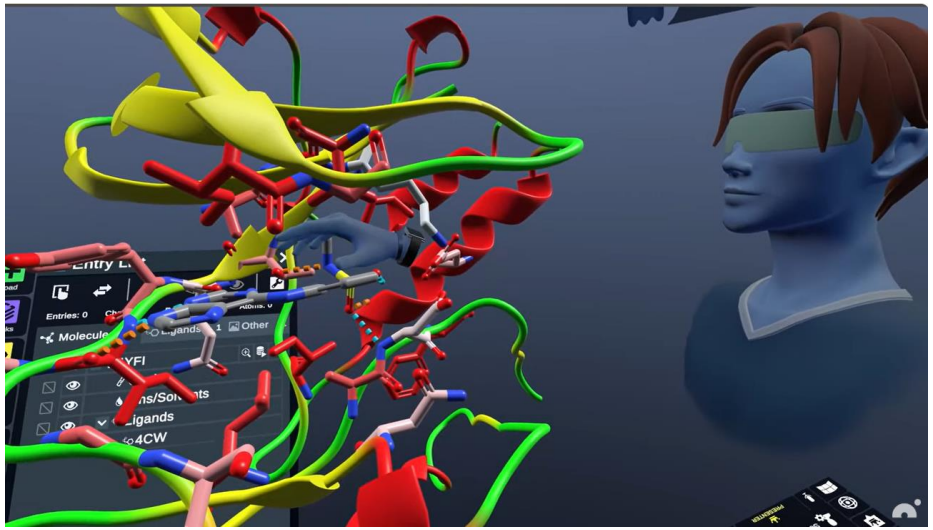
Suggested Solutions in Literature

Challenge	Suggested Solution
Limited Educator Training	Develop professional development programs focused on AI/ML literacy and hands-on tool usage
Curriculum Misalignment	Introduce interdisciplinary modules that merge chemistry with data science and computational thinking
Data Privacy & Ethics	Implement classroom discussions and school policies addressing AI transparency, bias, and data protection
Dependence on Preexisting Data	Use open-access chemical datasets and create classroom-scale projects with simplified training models
Tool Complexity	Adopt accessible ML tools (e.g., Orange3, Top Hat Ace) or scaffold research-grade tools for student use
Infrastructure Gaps	Provide cloud-based platforms and low-tech simulations to accommodate limited hardware
Assessment Difficulties	Create rubrics that evaluate conceptual understanding of ML applications alongside chemistry content

Iyamuremye, A.; Niyonzima, F. N.; Mukiza, J.; Twagilimana, I.; Nyirahabimana, P.; Nsengimana, T.; Habiyaremye, J. D.; Habimana, O.; Nsabayezu, E. Utilization of Artificial Intelligence and Machine Learning in Chemistry Education: A Critical Review. Discover Education 2024, 3, 95. https://doi.org/10.1007/s44217-024-00197-5 (accessed July 15, 2025).

Planned Pedagogical Intervention: Machine Learning Integration in Nanome

- Nanome is a virtual reality platform for molecular modelling and drug design that integrates machine learning through its AI-powered assistant, MARA.
- MARA uses natural language processing and AI to help users analyze molecular structures, query chemical data, and interact with computational tools.
- Nanome supports plugins that allow integration with ML-powered platforms like AutoDock, DSX, and other scoring or docking tools.
- Researchers can visualize ML-generated molecules, analyze binding affinities, and explore protein-ligand interactions in immersive 3D environments.



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(2) Nanome Inc. Overview of MARA: The Agentic System for Scientific Informatics. https://docs.nanome.ai/mara/overview.html
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Comparison Table of Popular Machine Learning Platforms in Chemistry

Platform	Core Functionality	ML Integration	Educational Use	Research Use
Nanome	VR-based molecular modeling and collaboration	Integrates ML via MARA assistant and plugins	Interactive visualization of ML-generated molecules	Real-time analysis of docking scores, protein-ligand interactions
Chemprop	Molecular property prediction using graph neural networks (GNNs)	Deep learning models trained on chemical datasets	Teaching structure–activity relationships and ML modeling	Predicting solubility, toxicity, and reactivity for drug design
IBM RXN	Reaction prediction and retrosynthesis planning	Transformer-based sequence-to-sequence models	Demonstrating reaction mechanisms and synthesis planning	Designing synthetic routes and validating reaction outcomes

(1) Nanome Inc. MARA: Your Scientific Discovery Co-pilot. https://nanome.ai/mara/ .(2) Nanome Inc. Overview of MARA: The Agentic System for Scientific Informatics. https://docs.nanome.ai/mara/overview.html.(3) Chemprop. GitHub Repository. https://github.com/chemprop/chemprop.(4) IBM Research. IBM RXN for Chemistry. https://rxn.res.ibm.com/ .(5) Schwaller, P.; Laino, T.; Gaudin, T.; Bolgar, P.; Hunter, C. A.; Bekas, C.; Lee, A. A. Molecular Transformer: A Model for Uncertainty-Calibrated Chemical Reaction Prediction. ACS Cent. Sci. 2019, 5(9), 1572–1583. https://doi.org/10.1021/acscentsci.9b00576.(6) Yang, K.; Swanson, K.; Jin, W.; Coley, C.; Eiden, P.; Gao, H.; Guzman-Perez, A.; Hopper, T.; Kelley, B.; Mathea, M.; Palmer, A.; Settels, V.; Jaakkola, T.; Jensen, K.; Barzilay, R. Analyzing Learned Molecular Representations for Property Prediction. J. Chem. Inf. Model. 2019, 59(8), 3370–3388. https://doi.org/10.1021/acs.jcim.9b00237.

Future Applications of Nanome in Teaching Advanced Chemistry Courses

Research Area	**Nanome Capabilities**
Molecular Design & Optimization	Real-time 3D visualization of complex organic molecules and reaction intermediates
Enzyme–Substrate Interaction	Immersive modeling of binding pockets and conformational changes in bio-catalysis
Reaction Mechanism Exploration	Collaborative mapping of multi-step organic reactions with spatial annotations
Stereochemistry & Chirality	Intuitive manipulation of chiral centers and stereoisomers for drug-like molecules
Ligand–Receptor Docking	Integration with ML plugins to simulate binding affinities and predict bioactivity

Future Applications of Nanome in Hydrogel Synthesis

Hydrogel Focus	**Nanome Utility**
Polymer Network Visualization	3D modeling of cross-linked hydrogel matrices and nanoparticle dispersion
Nanocomposite Design	Integration of carbon-based, metallic, or ceramic nanoparticles into hydrogel scaffolds
Drug Delivery Simulation	Spatial analysis of encapsulated molecules and release pathways within hydrogel pores
Tissue Engineering Scaffolds	Collaborative design of bio-inspired hydrogel architectures for regenerative medicine
Stimuli-Responsive Systems	Modeling of pH-, temperature-, or light-sensitive hydrogel behavior

Summary & Future Directions

- Machine learning is revolutionizing chemistry education and research, enabling predictive modeling, retrosynthesis design, and personalized learning experiences.
- Adaptive platforms like Mastering Chemistry provide foundational support, while ML tools such as Chemprop, IBM RXN, and Nanome drive innovation in molecule generation and reaction analysis.
- Nanome's integration with MARA and ML plugins offers immersive, collaborative environments for drug design, hydrogel synthesis, and advanced molecular visualization.
- Successful classroom integration demands thoughtful pedagogy, ethical awareness, curriculum redesign, and ongoing teacher training.
- By embracing AI responsibly, we equip the next generation of chemists to thrive in a data-driven, interdisciplinary scientific landscape.

Discussion Questions

1. How do we evaluate student understanding and engagement when using AI-enhanced chemistry tools that move beyond traditional assessment methods?

2. How can AI and ML tools be used to promote more inclusive and accessible chemistry learning experiences, particularly in under-resourced settings?

3. How can chemistry educators balance foundational content with emerging machine learning tools to prepare students for future scientific careers?

4. What ethical considerations should guide the use of AI/ML in chemistry education, particularly regarding data privacy, bias, and equitable access?

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