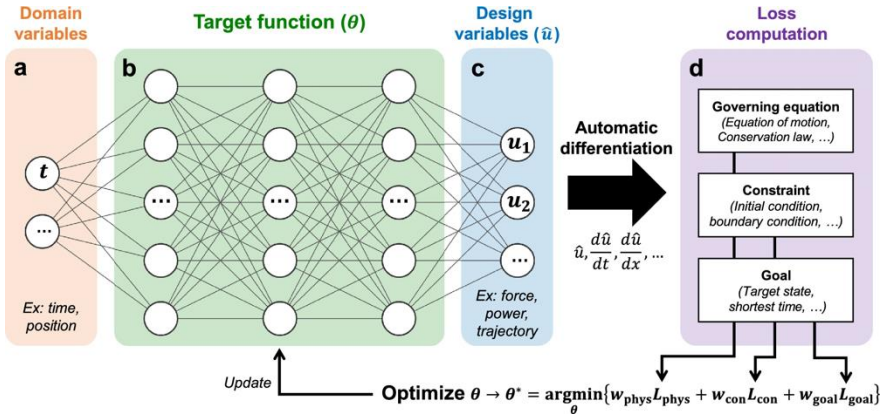
Dr. Clara Kirkvold | 11.06.2026

Physics-Informed Machine Learning: Putting the Science in Data Science

What is Physics-informed Machine Learning

Physics-informed machine learning (PIML) combines physical and chemical principles with machine learning models. PIMLs embed physical laws and constraints into model architecture or training to enable interpretable and scientifically consistent predictions.[1]



Schematic of a PINN. In PINN"s solving a PDE system is treated as an optimization problem.
Reprinted from Ref [2] under CC-BY license

For example, **Physics-informed Neural Networks (PINNs)** include partial differential equations (PDE) in the loss function. During training, both data error and physics-based error is minimized.[2]

Advantages of PIML[3]

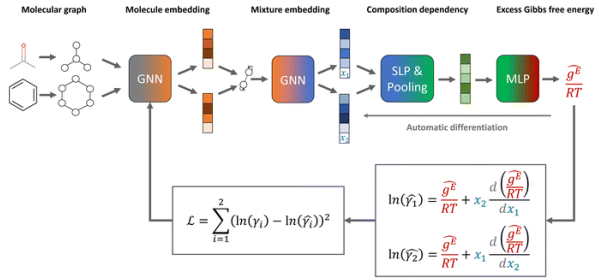
- Less data required
- Physically consistent predictions
- Better generalization
- Increased interpretability

Limitations of PML[4]

- Higher computational cost
- More complex training
- Requires domain expertise
- Sensitive to physics formulation

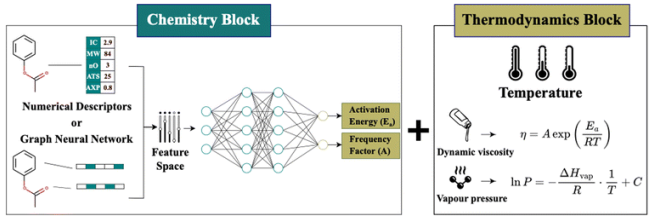
Examples of Physics-informed Machine Learning in Chemistry

Rittig *et al.* used a graph neural network (GE-GNN) for predicting composition-dependent activity coefficients of binary mixtures.



Schematic of physics-informed ML Framework designed by Rittig *et al.* Reprinted from Ref [5] under CC-BY-3.0 license

GE-GNN predicts excess Gibbs free energy, then uses automatic differentiation together with thermodynamic relationships to calculate activity coefficients, which ensures thermodynamic consistency.



Schematic of physics-informed ML Framework designed by Rajabi-Kochi *et al.* Reprinted from Ref [6] under CC-BY-3.0 license

Rajabi-Kochi *et al.* developed a physics-informed ML framework that predicts temperature-dependent properties, such as dynamic viscosity. An ML model to predict chemistry-dependent coefficients, which are used in thermodynamic equations that capture temperature and pressure dependence.

References

[1] Deng *et al. Appl. Math. Model* **2023**, *124*, 325–352.
[2] Seo, J. *Sci. Rep.* **2024,** *14, 202*
[3] MathWorks, *What Are Physics-Informed Neural Networks (PINNs)?* (accessed June 10, 2026).
[4] Meng *et al. Mach. Learn. Comput. Sci. Eng* **2025**, *1*, 20
[5] Rittgi *et al. Chem. Sci.*, **2024**, *15, 18504–18512*
[6] Rajabi-Kochi *et al. Digital Discovery* **2026**