# Machine learning and experiments: A synergy for the development of functional materials

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With machine learning (ML) and artificial intelligence (AI) becoming increasingly refined and accessible, computer engineers and materials scientists are utilizing these data-driven techniques to design new functional materials more efficiently. Additionally, the advancement of simulation software and computing power has substantially lowered the cost of obtaining training data. However, using only simulation data presents a difficulty in the eventual realization of a material design due to possible misalignment of the simulation setup and physical laboratory conditions. Therefore, it is mutually beneficial to also improve the experimental aspect of functional materials development using ML and AI techniques. In this article, we survey the current state of ML/AI involvement in functional materials design, focusing specifically on acoustic/mechanical metamaterials, piezoelectric materials, and biological materials. The macroscopic nature of these functional materials lends well to additive manufacturing fabrication, which makes optimizing the synthesis process of these materials highly desirable. We conclude by pointing out a few promising directions for future investigation of functional materials and their place in societal applications.

## Introduction

Functional materials possess both native properties and special functionalities tailored toward specific applications. For example, metamaterials can interact with electromagnetic/acoustic waves or exhibit unconventional structural behaviors;[1–5] piezoelectric materials can accumulate electric charges in response to mechanical stress;[6,7] biological materials can interface with living cells, tissues, and organs.[8–11] These advancements have greatly expanded the usage of engineering materials past the limitation of traditional mediums such as steel and concrete. Metamaterials can be used in the defense industry as miniature and lightweight microwave absorbers or cloaks to shield military aircrafts from radar detection;[12] piezoelectric materials can be used in a variety of sensors and actuators;[13,14] biocompatible materials can be used as bone implant materials.[15]

The astronomical rise of machine learning (ML) and artificial intelligence (AI) techniques has been observed through their massive popularity among computer engineers and materials scientists to aid in designing novel functional materials.[16–20] A main reason is that ML offers an avenue to bypass traditional engineering thinking, which emphasizes the notion that people need to understand a sophisticated topic before designing with it. When the design task is highly complex and involves too many variables, artificial neural networks can solve the problem through millions of neurons that encode the physics of the problem, saving on both financial expenditures and near-impossible manual calculations. ML is also top-notch at exploring vast design spaces to come up with solutions unintuitive to human engineers, such as highly complex digital materials[21–23] and graphene oxide functional group distributions that result in enhanced mechanical toughness.[24] Additionally, with more computing power, cheaper numerical

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simulations, and abundant training data for ML tasks, researchers reduce the need for expensive, time-consuming, and tedious laboratory experiments. This advancement is critical for the success of ML implementation because the methods typically require a large amount of data during the training process.

Despite flourishing ML and numerical simulations, there exists a weak link in the development chain of ML-assisted functional materials design. For example, little attention has been devoted to resolving the discrepancy between numerical simulations and laboratory experiments. Researchers must acknowledge that not all numerical simulations accurately reflect reality, nor do we have the capability to design experiments that perfectly reflect simulation scenarios. Therefore, it is essential that experimental measurements are consistently used to guide and correct the course of computational predictions throughout the production process. Furthermore, it may be worth considering how researchers can also improve the experimental aspect of functional materials development using insights from ML algorithms, which remains a relatively unexplored territory.

In this article, we review the current state of ML-assisted development of functional materials through an experimental lens. We focus specifically on three types of functional materials: acoustic/mechanical metamaterials, piezoelectric materials, and biological materials. These types of functional materials are mostly macroscopic, which means they can be fabricated by additive manufacturing techniques, making improvements in the experimental aspect of their development a particularly urgent and rewarding goal. We will conclude by pointing out a few promising directions for future investigation of functional materials and next steps to integrate them into industrial settings.

## Experimental aspects of ML implementation in functional materials development

### *Acoustic and mechanical metamaterials*

Metamaterials are intricately engineered materials that possess properties going beyond their natural constituents.[2,25,26] Many acoustic and mechanical metamaterials can interact with different types of waves in an unconventional fashion[27–30] (**Figure 1**a), while others exhibit unique structural properties such as a negative Poisson's ratio,[31–34] a superior strength-to-density ratio,[35,36] or an enhanced energy absorption[37–40] (Figure 1b). With the development of additive manufacturing and computational techniques, a broad range of scientific interests has gone to realizing materials with exceptional performance and versatility. The physical size of the metamaterial is often determined by its functionality. For example, electromagnetic metamaterials are nanoscopic or microscopic to interact with electromagnetic waves, whereas acoustic metamaterials (AMs) are macroscopic to interact with acoustic waves or to shield infrastructure from seismic waves.[41] The size of mechanical metamaterials (MMs) is also determined by use cases, which are usually macroscopic in structural applications. Existing at the macroscale (as opposed to smaller scales) makes the fabrication and testing of AMs and MMs more promising and

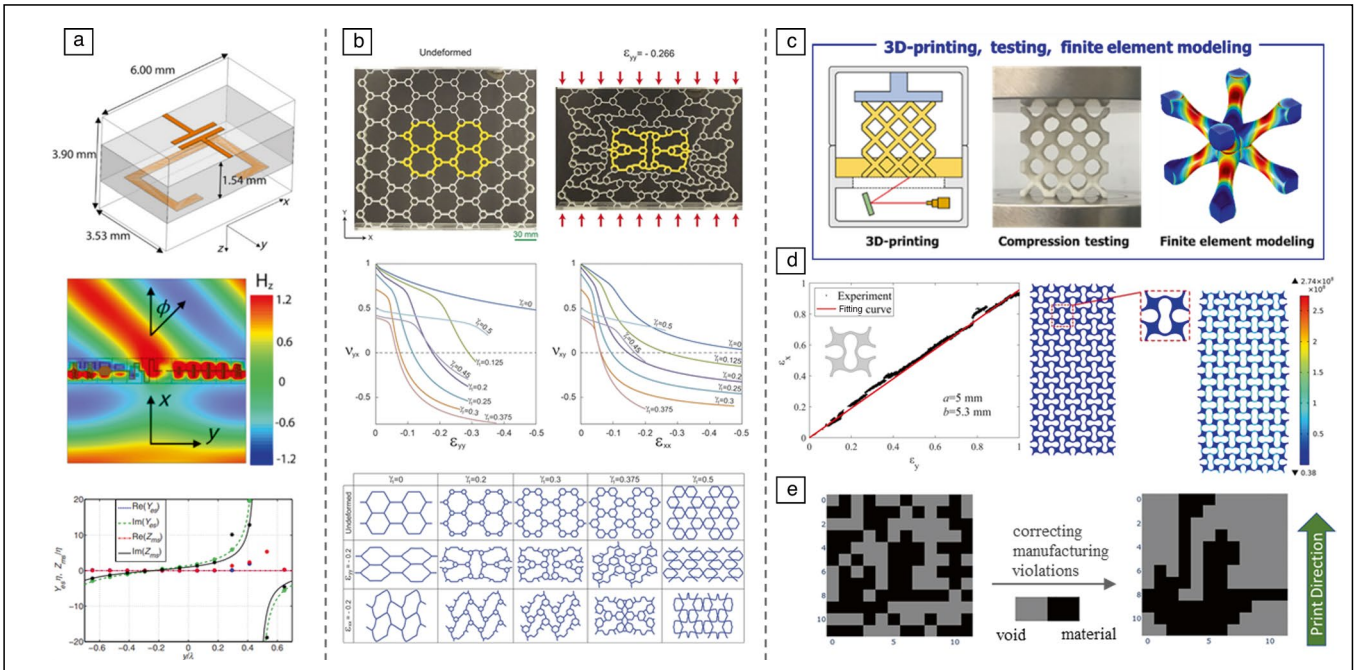


**Figure 1.** (a) An example of metamaterials for tailoring wavefronts with reflectionless sheets. Adapted with permission from Reference 27. (b) An example of mechanical materials (MMs) designed with hierarchical honeycomb, adapted from Reference 33. (c) Illustration of using compression tests to validate the machine learning (ML) generated design, adapted from Reference 50. (d) Illustration of using experiments to verify the simulation before training a simulation-based ML model, adapted from Reference 56. (e) Illustration of adding fabrication constraints on the design to ensure manufacturability. Adapted with permission from Reference 60.

therefore more important, because the manufacturing techniques at this scale are much more mature and feasible than microscale and nanoscale. However, ML-based studies, such as achieving a target operating frequency,[42–44] maximizing the acoustic bandgap for AMs,[45–47] and tailored deformation behavior for MMs,[48] are often based on simulation data alone. Reliable fabrication and experimental testing are relatively overlooked, which hinders optimal designs from being realized and deployed in critical, real-world applications. In the following, we will discuss the usage of experimental approaches in ML-based AM and MM designs.

The simplest synergy of experiments with ML-based design is using experimental measurements to validate results. Liu et al. conducted fabrication and mechanical tests to verify ML-designed multistable MMs with curved beams.[49] First, they ran finite element (FE) simulations based on randomly generated beam profiles to provide training data, which were later used to train a neural network surrogate model. With the surrogate model, they performed an efficient optimization of curved beams with varying thickness, objectives being stiffness, forward snapping force, and backward snapping force. Finally, they validated the optimal design of multistable MMs with 3D printing and compression tests. Lee et al. also verified generative ML-designed Bézier curve-based lattice MMs using additive manufacturing and compression tests, as shown in Figure 1c.[50] The authors modeled the beams of the lattice structure as highly flexible and smooth Bézier curves to augment the design space, and then used a combination of deep learning and genetic algorithms to solve the optimization problem. They showed in experiments that the optimal design of lattice MMs with Bézier-curve beams outperformed those with cylindrical and graded-density beams in terms of stiffness and strength. Other examples include ultrathin acoustic absorbing metasurfaces,[51] acoustic sinks,[52] AM absorbers,[53] auxetic MMs,[54] and lightweight lattice MMs,[55] among others.

Another approach is to use experiments to calibrate simulations before providing training data for ML. For example, Zhang et al. performed experiments to verify their FE model for planar auxetic MMs before running extensive simulations to generate data, as shown in Figure 1d.[56] In the ML design of strut-based multimaterial MMs, Mirzaali et al. calibrated FE simulations with tensile tests before data generation.[57] The two approaches described so far are not mutually exclusive, and some researchers use both to solidify ML-optimized designs. For example, Lee et al. used experiment-calibrated simulations to provide training data and experimentally tested the final design of gradient-index phononic crystals for energy focusing and harvesting.[58]

More creative approaches that integrate ML and experiments can be considered. One such approach includes manufacturing constraints in ML. Bessa et al. placed constraints in the ML algorithm to penalize slender elements in MMs, which are hard to 3D-print without defects.[59] They then applied sensitivity analysis to determine the combinations of parameters that have more impact on the desired properties to reduce the number of design parameters before training an ML model. Figure 1e also shows an example of adding fabrication constraints as part of the design process. From the figure, we can see that Garland et al. enforced multiple rules in the ML-generated MM unit-cell designs to ensure manufacturability, including restricting unit cells to have a contiguous body connected from top to bottom, disallowing hinge point connections, and keeping the effective density high enough for printing.[60] The constrained unit cells are then tiled into a lattice and boundary conditions are applied to the entire structure. Wang et al. ensured the fabricability of optimized cloaking MMs by constraining the properties within the precomputed unit-cell database during the optimization process.[61] Cloaking MMs are a novel type of MMs that can manipulate the elastic response around objects to make them indistinguishable from their homogeneous surroundings. The authors demonstrated the successful data-driven development of the cloaking MM via 3D printing and digital image correlation (DIC). Yet another way is to use experiments to explain ML-optimized designs. Researchers have also used DIC techniques to uncover the mechanisms of ML-designed tough bioinspired hierarchical MMs.[62] By inspecting the DIC results, they found that the strain fields of the more optimal sample are more uniform and distributed compared to that of the sample with lower toughness with a high strain concentration at the crack tip. This shows that the ML model has learned the patterns for generating designs with desired performance, the desired performance relating to material toughness and strength, in this case.

Integration of experiments and ML algorithms has greatly assisted the development of AMs and MMs by verifying optimal designs, calibrating training data, applying practical manufacturing constraints to the algorithms, and bringing insight to black-box models. Incorporating fabrication and experiments into the model training process can effectively bridge the gap between model-proposed designs and real-world applications. Potential future research directions include using experimental results as training data directly with data-efficient algorithms and learning design principles to iteratively improve functionality. Promising progress has been made in this direction. Gongora et al. used active learning to select experiments to design structures with superlative toughness.[63] Combined with a database of simulations, active learning-guided experiments can further accelerate the discovery of tough and resilient materials.[64] The same research group has also shown that transfer learning can make use of large databases of simple experimental measurements to predict complex properties.[19]

## Piezoelectric materials

Piezoelectric materials can generate an electric field by mechanical deformation (stress and strain) through what is referred to as the direct piezoelectric effect. Conversely, mechanical deformation in response to an electric field is known as the indirect piezoelectric effect. Due to this property,

piezoelectric materials have been used as highly effective sensors,[65–68] actuators,[66,69] and energy harvesters.[66,70] There are two main types of piezoelectric materials, ceramics and piezoelectric polymers. Ceramics possess a high piezoelectric coefficient and considerable energy-storage capability, whereas polymeric piezoelectric materials have comparably high flexibility, high breakdown strength as well as lighter weight. These tradeoffs between the two types of piezoelectric materials pose a challenge to their general application. Therefore, developing various approaches to finding an optimum ceramic mixing or polymer/nanoparticle composite ratio is necessary for achieving superior properties.

So far, many new material developments have been time-consuming and mainly based on trial-and-error experiments. However, the synergy between rapid advancements of computation and materials science has enabled an efficient computation-aided material design approach. In addition, the explosive growth of material databases, such as the Materials Genome Initiative (MGI)[71,72] and the Materials Project,[73] expedites migrating into a modeling-driven era in which trial-and-error experiments can be replaced by systematic, predictive material design methodology. Furthermore, ML methods can be used to learn from existing data. For example, Li et al. conducted physics-based simulations of polymer/nanoparticle composites using the phase-field method with regression ML.[74,75] The influence of the morphological orientation of the nanofiller in the polymer matrix was observed in terms of the composite's piezoelectric, mechanical, and dielectric properties. However, ML techniques solely based on simulations cannot include the variety of processing conditions and chemistry from real-world experiments. Therefore, employing comprehensive experimental data approaches has been attracting attention.[76]

The first approach is to validate ML-optimized material compositions and mixing ratios through experimental data. To tackle the challenge of low charge storage in piezoelectric polymers, Shen et al. designed polymer nanocomposites with high energy density, which is essential in energy-storage devices, by using ML.[77] Identifying the proper mixing ratio and type of nanofillers in polymer piezoelectric materials is critical in overcoming these limitations and creating high energy density materials. Five typical nanocomposites with 0D, 1D vertical nanofibers, 1D parallel nanofibers, 2D vertical nanosheets, and 2D parallel nanosheets are used to create the phase-field model to study the nanofiller effect, as shown in **Figure 2**a. Shen et al. performed 6615 high-throughput phase-field calculations to quantify the energy density, and constructed, using these calculation results, a data set mapping the microstructures to the properties of polymer nanocomposites as the ML training data. The energy-storage capabilities of 2205 polymer nanocomposites were evaluated using a scoring function, and some potential nanofillers were screened using a back-propagation algorithm. Finally, the authors fabricated P(VDF-HFP)/$Ca_2Nb_3O_{10}$ (poly(vinylidene fluoride-hexafluoropropylene) copolymer/$Ca_2Nb_3O_{10}$ perovskite nanosheets) nanocomposites to verify the design. As a result, Shen et al. nearly doubled energy density of the materials through this method with a modest increase in efficiency.

The second approach is to use experimental data as the training and test data for the ML algorithm. Yuan et al. suggested a method for determining superior energy-storage capability in the specific region between the ferroelectric phase and the relaxor ferroelectric phase, which was previously limited in complicated multicomponent systems due to the requirement of prior phase diagram knowledge.[78] This study examined the effectiveness of two ML techniques to find multicomponent solid solutions with higher energy-storage density in $BaTiO_3$-based ceramics using experimental data. Yuan et al. used two different kinds of strategies, as depicted in Figure 2b. The first deployed an ML algorithm based on support vector machines with a radial-based kernel function (SVR.rbf) and adaptive design to evaluate a massive virtual space with nine million compounds. The second strategy employed ML classification and regression models, as well as adaptive design, which allowed only a subclass of compounds to be evaluated in the virtual space. A compound with the highest energy-storage density of 73 mJ/cm$^3$, $(Ba_{0.86}Ca_{0.14})(Ti_{0.79}Zr_{0.11}Hf_{0.10})O_3$, in an electric field of 20 kV/cm was obtained. The same researchers also provided a data-driven paradigm to search for ferroelectric ceramics with an increased piezoelectric constant.[79] In this study, four different kinds of surrogate models were compared using SVR.rbf for the incremented piezoelectric constant as shown in Figure 2c. The feature selection technique was demonstrated by two approaches. One is finding the best $d_{33}$ among a group of 98 compositions using numerical simulations, and the second one is developing new compositions with enhanced $d_{33}$ through experimental synthesis. Finally, three iterations of a closed feedback loop using experimental synthesis led to the discovery of a configuration with a 430 pC/N piezoelectric constant, which is an improvement over the raw data.

The use of non-centrosymmetric (NCS) materials such as $BaTiO_3$ is of wide interest in both academia and industry owing to their exciting properties, including piezoelectricity, ferroelectricity, and nonlinear optical activity, which are allowed from the lack of inversion symmetry in these materials. This inversion symmetry breaking originates from distortions in d0 early transition-metal (ETM) octahedra. However, the development of new NCS material derived from d0 ETM octahedra is challenging because polar ETM octahedra tend to adopt centrosymmetric arrangements.[80–84] Accordingly, racemic compounds have attracted attention to replace NCS materials as these compounds contain chiral basic building units to guarantee the inversion symmetry breaking.[85,86] Nisbet et al. presented the targeted synthesis of a series of polar racemates based on d0 ETM octahedra and racemic combinations of chiral copper-bipyridine coordination complexes, as shown in Figure 2d, and showed they possess comparable piezoelectric properties to those of commercial NCS materials.[87] They applied supervised ML models and trained them

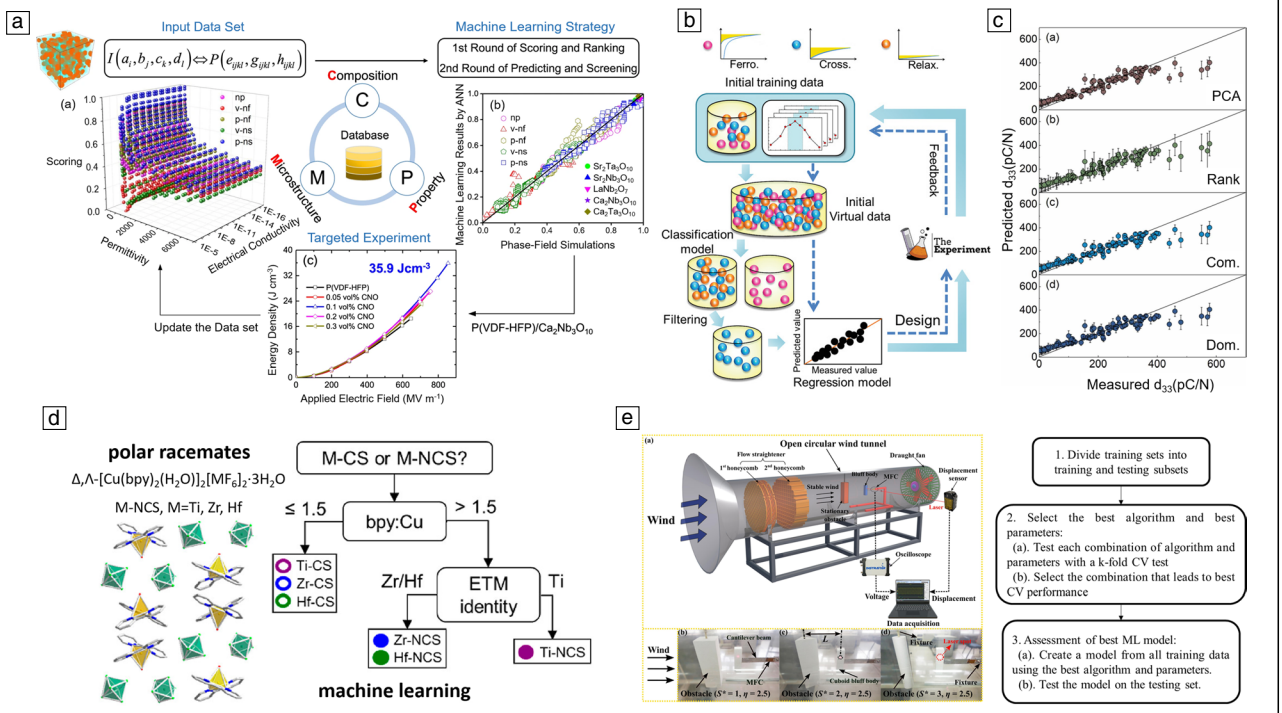


**Figure 2.** (a) Schematic diagram of the progression of simulation-guided material design from theoretical prediction to specialized experiment, adapted from Reference 77. (b) Schematic flow chart of adding experimental data set into the training data set for two different machine learning (ML) algorithms. The inner loop is based on SVR with only the regression ML model. The outer loop is based on a combination of classification and regression ML models. Adapted with permission from Reference 78. (c) Four experiment-based surrogate models trained with different feature selection strategies, including SVR.rvf ML, principal component analysis (PCA), gradient boosting tree, composition and domain knowledge, adapted from Reference 79. (d) Crystal structure of Δ, Λ-$[Cu(bpy)_2(H_2O)]_2[MF_6]_2{\cdot}3H_2O$ (M-NCS, M = Ti, Zr, Hf), and polar structure composed of chiral Δ, Λ-$Cu(bpy)_2(H_2O)^{2+}$ cations and weakly polar $MF_6^{2-}$ anions. Composition space of these structures is optimized with decision tree. Adapted with permission from Reference 87. (e) Schematic of the wind tunnel experiment to obtain input parameters used in tenfold cross-validation method with three-stage evaluation process. Adapted with permission from Reference 106.

on reaction parameters to gain unbiased insight for the composition space, as the relevant hyperparameters such as tree depth and leaf sample splits were optimized via a permuted grid search. The data set used in this ML model consisted of 51 experiments transcribed from laboratory notebook records using the ESCALATE ontology.[88] Moreover, additional stoichiometric features such as molar amounts and molar ratios were calculated directly from the raw experimental data on the $TiF_6^{2-}$, $ZrF_6^{2-}$, and $HfF_6^{2-}$ anionic building units to provide data on geometry, energetics, and charges. Their ML model predicted that formation of the Ti-NCS compound requires the amount of HF present in the reaction to decrease to raise the pH, which was later verified experimentally. Furthermore, the ML-aided composition space visualization captured the unique character of $TiF_6^{2-}$ anion for the out-of-center distortion due to a strong bonding interaction that gives the second-order Jahn–Teller character, in which decision tree classification and predictive ML models identified statistical differences in the three composition spaces examined in this work.

Despite the intriguing property of piezoelectric materials as electromechanical transducers, tradeoffs still exist when using these materials in such applications. For instance, piezoelectric materials often contain lead in the form of lead zirconate titanate (PZT) that is biologically harmful and therefore limits their application in the biomedical field.[89–92] Recently, as a comprehensive design approach to consider tradeoffs in materials, density functional perturbation theory (DFPT) has been widely employed to effectively calculate the second-order derivatives of total energy with respect to atomic displacement.[93–97] Choudhary et al. developed accurate classification and regression ML models to prescreen high-performance materials for the next set of DFPT calculations, without performing additional expensive first-principles calculations.[98] They used classical force-field inspired descriptors (CFIDs) and gradient-boosting decision trees (GBDTs) for the ML classifiers to predict whether a material has a high piezoelectric coefficient (>0.5 $C/m^2$) and dielectric constant (>20). Using 10,305 materials list in the ML models, which are selected from material experiment data such as the JARVIS-DFT database (with OptB88vdW bandgaps >0.1 eV and energy above convex hull <0.5 eV/atom), they found examples of predicted lead-free high-piezoelectric materials that have not been reported in the literature, such as $MoO_3$ (JVASP-30103), $YWN_3$ (JVASP-38813), $W(BrO)_2$, etc. In this study, piezoelectric coefficients were validated by comparing with experimental ones for several

classes of materials such as oxides, nitrides, and sulfides, and in several crystal structures.

Energy generated via vibrations from the natural environment is an attractive form of the renewable clean energy with immediate impacts in our daily life.[99,100] Moreover, this energy can be converted into usable electrical energy through various electromagnetic[101–103] and electrostatic[104,105] pathways. Among them, piezoelectric energy harvesters made of piezoelectric materials have been considered as a strong candidate due to their relatively high power density and simple implementation. Particularly, wake-galloping piezoelectric energy harvesters (WGPEHs) have been proposed for efficient energy harvesting. Wake-galloping is a phenomenon of the aerodynamic instability that induces large vibrations, such as wind-induced vibration of offshore risers. Zhang et al. studied the vibration response of WGPEHs by using ML models to predict the harvester's voltage and displacement output.[106] To specify input parameters used in ML models, they conducted wind tunnel experiments, as shown in Figure 2e. As a result, they found four parameters that have a significant effect on the vibration response—cross section, diameter ratio, distance between two object centers, and velocity span of WGPEHs. Overall, their experimental results showed that with the increase of the diameter ratio, the velocity span at the maximum voltage and displacement of WGPEHs gradually increased, and those maximum voltage and displacement values also gradually increased. Similarly, with the increase of the distance between two object centers, the velocity span at the maximum voltage and displacement gradually increased, but those maximum voltage and displacement values presented a trend of first increasing and then decreasing. Using these four parameters as input features, they applied and compared three different ML algorithms of decision tree regressor (DTR), random forest (RF), and gradient boosting regression trees (GBRTs). Their study showed the GBRT model performs best in predicting both the voltage and displacement output of WGPEHs. For piezoelectric nanogenerators, see a review paper by Jiao.[107]

ML models used in piezoelectric material designs can provide helpful statistical information to qualitative inferences made by human inspection. Furthermore, ML models can quantify the conventional qualitative arguments of material design space and capture the salient phase-boundary information in small experimental data sets.

## Biomaterials

Biological functionality is an indispensable attribute with essential benefits for healthcare technologies. Constructing personalized biomaterials for translational medicine already entails massive hurdles due to the interplay between the material composition, surface properties, and biological responses.[108] However, ML has already proven indispensable to facilitate numerous aspects of materials innovation, from data mining of literature to identify specific features to investigating nanobiotechnologies and their cellular interactions in clinical studies.[109]

Bioinspired synthetic functional materials have been developed with great success by taking the ingenuity of nature's evolutionary optimization to achieve enhanced biological performance. For example, superhydrophobic materials have been created from fine branch-like nanostructures on the surface of a lotus leaf,[110] antibiofouling can be realized based on placoid scales structures from shark skin,[111] and stronger adhesives have been invented with the efficacy of mussels,[112] geckos,[113] and slugs.[114] However, it is often challenging to mimic bioinspired materials because they require comprehensive understanding of biological operation principles, and reproducing the outcome may necessitate both sophisticated simulation models as well as trial-based experiments. ML-aided computational methods have provided enormous benefits to the understanding and exploration of better biological functional materials, which has advanced materials discovery, materials synthesis, and protein structure predictions.[115–117]

In addition to computational approaches, ML-powered experimental methods have shown promising results in creating advanced functional biomaterials. Wu et al. designed a neural network-based ML method to recommend an affordable new Ti alloy with a bone-like modulus.[118] The model is trained using a small amount of data from high-throughput experiments, as shown in **Figure 3**a. The best synthesized Ti-12Nb-12Zr-12Sn (in wt%) composite alloy shows superior biocompatibility, a modulus close to cortical bone, and lower cost (Figure 3b).

Besides improving the target properties of biomaterials, ML methods can monitor and correct for the quality of the prototype *in situ* by rapidly stabilizing various printing processes during fabrication. For example, using a high-resolution camera and machine vision system to monitor jet angle and Taylor cone volume enabled highly accurate melt electrowriting (MEW) of small diameter fibers in tandem with SEM imaging for real-time diameter measurement verification.[119] The 12-mm-thick collapsible MEW tubes developed exhibit a distinct elastic snap-through property often associated with MMS. Jin et al. also established a novel anomaly detection system using advanced convolutional neural network (CNN) models evaluated on real-time images captured by a commercially available bioprinter, which showcased how the transparent biomaterial gelatin methacrylate (GelMA) could be monitored and corrected for defects in the extruded hydrogel.[120] Kang et al. introduced a micro/nano current detection module and data processing program shown in Figure 3c to recognize different jet ejection modes of electrohydrodynamic direct-writing (EDW), a novel update that promotes precise patterning of structures for wearable electronics and biosensors.[121]

Moreover, living biological states are also considered as target objectives for ML models to assist in creating biocompatible materials. Recently, Xu et al. developed a predictive model for stereolithography-based bioprinting using an

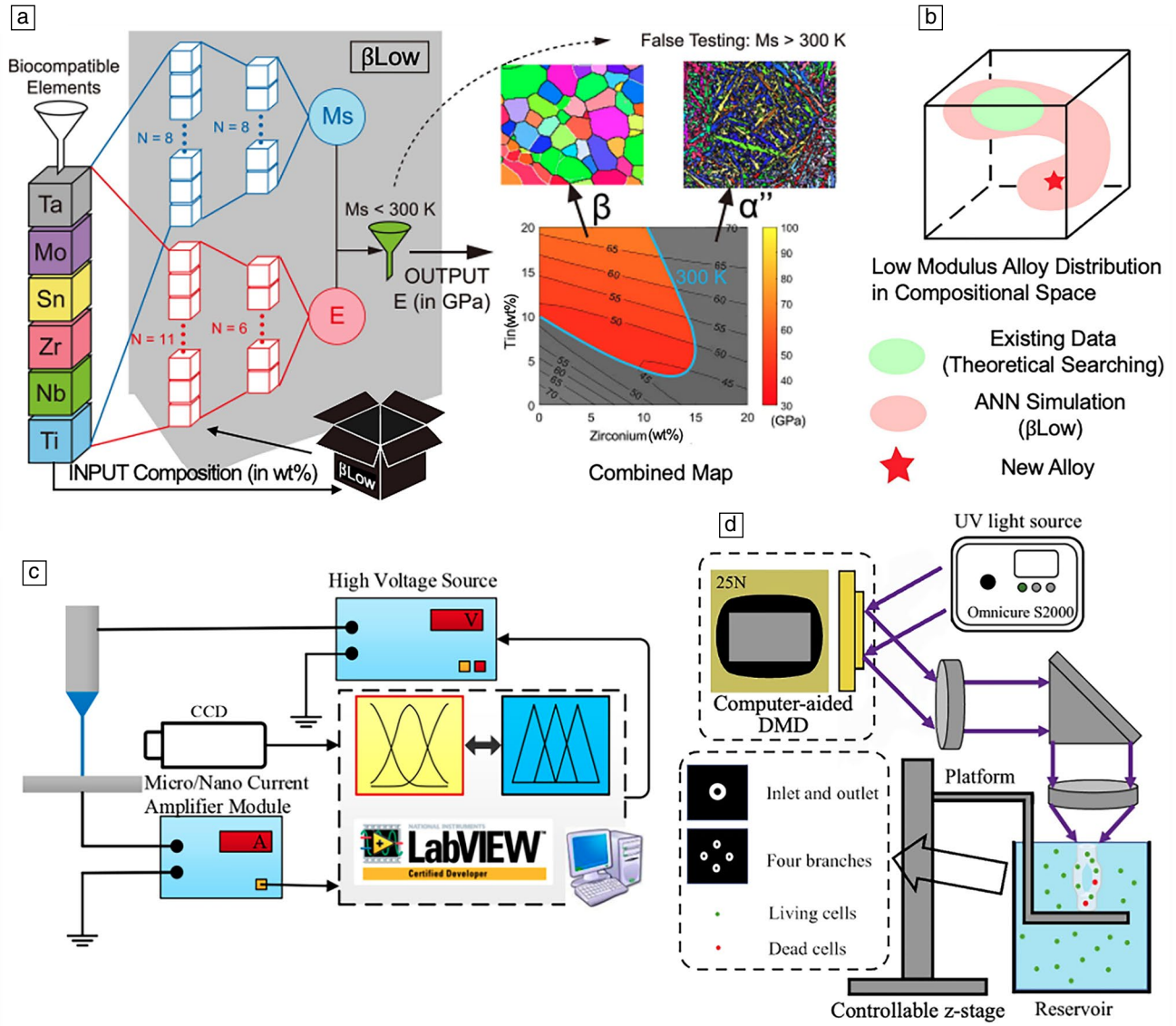


**Figure 3.** (a) Schematic flow chart of machine learning (ML)-assisted approach (βLow) for Ti alloy discovery, which includes property prediction, Ms temperature filtering, and generating combined maps, adapted from Reference 118. (b) Illustration of the ML guided alloy discovery, adapted from Reference 118. (c) Schematic setup of the current detection and measurement system synchronized with a data processing program for electrohydrodynamic direct-writing, adapted from Reference 121. (d) Illustration of experimental setup for bioprinting system with the 2D patterns of a four-branch vascular structure and cell condition during printing, adapted from Reference 122.

ensemble learning algorithm to predict cell viability via an experimental approach, in which traditional physics-based models are constrained due to the complexity of cellular structures and cell recovery (Figure 3d).[122] Here, physics-based models are not applicable due to the complexity of cellular structures and cell recovery. Four critical process parameters (UV intensity, UV exposure time, gelatin methacrylate concentration, and layer thickness) were studied and 405 experimental data points were collected by varying these four printing settings. Cell viability was predicted with high accuracy (R-squared value of 0.953) using the process parameters as inputs through an ensemble learning approach that combines neural networks, ridge regression, *k*-nearest neighbors, and random forest methods. A study by Barrera et al. also made key contributions to the field of tissue engineering, where they employed 3D CNNs (trained using digital tomographies obtained from CAD models) to accelerate the design process of complex scaffolds with tunable porosity and geometries. Their ML intensive strategy circumnavigates the limitations of using traditional finite element modeling simulations alone, which ultimately allows them to achieve multi-objective optimizations to forecast the biomechanical properties of a new set of engineered tissue scaffolds and expand on the larger metamaterials sphere.[123]

## Discussion and future perspectives

A variety of functional materials have been achieved with experimentally aided ML approaches, using state-of-the-art algorithms, as presented in the previous sections. Although some methods could be specific to a particular problem, other methodologies have a broader application domain, which are worth mentioning. For example, Raccuglia et al. utilized failed experimental data to develop a support vector machine-derived decision tree model to predict reaction outcomes for the crystallization of templated vanadium selenites.[124] It is illuminating that ML models can take advantage of perceived negative results and learn toward the desired targets like an experienced experimental operator. As ML models usually require a massive amount of training data, automated high-throughput experimentation methods have been actively deployed in materials synthesis, characterization, and measurement.[125–127] For example, thermal conductivity measurements are conducted by time-domain thermoreflectance using a femtosecond laser in a pump-probe configuration.[128] Using the same laser system, coefficients of thermal expansion are measured through high spatial resolution techniques.[129,130] Moreover, high-throughput experimentation methods have shown great success in exploring other materials properties including elastic modulus,[131] specific heat capacity,[132] and toxicity.[133] By combining ML algorithms, process–structure–property relationships can be revealed based on data obtained from high-throughput experimentation.

In addition to pure experimental approaches in the ML implementation, studies are also developed by adopting both experiments and numerical simulation models to reach the objectives, such as superior materials properties and better process parameter combinations.[59,134] However, most studies treat the experimental approach as a validation procedure when evaluating the performance of the simulation model or the optimization outcome. It is worth noting that the nature of data from simulations and experiments are distinct. Simulation data are considered biased, dense, and mostly low-fidelity due to the assumptions deviating from real-world conditions. Experimental data are unbiased, sparse, and noisy due to the error introduced during experiments. Experimental data can be treated as high-fidelity after repeated experiments. It offers great value if both types of data structures are fused effectively when building predictive ML models. Similar ideas have been developed in recent studies such as FE analysis-informed Bayesian optimization (BO) achieving accelerated exploring speed compared to the conventional BO method.[64] Another generalizable framework, Multi-fidelity BO, is also emerging for successfully addressing material design problems, such as searching for optimal bulk modulus in alloy composition[135] and mechanical structural optimization.[136]

## Summary

The frontier of materials development still has vast expanses to explore, and computationally driven processes are bound to accelerate the pace of innovation across all categories of functional materials. The integration of experiments and ML algorithms has shown a promising synergy to develop acoustic and mechanical metamaterials through multiple channels: calibrating training data, manufacturing constraints for algorithms, bringing insights to black-box models, and verifying optimal design parameters. Furthermore, the ability to rapidly optimize materials composition and geometric parameters of composites has demonstrated the strengths of ML models in realizing increased piezoelectricity or energy-storage density of synthesized materials. In the realm of functional biomaterials, employing computers to evaluate the various degrees of uncertainty inherent to cell culture studies and living organisms is critical to developing biocompatible, biodegradable, and effective structures. ML algorithms can be used to tune the mechanical properties of biomaterials to better mimic *in vivo* conditions, which can lead to effective pharmaceutical delivery and enhanced cell viability of biomedical devices.

Across the research domain, an overarching goal is to also take advantage of experimental training data in combination with data-efficient algorithms to iteratively improve the accuracy of ML models over time. Generalizable approaches such as high-throughput experimentation and Bayesian optimization have been actively applied to experimental ML methods in creating functional materials. Future directions include utilizing multi-fidelity data from both experiments and numerical simulation to accelerate and improve ML model performance. The bridge connecting materials science and computational engineering is narrowing the gap between theoretical and empirical findings, and thus, we hold an optimistic outlook toward societal implementation of advanced functional materials.

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## Conflict of interest

The authors declare no conflict of interest.

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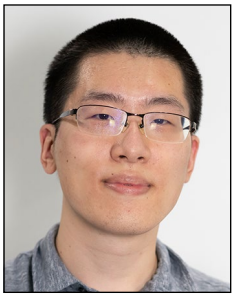

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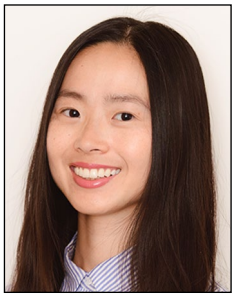

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