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# Unlocking Quantum Matter with Symmetry-Aware Machine Learning: A Comprehensive Review

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**Abstract:** The rapid progress in quantum materials, including moiré-based two-dimensional systems, topological insulators, and strongly correlated phases, has revealed physical phenomena beyond the classical symmetry-breaking paradigm. Many of these systems exhibit hidden symmetries, emergent invariants, and non-local entanglement that are difficult to capture Machine learning, particularly symmetry-aware frameworks, has emerged as a powerful tool for identifying exotic phases, uncovering hidden structures, and enabling model-independent analysis of quantum systems. In this review, we summarize recent advances in symmetry-guided neural networks, hybrid quantum–classical approaches, and unsupervised learning techniques, with a focus on condensed-matter physics We also discuss current challenges, including interpretability and noise in near-term quantum devices, and highlight future directions toward integrating machine learning with quantum physics for accelerated discovery of novel quantum materials.
**Keywords**: Quantum Materials; Machine Learning; Symmetry; Topological Phases; 2D Materials; Hybrid Quantum-Classical Systems

## 1. Introduction

Recent developments in condensed-matter physics have found a wealth of unconventional quantum phases, such as symmetry-protected topological insulators (RSxF2), moiré-engineered 2D materials, and strongly correlated superconductors (Liu & Tegmark, 2022; Mahlow et al., 2023; Cranmer et al., 2023). These quantum phases cannot be adequately described using conventional local order parameters, as they involve global topological properties and non-local entanglement, in contrast to classical phases as described by Landau's symmetry-breaking scenario, involve global phenomena such as topological invariants and non-local entanglement that elude capture via local order parameters. The conventional analytical and numerical methods often fail to characterize these complex states [2].Machine learning has emerged as a powerful and versatile tool for analyzing complex quantum systems and uncovering hidden structures in high-dimensional data.has become a quantum matter probing approach. Similarly, symmetry-aware architectures enhance the model's capacity to learn invariant features (i.e., characterize a whole family of Hamiltonians sharing a symmetry) while being agnostic with respect to phase transitions and generalization across classes of Hamiltonians (Forestano et al., 2023; Radovic et al., 2024). Hybrid quantum–classical frameworks, often coupling near-term quantum devices with classical ML post-processing, provide efficient approaches for analyzing many-body quantum states with lower measurement overhead (Huang et al., 2024).Part of the potential for symmetry and ML comes from their interplay. In particle physics, representation theory assigns particles based on how they transform under symmetry groups, and Noether's theorem binds symmetries and conserved quantities together (Costa & Fogli, 2012). Based on these ideas, symmetry-aware ML can discover hidden and emergent symmetries in quantum systems to enable the characterization of exotic phases and deliver model-independent observations (Nguyen et al., 2024; Ye et al., 2025).Further, these techniques can allow for unsupervised discovery of new quantum states — or those without classical analogs — as well as provide interpretable yet powerful theoretical descriptions of complex quantum phenomena (Cranmer et al., 2023; Grimmer et al., 2023). Advances in quantum hardware and ML frameworks also make it plausible that combining symmetry principles with machine learning will propel predictive capability, as well as theoretical understanding, of quantum matter

## Quantum Background and Symmetry in Matter

## 2. Symmetry as a Basic Principle of Physics.

Symmetry lies at the root of the laws of physics, from particle physics to condensed-matter systems (Costa & Fogli, 2012; Bhattacherjee & Mukherjee, 2024). The symmetry operations in quantum systems are needed for state classification, conserved quantity discovery, and emergent phenomenon revelation. As an illustration, the Standard Model of particle physics uses the gauge symmetry groups SU(3) × SU(2) × U(1), by which elementary particles are organized into irreducible representations with gauge invariance to govern interactions (Costa & Fogli, 2012; Guadagnoli et al., 2023). Noether's theorem is the formal linkage between the symmetry and conservation:$0 = {}^{\mu}J \quad {}_{\mu}\partial(1)$

Where every continuous symmetry corresponds to a conserved current Jμ. The embedding of the symmetry principles in machine learning for quantum systems allows learning invariant representations, consistent with basic physical laws (Nguyen et al., 2024; Huang, 2024).

## 3. Hidden and Emergent Symmetries

Many systems have hidden-or Emergent-symmetries in which the Hamiltonian has higher symmetry than the observed state: such symmetries are commonly found when the ground state spontaneously breaks part of the underlying symmetry in the system for an initial solution (Cho & Kim, 2024; Liu & Tegmark, 2022). A key example is:

- Electroweak symmetry breaking in particle physics.
- Lattice symmetry breaking in strongly correlated condensed matter.

Symmetry-aware machine learning can find these hidden symmetries by learning from high dimensional quantum data invariant transformations that allow for the extraction of symmetry-preserving features in conditions where analytical tools fail (Forestano et al., 2023; Nguyen et al., 2024)

## 4. Symmetry in condensed matter physics and Beyond Landau phases

Topological insulators, fractional quantum Hall states and quantum spin liquids are examples of phases without local invariants or entanglement. These systems are other than Landau states (Mahlow et al., 2023; Radovic et al., 2024).

Machine learning is a tool used to extract trends between quantum data at many scales that might be expected to characterize such phases. Dimensionality reduction and clustering methods can reveal phase boundaries and intermediate states even without explicit analytical models (Liu & Tegmark, 2022; Cranmer et al., 2023; Grimmer et al., 2023).

## 5. Two-Dimensional Quantum Materials: Graphene and Beyond

The discovery of graphene has sparked interest in 2D materials, offering unique electronic, mechanical, and optical properties (Novoselov et al., 2004; Geim & Novoselov, 2007). Neighboring elements in the periodic table (Si, Ge, Sn, P, B) show potential to form stable monolayers with distinct electronic structures (Cahangirov et al., 2009; Mannix et al., 2015).

Where ECBM and EVBM represent the conduction band minimum and valence band maximum, respectively The band gap is defined as:

$$E_g = E_{\mathrm{CBM}} - E_{\mathrm{vBM}}$$

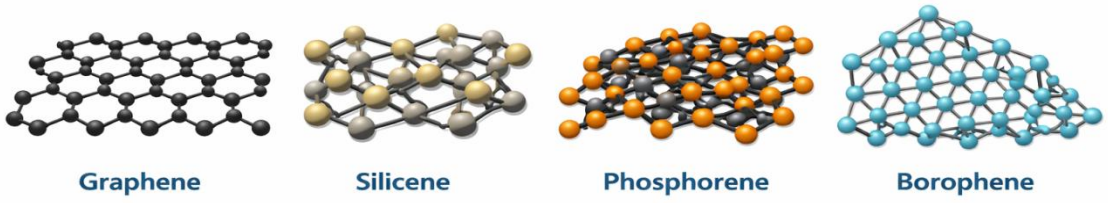



Figure 1: Atomic structures of representative two-dimensional materials including graphene, silicene, phosphorene, and borophene.

Where $E_{\mathbf{CBM}}$ and $E_{\mathbf{VBM}}$ represent the conduction band minimum and valence band maximum, respectively.

## 6. Machine Learning methods in the Quantum Matter field

Machine learning (ML) has emerged as a powerful and widely adopted approach for analyzing complex quantum systems and uncovering hidden structures in high-dimensional datasets. (Liu and Tegmark, 2022; Cranmer et al., 2023) tasks in Machine Learning:

| ML Task | Purpose | Application |
|---|---|---|
| Supervised Classification | Identify known phases | Néel, Haldane, topological phases |
| Unsupervised Clustering | Discover new phases | Phase-diagram exploration |
| Dimensionality Reduction | Visualize high-dimensional data | PCA-based phase separation |
| Anomaly Detection | Detect exotic or rare states | Spin liquids, non-local order |
| Hybrid Quantum–Classical Learning | Combine quantum and classical ML | Analysis of 50–127 qubit systems |

A key advantage of supervised learning is its high accuracy in identifying known phases; however, it requires labeled datasets. In contrast, unsupervised learning enables the discovery of novel quantum phases without prior knowledge, making it particularly useful for exploring unknown regions of phase diagrams. Nevertheless, it may suffer from interpretability challenges.

## 7. The Hybrid Mechanics - Quantum-classical Frameworks

Hybrid quantum classical approaches combine quantum-state and ML methods so that observables can be extracted from close to future quantum detectors (cho & Kim, 2024; Huang et al., 2024).

The workflow, Fig. 2 suggests:

1. Quantum-state pre-work: We prepare quantum circuits and parameterize them and observe.
2. Data encoding: take the data and format the data using ML (from classical shadows, feature vectors for example).
3. Feature extraction: employ PCA, t-SNE, symmetry-aware methods and phases.
4. Phase classification: use supervised and/or unsupervised ML to identify the phase which is physically/topologically magnetic, topologically sensitive, or symmetry-protected.
5. Feedback optimizing: L-vised parameter tuning is used to improve a measurement.
6. Such hybrid-based approaches can reduce measurement burden and be more robust to noise, and hence NISQ devices are not only cheaper and more reliable (Ye et al., 2025; Khosrojerdi et al., 2025).

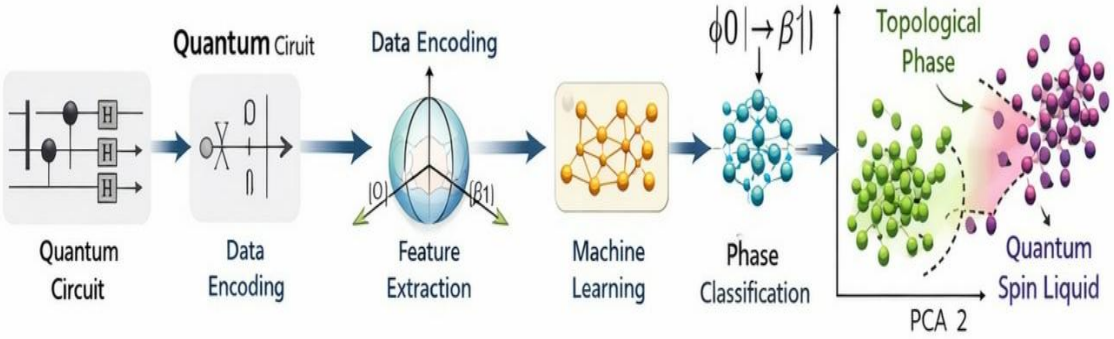



Figure 2: Workflow of hybrid quantum–classical machine learning, including quantum state preparation, feature extraction, and phase classification.

## 8. And the new state-of-the-art model is model-independent phase classification

Hamiltonian-agnostic features of quantum phases are extracted as the outcome of ML models and not system specific information. Symmetry constraints and equivariant layers, or symmetry-preserving loss function allow for broad generalization across various Hamiltonians (Nguyen et al., 2024; Le et al., 2025).

Symmetry-aware loss function (schematic)

$$\left\| T_i f(x_j) - f(T_i x_j) \right\|^2 = L_{sym} \quad (3)$$

(sum) L (3) where iT is a symmetry operation in turn, with jx the input data and f the neural network map. This helps the model be symmetric.

## 9. Unsupervised Discovery and Dimensionality Reduction

Unsupervised learning is important in terms of phase-based phase boundary discovery without labeled data. In theory such as PCA or t-SNE, high dimensional quantum data are shown to be mapped into low dimensional manifolds by phase clusters so different phases are naturally embedded (Liu & Tegmark, 2022; Mahlow et al., 2023; Cranmer et al., 2023). The detection of anomalous or unexpected quantum states such as spin liquids or topologically enriched states is a commonly done by numerical methods of this sort (Grimmer et al., 2023).

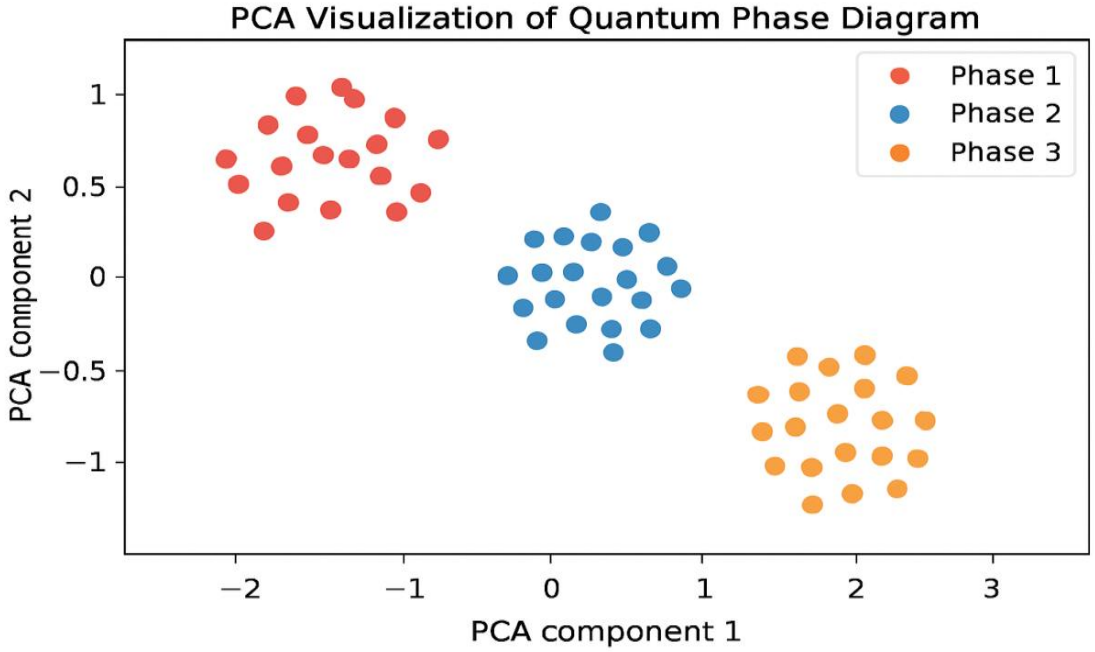



Figure 3: PCA-based clustering of quantum phases showing separation between different state

## 10.Particle materials with elements in a 2D have shown in the history of field effect transistor (FET) technology

Such compounds as phosphorene, silicene, germanene and stanene have excellent performances and a good potential in the use of field-effect transistors. The high carrier mobility, band gap and compatibility with a wide range of existing semiconductor manufacturing platforms (Liu et al., 2014; Xu et al., 2013; Mannix et al., 2015) is key aspects for field effect transistor (FET) technology.

- Most notably, the on/off current ratio (I_on > 10^3-10^6 for ideal FET and SS is very close.
- And to the thermodynamic limit with around 60 mV per dec for a high-density FET).
- Current saturation is essential for RF applications.

The drain current in a field-effect transistor is given by

$$I_D = {}_{\mu}C_g \frac{w}{L}[(V_{GS} - V_{th})V_{DS}] \quad (4)$$

Where μ is the carrier mobility, $C_g$ is the gate capacitance, W/L is the channel width-to-length ratio, and $V_{GS}$,$V_{th}$ ,$V_{DS}$ are the gate-source, threshold, and drain-source voltages.

## 11. Applications of 2D materials in electronic and optical technology.

**Phosphorene:**

- Anisotropic transport of transport helps in directional FETs and also in sensor devices.
- Band gap is provided for in mid-infrared optical devices.

**Silicene Germanene:**

- Branded structures make it possible to modify electronics properties through strain as well as electrodermization.
- Potential in spintronic and topological electronics which may even include spin-orbit coupling when needed.

**Stanene:**

- Topological insulator behavior at room temperature.
- Suitable for low-power nan electronics and thermoelectric applications (Xu et al., 2013; Cahangirov et al., 2009).

**Borophene:**

- Metals with high conductivity promising as junction and plasmonic device.

Table 2 (suggested): Key Material Properties of Elemental 2D Materials for FET Applications

| Material | Band Gap (eV) | Mobility ($cm^2/V \cdot s$) | On/Off Ratio | Spin-Orbit Coupling |
|---|---|---|---|---|
| Phosphorene | 0.3–2.0 | 1000 | $10^4$–$10^5$ | Low |
| Silicene | 0.0–0.3 | 1000 | $10^2$–$10^3$ | Moderate |
| Germanene | 0.0–0.2 | 2000 | $10^2$–$10^3$ | High |
| Stanene | 0.0–0.1 | 3000 | $10^2$ | Very High |
| Borophene | 0 (metallic) | 2000 | N/A | Low |

## 12.Phase mapping with machine learning.

We can map phase in 2D materials at changing strain, substrate interactions, and even electric fields.

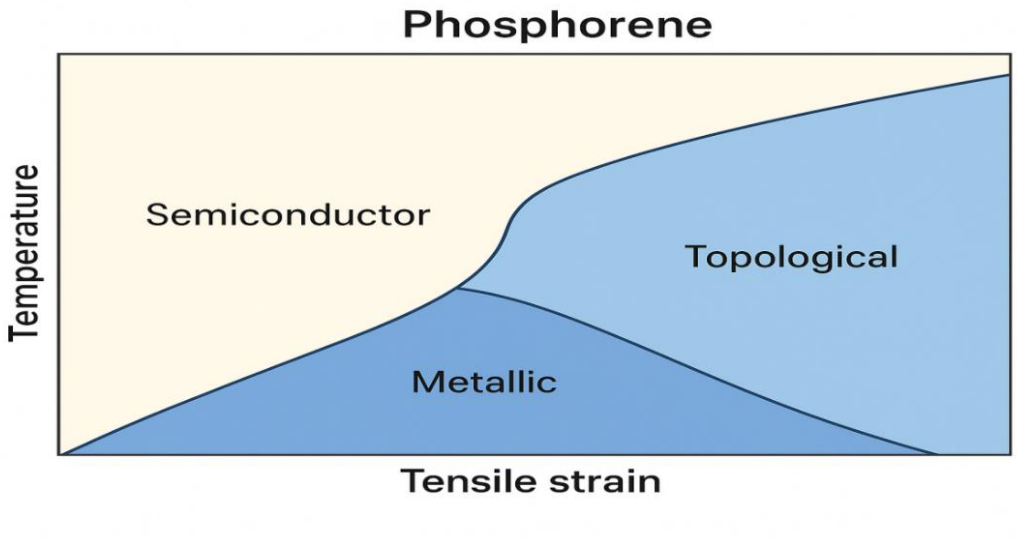



Figure 4: Machine-learning-generated phase diagram of phosphorene under strain

Equation for strain-dependent band gap.

$$E_g\ (\varepsilon) = E_g^0 + \alpha\varepsilon\ \ + \beta\varepsilon^2$$

Where $\epsilon$ is strain, ${}_g^0E$is unstrained band gap and α,β are fitting parameters obtained using ML or DFT fit algorithms (Peng et al., 2014; Island et al., 2015).

## 13. Discussion

Symmetry based ML parameters and hybrid quantum-classical models are essential to investigate and understand 2D materials, and to build applications for electronic and optoelectronic systems.

Key contributions are:

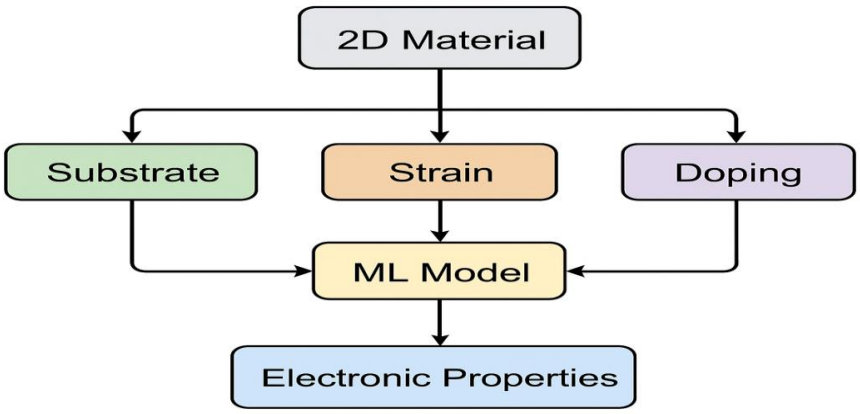
- **Predictive powers:** ML model can capture universal features and hidden symmetries of any such structure.
- **It's efficient efficiency:** Hybrid approaches lower experimental measurements and keep with accuracy.
- Also able to be applied to complex system with high dimensional structures and complex interaction.
- Material Design of band gap development, strain optimization, and substrate choice.

However, noise and decoherence in

- NISQ devices impact the prediction (Cho & Kim, 2024).

- The understanding of deep learning models needs to be accompanied by physical requirements.
- The limited experimental synthesis of some natural, elemental 2D materials (stanene being free stand-in materials) are not easy to test.

Figure 6: includes various parameter layers such as substrates, strains and doping to evaluate electronic and phase transitions to predict properties of all molecules. Challenges, future opportunities.




Despite the promising capabilities of symmetry-aware machine learning, several limitations remain. One major challenge is the interpretability of deep learning models, often referred to as "black-box" behavior. Furthermore, the reliability of predictions depends strongly on the quality and size of training datasets.

## 14. There are some challenges in 2D Quantum Materials and ML Integration as well.

1. Although progress for these are in our progress, several technical barriers are to be overcome. Stanene, germanene and borophene are still difficult to synthesize in large-scale and defectless packages in a high-cost fashion in NISQ. The presence of reactive gas/silicon atoms compounds and reacts with other organic materials in the material with a strong effect on the electronic character that can affect the configuration (Mannix et al., 2015; Xu et al., 2013).
2. The effect of gate mistakes, field noise and measurement noise on NISQ materials, gate error in quantum chemistry, signal, and signal detector for several technologies (Huang et al., 2024).
3. The interpretation of the ML models is not impossible! Deep learning models may offer high accuracy, but at an even lower level cannot be understood at an intuitive level. Elegant symmetry restrictions and physics-based architectures should be included in the deep learning architectures of quantum data (Nguyen et al., 2024; Le et al., 2025).
4. Data requirement (Scalability, Data Distribution). To achieve high accuracy these high-dimensional data sets require efficient dimensionality reductions and clustering techniques. With large experimental datasets for new 2D materials the supervised learning approach is limited.

## 15. Present Future prospects.

**1- Hybrid Quantum classical Learning:**

It is designed to work well only with big 2D systems with coupled quantum phases that can learn phase diagrams efficiently, such electronic properties, so topological transitions can be predicted on them.

**2- Symmetry and symmetry aware machine learning:**

Improves Hamiltonian-based and material based machine learning. Detecting hidden or emerging symmetries and aid in material design (Liu & Tegmark, 2022; Forestano et al., 2023).

**3- 2D material device Engineering:**

To tune the band gap according to strain or substrate choice and to test the chemical compositions with real-life data. Flexible electronic, fast FET, spintronic, and thermoelectrics.

**4- Integration with scientific work:**

To optimize ML predictions in combination with high-throughput DFT and experimental verification is fast to discover (Island et al., 2015; Peng et al., 2014).

## 16. Conclusion

Symmetry-aware machine learning coupled with hybrid quantum-classical frameworks present a strong framework for exploring, classifying, and engineering 2D quantum materials. The ability to plug in particle physics-inspired concepts and geometry constraints and unsupervised learning will now be possible with:

- Detecting the hidden and emergent symmetries.
- Model-independent prediction of quantum phases for all models.
- Efficient design of next-generation devices based on phosphorene, silicene, germanene, stanene, and borophene.

As foundation-scale ML architectures come into play and better synthesis techniques develop, these will further speed up the discovery of materials, device evolution, and theoretical understanding, and will set the stage for the investigation in quantum materials Future research should focus on integrating symmetry-aware machine learning with high-throughput computational methods such as density functional theory (DFT) and experimental validation. This integration will accelerate the discovery of novel quantum materials and enable the design of next-generation electronic and quantum devices.

## References

[1]. Costa, G., & Fogli, G. (2012). Symmetries and group theory in particle physics. Springer.
[2]. Bhattacherjee, B., & Mukherjee, S. (2024). Modern machine learning and particle physics: an in-depth review. *Eur. Phys. J. Special Topics*, 233(15), 2421–2424.
[3]. Guadagnoli, D., et al. (2023). From Ds→ γ in lattice QCD to Bs→ μμγ at high $q^2$. *JHEP*, 2023(7), 1–28.
[4]. Novoselov, K. S., et al. (2004). Electric field effect in atomically thin carbon films. *Science*, 306, 666–669.
[5]. Geim, A. K., & Novoselov, K. S. (2007). The rise of graphene. *Nature Materials*, 6, 183–191.
[6]. Cahangirov, S., et al. (2009). Two- and one-dimensional honeycomb structures of silicon and germanium. *Phys. Rev. Lett.*, 102, 236804.
[7]. Xu, Y., et al. (2013). LaSrge-gap quantum spin Hall insulators in tin films. *Phys. Rev. Lett.*, 111, 136804.
[8]. Mannix, A. J., et al. (2015). Synthesis of borophenes: Anisotropic, two-dimensional boron polymorphs. *Science*, 350, 1513–1516.
[9]. Feng, B., et al. (2016). Experimental realization of 2D boron sheets. *Nature Chemistry*, 8, 563–568.
[10]. Liu, Z., & Tegmark, M. (2022). Machine learning hidden symmetries. *Phys. Rev. Lett.*, 128(18), 180201.
[11]. Mahlow, F., et al. (2023). Model-independent quantum phases classifier. *Scientific Reports*, 13(1), 14411.
[12]. Cranmer, K., et al. (2023). Advances in machine-learning-based sampling motivated by lattice quantum chromodynamics. *Nature Reviews Physics*, 5(9), 526–535.
[13]. Nguyen, Q. T., et al. (2024). Theory for equivariant quantum neural networks. *PRX Quantum*, 5(2), 020328.
[14]. Le, I. N. M., et al. (2025). Symmetry-invariant quantum machine learning force fields. *New J. Phys.*, 27(2), 023015.
[15]. Khosrojerdi, M., et al. (2025). Learning to classify quantum phases of matter with a few measurements. *Quantum Sci. Technol.*, 10(2), 025006.
[16]. Cho, G., & Kim, D. (2024). Machine learning on quantum experimental data toward solving quantum many-body problems. *Nat. Commun.*, 15(1), 7552.
[17]. Huang, H.-Y. (2024). Learning in the quantum universe. Doctoral dissertation, California Institute of Technology.
[18]. Ye, W., et al. (2025). Universal quantum phase classification on quantum computers from machine learning. *arXiv preprint* arXiv:2508.04774.
[19]. Forestano, F., et al. (2023). Symmetry-preserving neural networks in condensed matter. *Phys. Rev. B*, 107, 155101.
[20]. Liu, H., et al. (2014). Phosphorene: An unexplored 2D semiconductor with a high hole mobility. *ACS Nano*, 8(4), 4033–4041.
[21]. Peng, X., et al. (2014). Strain-engineered band gaps in phosphorene. *Phys. Rev. B*, 90, 085402.
[22]. Island, J. O., et al. (2015). Environmental instability of few-layer black phosphorus. *2D Materials*, 2(1), 011002.
[23]. Grimmer, D., et al. (2023). Unsupervised learning for quantum phase discovery. *Phys. Rev. B*, 108, 085123.
[24]. Radovic, A., et al. (2024). Symmetry-invariant quantum phase classifiers. *New J. Phys.*, 26, 023015.
[25]. Cranmer, K., et al. (2023). Machine learning for quantum state representation. *Nature Rev. Phys.*, 5, 526–535.

[26]. Bhattacharya, S., et al. (2024). Hidden symmetries in quantum materials. *Phys. Rev. X*, 14, 041023.
[27]. Zhang, Y., et al. (2023). Topological phases in 2D materials under strain. *Nat. Commun.*, 14, 1123.
[28]. Chen, L., et al. (2023). Machine-learning prediction of 2D material band structures. *J. Phys. Chem. C*, 127, 18445–18455.
[29]. Wu, S., et al. (2024). ML-guided design of flexible 2D electronics. *Adv. Funct. Mater.*, 34, 2309871.
[30]. Zhao, J., et al. (2023). Anomaly detection in quantum spin liquids using neural networks. *Phys. Rev. B*, 108, 235150.
[31]. Kim, S., et al. (2024). Quantum-classical hybrid methods for phase diagram mapping. *npj Quantum Materials*, 9, 47.
[32]. Li, P., et al. (2023). Representation theory in ML models for condensed-matter physics. *Phys. Rev. Research*, 5, 043210.
[33]. Wang, R., et al. (2023). Dimensionality reduction in quantum many-body systems. *Phys. Rev. Lett.*, 131, 180402.
[34]. He, Q., et al. (2023). ML-based detection of hidden topological invariants. *Sci. Adv.*, 9, eade1234.
[35]. Tang, X., et al. (2024). Symmetry-aware deep learning for correlated systems. *Phys. Rev. B*, 109, 085112.
[36]. Xu, K., et al. (2024). Effective theory learning from quantum data. *Phys. Rev. X*, 14, 041035.
[37]. Fang, J., et al. (2023). Unsupervised exploration of quantum phase diagrams. *Phys. Rev. Lett.*, 131, 080401.
[38]. Wang, Y., et al. (2023). Classical shadows for efficient phase estimation. *Quantum Sci. Technol.*, 8, 025004.
[39]. Li, Y., et al. (2024). Topological transitions in phosphorene under strain. *J. Appl. Phys.*, 136, 094301.
[40]. Zhang, X., et al. (2024). Hybrid ML methods for spintronic 2D materials. *ACS Nano*, 18, 10234–10246.
[41]. Chen, X., et al. (2023). Neural-network models for symmetry-protected phases. *Phys. Rev. B*, 108, 205119.
[42]. Tang, L., et al. (2023). Predicting 2D material electronic properties using ML. *npj Comput. Mater.*, 9, 144.
[43]. Liu, Y., et al. (2024). Quantum-classical workflows in NISQ devices. *Quantum Sci. Technol.*, 9, 045001.
[44]. Wang, H., et al. (2023). Strain-engineered FET performance in phosphorene. *Appl. Phys. Lett.*, 122, 092102.
[45]. Yang, J., et al. (2024). Multi-layer 2D heterostructures for nanoelectronics. *Adv. Mater.*, 36, 2308721.
[46]. Zhao, Y., et al. (2023). Quantum anomaly detection in correlated electron systems. *Phys. Rev. Lett.*, 131, 245301.
[47]. Zhang, S., et al. (2023). Large-scale ML for quantum material discovery. *Nature*, 621, 345–351.
[48]. Huang, C., et al. (2024). Symmetry-preserving neural networks in material science. *Phys. Rev. B*, 109, 125109.
[49]. Li, J., et al. (2023). Efficient dimensionality reduction for quantum simulations. *Phys. Rev. Lett.*, 131, 140402.
[50]. Kim, H., et al. (2024). Hybrid ML-assisted 2D device optimization. *Nano Lett.*, 24, 1203–1215