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Maximizing Triboelectric Nanogenerators by Physics-Informed AI Inverse Design

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Triboelectric nanogenerators offer an environmentally friendly approach to harvesting energy from mechanical excitations. This capability has made them widely sought-after as an efficient, renewable, and sustainable energy source, with the potential to decrease reliance on traditional fossil fuels. However, developing triboelectric nanogenerators with specific output remains a challenge mainly due to the uncertainties associated with their complex designs for real-life applications. Artificial intelligence-enabled inverse design is a powerful tool to realize performance-oriented triboelectric nanogenerators. This is an emerging scientific direction that can address the concerns about the design and optimization of triboelectric nanogenerators leading to a next generation nanogenerator systems. This perspective paper aims at reviewing the principal analysis of triboelectricity, summarizing the current challenges of designing and optimizing triboelectric nanogenerators, and highlighting the physics-informed inverse design strategies to develop triboelectric nanogenerators. Strategic inverse design is particularly discussed in the contexts of expanding the four-mode analytical models by physics-informed artificial intelligence, discovering new conductive and dielectric materials, and optimizing contact interfaces. Various potential development levels of artificial intelligence-enhanced triboelectric nanogenerators are delineated. Finally, the potential of physics-informed artificial intelligence inverse design to propel triboelectric nanogenerators from prototypes to multifunctional intelligent systems for real-life applications is discussed.

1. Introduction

Triboelectric nanogenerators (TENGs) are devices that can convert mechanical excitation into electrical signals via triboelectrification effect and electrostatic induction.[1] The combined capabilities of renewable energy generation, sustainability, and self-powering, coupled with the potential for widespread integration, have driven significant interest in TENGs over the past decade. TENGs have been extensively investigated for harvesting energy from various resources ranging from large-scale excitations induced by wind and ocean waves to subtle mechanical energy generated by heartbeat and breathing from life activities.[2,3] Electrical signal analysis has recently directed TENGs to the other main domain of active sensing such as microscale biocompatible electronics and ultra-flexibly multiscale sensors in biomedical and bioengineering applications.[4]

Contact electrification between solid–solid cases is typically characterized by electron transfer, which can be explained by, for example, the surface states model for dielectric materials and Fermi level for metal. Two atoms are likely to attract each other

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DOI: 10.1002/adma.202308505

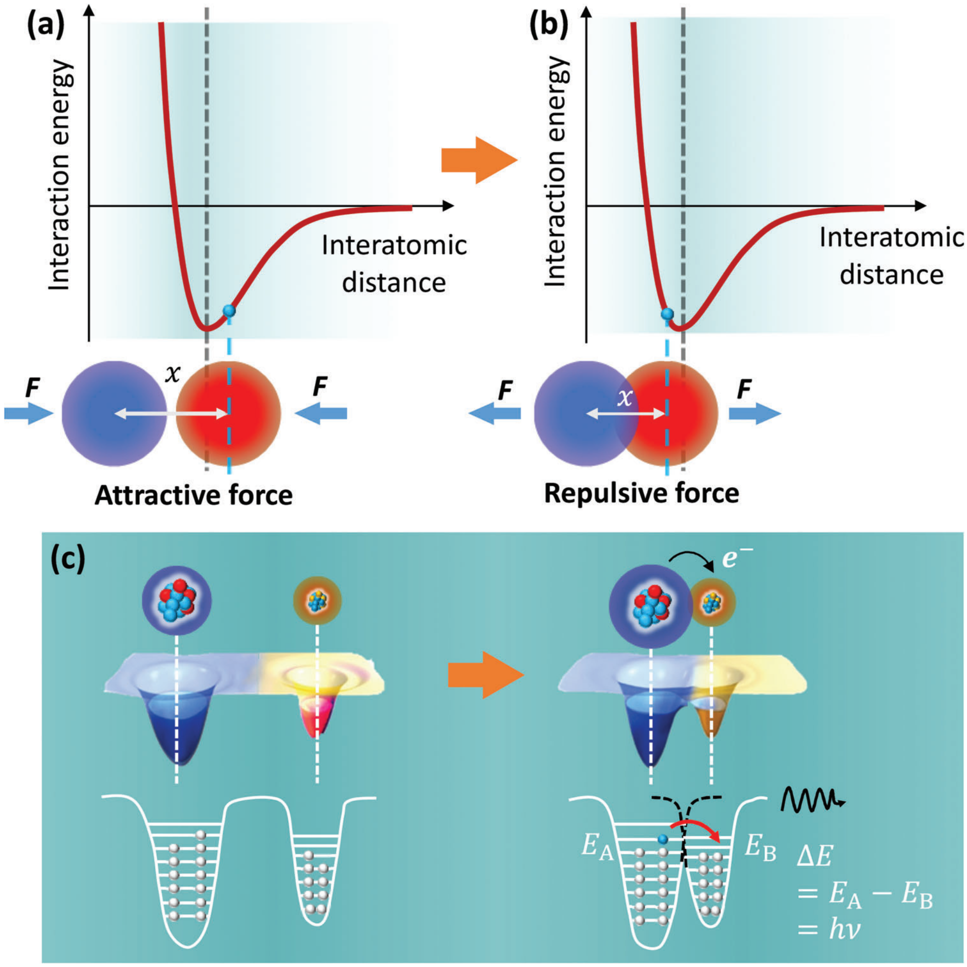

Figure 1. Contact electrification and triboelectrification. Two atoms are likely to a) attract each other when the distance between the two materials is larger than the bonding length, and b) repulse when the distance is smaller than the length. c) Strong electron cloud overlap occurs between the atoms when the atoms are adequately close and eventually contact, which results in the lowered potential barrier and eventually the electron transition.

when the distance of the two materials is larger than the bonding length, as shown in **Figure 1**a. Figure 1b displays the contact electrification exists in the repulsive force region between the interaction potential of atoms when the atomic distance is smaller than the bonding length. When the atoms are adequately close and eventually contact, a strong electron cloud overlap between the atoms results in the lowered potential barrier and thus the electron transition, as shown in Figure 1c. Due to the coupling effect of contact electrification and electrostatic induction, triboelectrification has been used to convert arbitrarily distributed mechanical energy into electric energy, such as TENGs with the merits of, through certain design, high energy efficiency, various material options, simple structures, low cost, etc.[2]

Compared with their counterparts in energy harvesting and sensing, TENGs have exhibited several advantages including wide material options, low cost, and high energy conversion efficiency.[1] To improve the electrical performance of TENGs, recent research trends have been shifted to the optimization of TENGs in three perspectives, that is, composition alteration of friction materials, promotion of dielectric properties, and optimization of interfacial microstructures.[5–7] Research efforts have been dedicated to determining the compositions of friction materials for advanced electrical properties of high conductivity and low resistance such as conductive elastomers.[8] Advanced material technologies have been used to tailor dielectric materials with tunable properties in triboelectric pairs such as computer-aided material discovery.[9] More recently, the periodic assembly essence of mechanical metamaterials has been applied to optimize the interfacial microstructures in TENGs.[10] Due to the need for high performance and well effectiveness for real-life application scenarios, however, TENGs have been facing the challenge of optimizing for specific output mainly due to the uncertainties associated with their complex structures.

Recently, there has been a growing interest in deploying artificial intelligence (AI) tools for enhancing the performance of TENGs.[11] However, the entire field of AI-enhanced TENGs is still in its infancy. **Figure 2** demonstrates the tree of research for TENGs in terms of integration with AI paradigms, including standard AI, generative AI (GAI), and physics-informed AI. In general, AI-maximized TENGs fall into the four categories of AI maintenance consisted of monitored and predictive

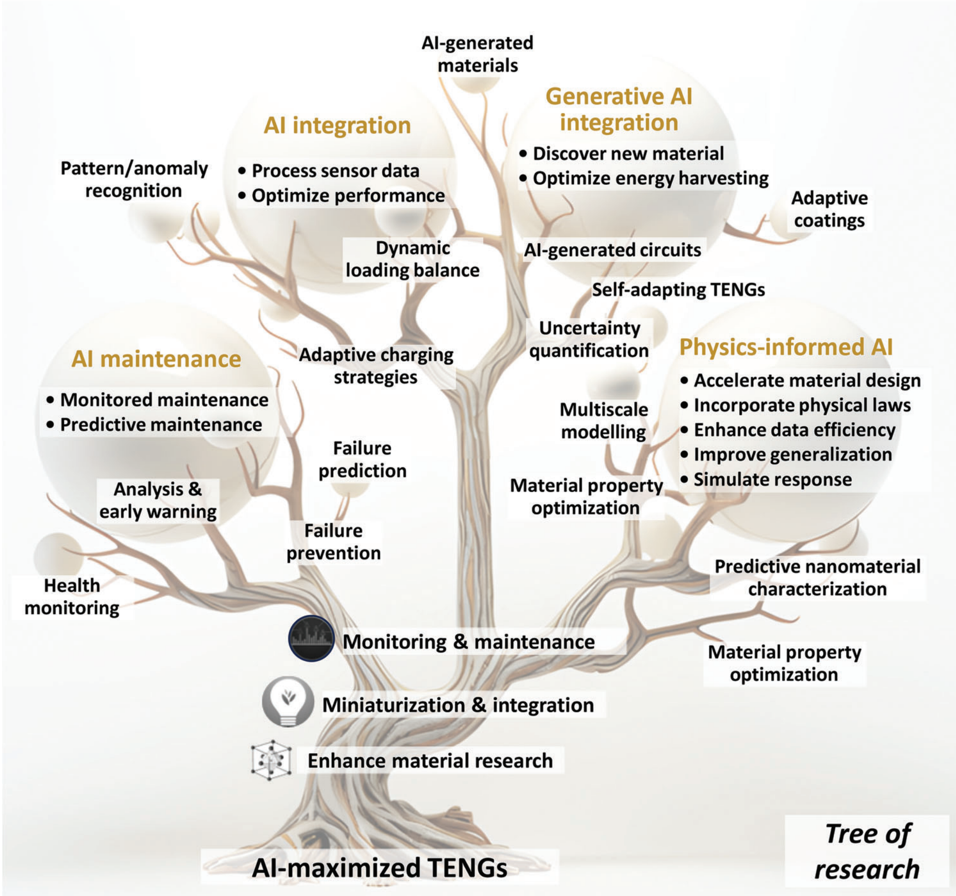

Figure 2. Tree of research for future development of TENGs with AI, generative AI, and physics-informed AI inverse design. The AI approach to TENGs design can expand their utility in monitoring and maintenance, accelerate their miniaturization and integration for various engineering and medical applications, and enhance the material research and discovery for more optimized designs.

maintenances, AI integration consisted of process sensor data and optimized performance, GAI integration consisted of discover new materials and optimize energy harvesting, and physics-informed AI consisted of accelerate material design, incorporate physical laws, enhance data efficiency, improve generalization, and simulate response. First of all, the limited studies with focus on using standard AI methods (e.g., neural networks (NN), deep learning DL) merely target optimizing or predicting the electrical output of TENGs.[11,12] Second, the standard AI methods can have broad applications in other areas including processing sensory data generated by TENGs, monitored maintenance, or predictive maintenance. Within the realm of AI, third, the GAI methods (e.g., generative adversarial networks (GANs), variational autoencoders) are other emerging tools with outstanding ability to learn complex patterns in the data and generate new contents, properties, or structures.[13] The GAI algorithms are particularly strong for inverse design of material systems.[13] Despite the significant capacity of the GAI methods in enhancing TENG systems in various aspects, their substantive application in this area is conspicuous by its absence. The major challenge with the implementation of AI and GAI methods is that they often require a large amount of data for calibration. Moreover, since they rely solely on data, there are concerns about the uncertainty associated with these models. To address these challenges, fourthly, physics-informed AI has been proven to be an efficient approach with various applications ranging from discovering advanced materials to optics.[14,15] Also, strategic inverse design has been proposed as a data-driven method for performance-oriented material response in recent years.[16] By incorporating domain-specific knowledge and constraints from physical laws into the AI simulation process, the physics-informed AI models can learn and extrapolate information from limited data more effectively. This capability makes them attractive approaches in various domains where data might be scarce or expensive to obtain. For the TENG systems, a physics-informed AI inverse design strategy could be the key to addressing the challenges associated with design and optimization, opening horizons for exploring new generations of TENGs.

This perspective overviews the working principles of TENGs, summarizes the current challenges of designing and optimizing TENGs, and presents insights into the strategic inverse design method to obtain physics-informed and performance-oriented TENGs systems. We particularly discuss the inverse design strategies in the context of the AI-based methods for expanding the principles from analytical modeling to physics-informed AI, discovering frictionally conductive compositions,

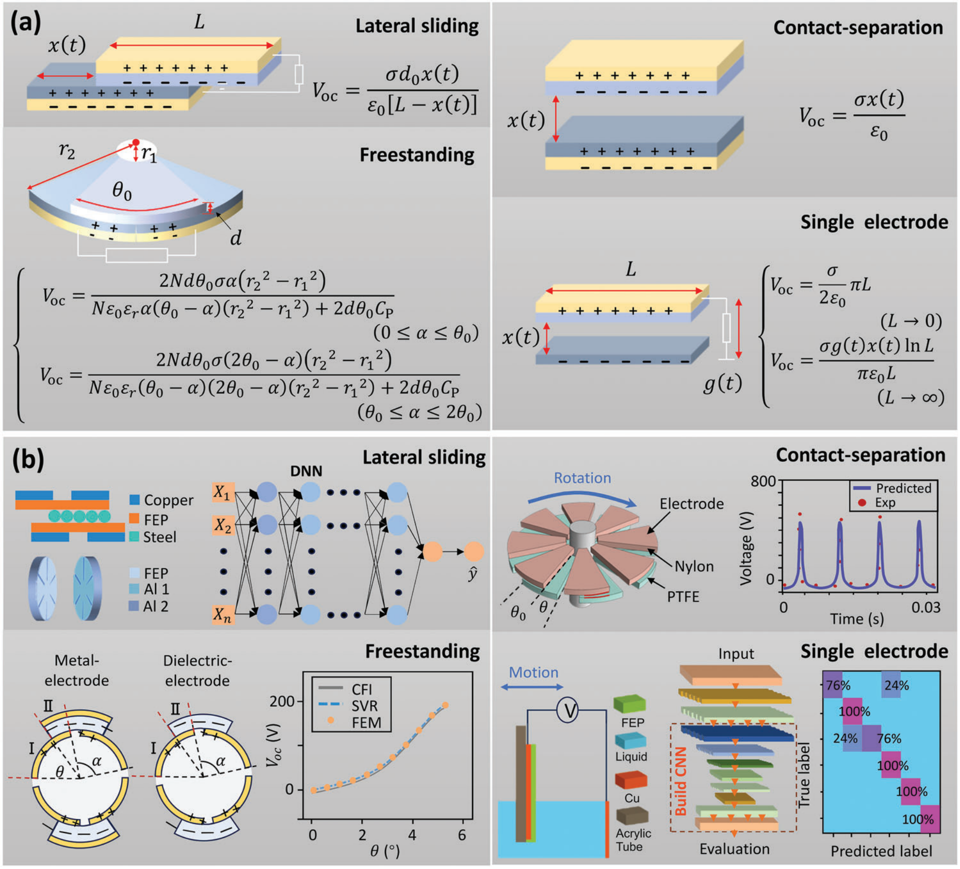

Figure 3. Analytical models of TENGs and technical challenges ahead of their design and optimization. a) Typical theoretical expressions of the lateral sliding,[18] contact-separation,[19] freestanding,[20] and single electrode[21] models. b) Existing AI models to predict the electrical performance of four modes of TENGs including lateral sliding,[12] contact-separation,[11] freestanding mode,[22] and single electrode[23] modes.

selecting ideally dielectric materials, and designing contact interfaces. Eventually, we discuss the strategic inverse design toward the next-generation integrated TENG systems with the electrical performance that meets the specific application conditions and requirements.

2. Current Progress and Limitations of Analytical Models of TENGs

TENGs have been reported to have the unique feature of high voltage and low current due to their high internal resistance. For instance, the voltage output can easily reach hundreds to thousands of volts while the current is typically at the scale of microamperes. Thus, TENGs have emerged as ideal high-voltage sources.[17] To investigate the electrical performance of TENGs with different working principles, four-mode of the lateral sliding,[18] contact-separation,[19] freestanding,[20] and single electrode[21] analytical models have been developed based on the fundamental theory of Maxwell's displacement current (**Figure** 3a). The displacement current is mainly caused by the reasons of time-varying electric field, time-varying movements of atomic bound charges, and polarization of the dielectric. According to the four-mode analytical models, the open-circuit voltage V_{OC} is affected by two types of parameters, including the material properties such as the surface charge density σ and the structural design such as the relative displacement changing with excitation time $x(t)$. Thus, the electrical performance of TENGs can be tailored by these material and structural parameters.

Various design and fabrication strategies have been proposed to optimize the electrical performance of TENGs. In material selection, for example, flexible contact surfaces are chosen as the triboelectric materials to reduce the surface wear of TENGs resulting in triboelectrification.[24] Dielectric elastomers with low stiffness and well stretchability are bonded with flexible electrodes on the top and bottom to form dielectric elastomer actuators.[25] In structural design, continuous charge replenishment is designed in TENGs to reduce the surface charge dissipation into the air.[26] Intermediate layers are designed as the blocking or charge storage layers between the triboelectric materials and electrode layers to prevent the surface electron drift to the bottom electrode under the action of electric field.[27] However, these design and fabrication strategies are neglected in the analytical models due to the assumed simplifications.[17] **Table** 1 summarizes the existing four-mode analytical models of TENGs with the typical design variables, simplifications, and application scenarios.

Figure 3b displays the existing AI models to predict the open-circuit voltage generated based on four operational modes of

Table 1. Summary of the existing analytical models with design variables, main simplifications, and application scenarios.

Mode	Working principles	Structural characteristics	Material selections	External excitations	Variables	Simplifications	Application scenarios	Refs.
Contact-separation	During contact-separation process, potential changes between two electrodes, and external current flow are created to balance the potential difference	• Relative displacement between contact surfaces x • Contact surface area • Overall size	• Surface charge density σ • Vacuum dielectric constant ϵ_0	• Applied force • Displacement distance • Triggering frequency	• Conductive materials with different σ and ϵ_0 • Structural design to control the displacement	• Uniform displacement • Surface wear is negligible • Surface charge dissipation is negligible • Performance degradation by fatigue is negligible	• Spacer • Arch • Spring-based contact-separation structures • Multi-layer contact-separation • Microporous-nanoparticle composites	[2,17,28–33]
Single electrode	External mechanical movement causes gap between two friction surfaces, and potential differences are created between two electrodes	• Gap between two triboelectric materials x • Board length l • Gap between main electrode and reference electrode g	• Charge density σ • Vacuum dielectric constant ϵ_0	• Applied force • Displacement distance	• Electrode spacing • Area size	• Neglect effect of thickness and simplify to a 2D model • Frictional charges are uniformly distributed on surfaces of dielectric layers	• Plane sliding structure	[2,28,31,33]
Lateral sliding	• Utilize relative displacement parallel to contact interfaces, and potential changes between two electrodes • Electrical output is generated through external circuit	• Lateral separation distance x • Thickness d • Board length l	• Surface charge density σ • Relative permittivity ϵ_1	• External force in horizontal direction of devices	• Sliding distance	• Distance between positively and negatively charged surfaces is negligible • Vertical distance between electrode layer and surface of friction charge is negligible • Thickness effect is negligible • Decay of friction charge with time is negligible • Edge effect is negligible	• Plane sliding structure • Grid-like electrode structure • Rotating disc structure • Rotating cylindrical structure	[2,21,28,29,32,33]
Freestanding	Potential difference is generated when independent layers move from one electrode to another	• Dielectric plate thickness d • Gap angle θ_g • Center angle θ_0 • Number of grating units N • Inner and outer radius of TENG r_1 and r_2	• Relative dielectric constant ϵ_{r1} • Surface charge density σ	• Rotation angle • Rotation rate	• Rotation rate • Number of grating units	• Negative tribo-charges uniformly distribute on dielectric surfaces • Influence of contact force between triboelectric surfaces is negligible • Electrode gap is negligible	• Rotating wheel structure • Grid-like electrode structure	[2,28,31,33,20,18]

TENGs. In particular, Jiang et al.[12] developed a deep neutral network (DNN) model to predict the output performance of the lateral sliding TENGs with different design conditions. A theoretical model integrated with an AI optimization model (grey wolf optimization method) was reported by Khorsand et al.[11] to characterize the output of the rotary TENGs in the contact-separation mode under various kinematics and geometric conditions. Wang et al.[22] presented a supported vector regression (SVR) model to optimize the average power of the cylindrical grating-structured TENGs in the freestanding mode.[22] A DL model was developed to detect and classify the microplastics in the liquid–solid TENG.[23] Satisfactory prediction accuracies were reported in all these existing studies.

3. Technical Challenges in Design and Optimization of TENGs

Electrical performance of TENGs is affected by factors at the material and structure level. The former consists of the factors related to conductive materials (e.g., triboelectric polarity and surface charge density) and dielectric materials (e.g., resistance). The structure level factors are related to contact interfaces such as surface roughness and deformation morphology.[4] Design and optimization of TENGs demand controlling the factors in these two categories. Although conductive materials can be optimized by mixtures, there are major difficulties in obtaining the optimal triboelectric polarity and surface charge density due to the uncertainty of the key factors in compositions.[34,35] In addition, several technical challenges still need to be addressed to expand the implementation of TENGs. These challenges include ensuring their biocompatibility, enabling their operation in extreme conditions (such as high temperature, humidity, moisture, and varying excitation amplitudes and frequencies), and addressing the lack of sufficient experimental data in these domains.

Figure 4 depicts the technical challenges in TENGs. Figure 4a demonstrates the technical challenges of TENGs in biocompatibility, performance, and data amount. This figure illustrates the biocompatibility and applicability of the selected triboelectric materials of wool, polypropylene (PP), silk, nylon, natural rubber (NR), aluminum (Al), silicon (Si), quartz, sulfur, polyethylene (PE), polytetrafluoroethylene, polydimethylsiloxane (PDMS) and polyvinyl chloride (PVC). The materials are particularly compared in terms of the triboelectric factor ξ, where the origin factor is $\xi = 0$ for metals or superconductors as the Seebeck coefficient is zero. Triboelectric materials are distributed along the positive and negative ξ. Figure 4a also depicts how typical triboelectric materials (i.e., Al, PDMS, and nylon) are analyzed with respect to their performance under extreme operation conditions such as high temperature, humidity, excitation amplitude, or frequency. High corrosivity, high responsiveness, low robustness, and low recovery have been reported as the main issues of the TENGs fabricated by these materials. These issues result in the loss of the devices' functionalities. Furthermore, the scarcity of data is a concern found in the entire procedures of developing AI models, including the insufficiency, error, noise, and complexity in data processing, inefficiency in data analysis, and inaccuracy and imprecision in data results. Figure 4b shows the uncertainty in characterizing the key factors in composition the lack of quantitative relationships by traditional statistical tools, and the difficulty in optimizing conductive and dielectric materials by composition mixtures while controlling structural response by design of contact interfaces. Resistance of dielectric materials can be critically affected by mixtures, but it is difficult to identify the key factors in compositions. The four-mode analytical models have been proposed to establish the quantitative relationships between the key factors (i.e., input variables) and electrical performance (i.e., output variables). However, intuitive guideline is still insufficient to achieve desirable electrical response as the complex nature of TENGs results in the difficulty of characterizing all the factors and accurately obtaining the relationships only using traditionally statistical tools. Addressing these technical challenges, AI-based performance prediction and optimization have recently been reported to tailoring the micro-compositions of functional materials to obtain desirably electrical response,[34] and unveil the relationships between the inputs and outputs without quantitatively modeling.[35,36] **Table 2** summarizes the existing AI models developed for the performance prediction and output data analysis of four modes of TENGs.[12,22,23,37–45]

4. Inverse Design of TENGs by Physics-Informed AI

The four-mode analytical models aim at unveiling the mechanism and key parameters of TENGs to improve their performance by determining advanced conductive and dielectric materials, designing optimal structures, and obtaining standardized electrical output. The analytical models are, however, inadequate due to the highly complex nature of material discovery and structural design. AI has been used as a powerful tool to expand the mechanism of triboelectrification and address the theoretical issues of TENGs. More recently, physics-informed AI and AI inverse design models have been reported for various applications in electrical energy fields.[46–48] For example, physics-informed AI models were developed for photovoltaic and solar energy,[49–51] wind energy,[52,53] power flow[54,55] and power system management.[56,57] **Figure 5** illustrates the principles and procedures of physics-informed AI inverse design for TENG systems, encompassing theoretical analysis, the selection of conductive and dielectric materials, and the design of the contact interface. **Table 3** compares the existing physics-informed AI models and AI inverse design models with other AI models in terms of the principle and mechanism, characteristics, application scenario, and applicability in TENGs.[12,58–65]

4.1. From Analytical Modeling to Physics-Informed AI

Four-mode analytical models have been developed to investigate the electrical outputs (e.g., voltage and charge) of TENGs in various application scenarios.[66] The four-mode models are limited due to their simplifications. For instance, they rely on relative displacement change $x(t)$ that is eventually distributed over time.[67] Therefore, most TENGs are qualitatively designed based on researcher experience or preliminary experiments. AI tools have recently been applied to design TENGs with optimal electrical performance, for example, electro-physiological sensors,[68] TENG arrays,[69] self-powered sensor networks,[70] etc. However,

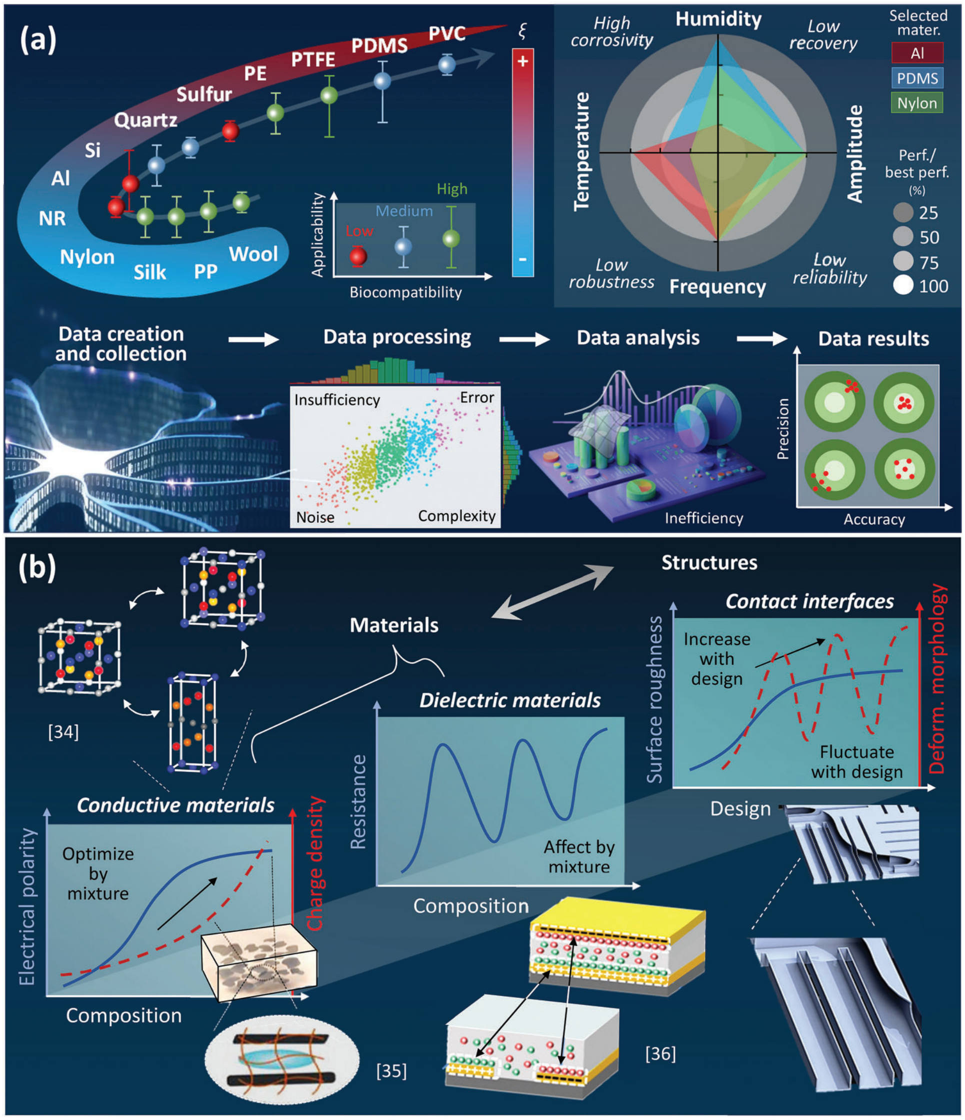

Figure 4. Technical challenges in TENGs. a) Technical challenges in biocompatibility, performance, and data amount. The scarcity of biocompatible triboelectric materials is especially significant when designing TENG-based implants that necessitate specific mechanical properties, such as high stiffness or softness. Ensuring the performance reliability and robustness of current triboelectric materials under extreme operational conditions is a crucial area for further research. The dearth of adequate data at every stage of developing resilient AI models for TENG-based systems continues to be a pressing concern. b) Uncertainty in characterizing the key factors in composition and the lack of quantitative relationships by traditional statistical tools, and the difficulty in optimizing conductive and dielectric materials by composition mixtures while controlling structural response by design of contact interfaces (Reproduced with permission [34-36], 2023, Wiley).[34–36]

the large amount of data required for calibrating the AI models has severely limited their development. This is particularly a challenge for the AI algorithms that significantly rely on data such as NN and DL. Given the expenses of experimentally expanding the database, numerical simulations have been used to quantitatively investigate the electrical response and develop adequate data for TENGs.[71]

To address these challenges and improve the uncertainty associated with AI model, realizing physics-informed AI combining the four-mode principles with AI prediction models is a viable approach. Physics-informed AI models have been reported to analyze complexly analytical equations, such as the physics-informed NN models for solving different nonlinearly partial differential equations[72–76] and their applications in structural identification,[77] nanoscale heat transport[78] and Motion estimation of moored buoys.[79] From the analytical modeling, the AI prediction to the physics-informed AI, electrically-tunable TENGs can be created by strategic inverse design to control the electrical performance and, more interestingly, to customize components that can be integrated in devices and assembled in intelligent systems.[2,80] Figure 5a shows the design path of TENGs from analytical modeling for the triboelectrification effect, AI-enabled prediction for TENG components to physics-informed inverse design for integrated TENG devices

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Table 2. Existing AI models developed for the performance prediction and output data analysis of TENGs.[12,22,23,37–45]

	Performance prediction	Data analysis
Contact-separation	• K nearest neighbor (KNN) and NN • KNN accuracy of 97.1% • NN accuracy of 97% • KNN provides better results than other ML models[37]	• Hierarchical NN • Real-time neuromorphic computing • Accuracy of 92.11%[38] • Multilayer deep belief network (DBN) • Analyze useful information from raw electronic signals • Generate keystroke dynamics identification results • High identification accuracy, stable, and reliable performance[39]
Single electrode	• Convolutional neural network (CNN) • Liquid–solid TENGs • Detect microplastic particles in water • Accuracy of 86.7%[23]	• Particles-laden droplet-driven TENGs • CNN to identify particle types • Accuracy >95%[40] • Classification coding and recurrent neural network • Sheath-core triboelectric nanogenerators (SC-TENGs) • Identify materials in real-time • Accuracy of 96.5%[41]
Lateral sliding	• DNN • Predict output power with structures of TENGs • Consistent with experiments and simulations[12] • Co-evolutionary particle swarm optimization and physical solver • Optimize key structural parameters (i.e., contact area, electric film thickness, and external resistance) • Optimize main characteristics of TENGs[42]	• 1D CNN • Detect various volatile organic compounds species • Accuracy of 54.286%[43]
Freestanding	• SVR • Investigate the influence of rotor-stator gap and parasitic capacitance on grating-structured TENGs • Obtain optimal grating number and average power[22]	• Long and short-term memory (LSTM) • Cantilever-structure freestanding TENGs • LSTM as a cantilever defect identification model for electric output of TENGs • Accuracy of 98.6%[44] • Continuous wavelet transform and CNN • Classify and identify typical faults of rotating machinery • Accuracy of 90%[45]

and assembled TENG systems. **Figure 6a** shows the framework of the physics-informed NN (PINN(t;θ)) for Maxwell's equations, where θ denotes the set of trainable weights w and biases b while Γ is a nonlinear activation function.[58] Specify the measurement data $\{t_i, \mathrm{B}_i, \mathrm{E}_i\}$ for **B** and **E**, and the residual points $\{t_j\}$ for the PDE. The loss L function can be specified by summing the weighted losses of the data and PDE, and the PINN model can be trained to find the best parameters by minimizing L.

4.2. Material Discovery for Frictionally Conductive Materials

AI has been playing a significant role in material discovery ever since its debut as AI can capture the subtle relationships between material compositions and properties without requirements on assuming prior form of the relationships. AI has been used to discover frictionally conductive materials with ideal conductive properties.[4,28,84] Frictionally conductive materials, typically found in synthetic compositions, have been used in TENGs due to the triboelectrically negative characteristics required to transfer charges. These compositions tend to bind electrons and thus seize electrons from others under contact friction. To improve the friction materials in TENGs, research efforts have been dedicated to finding the compositions with optimal triboelectric capability.[85]

To this end, physic-informed AI inverse design can be a powerful tool to characterize material properties,[86–88] obtaining advanced compositions by varying the compositions in their functional chemical groups (e.g., sulfur groups, hydroxyl groups, amine groups, etc.), material components, and functional fillers.[89] The electron-donating capabilities and microstructures can be tailored by varying the component ratios of different friction layers, which will lead to promising improvement of transferring charges for the friction materials with the same contact friction conditions. For example, physics-informed AI and AI inverse design models were reported on the functional materials of nanophotonics,[90] thermal materials,[91] and electromagnetic materials[92] with enhanced performance, and the composites of multi-materials[93] and heterogeneous materials.[94] Materials reliability, robustness, and fatigue resistance were improved with less defects in additive manufacturing.[95–98] Figure 5b demonstrates the application procedures of inverse design by physics-informed AI to determine the frictionally conductive materials with programmable triboelectric properties. Figure 6b shows the framework of the physics-informed DL for solving an elasticity problem in conductive materials.[81] The DNN of displacement takes the position at each material point

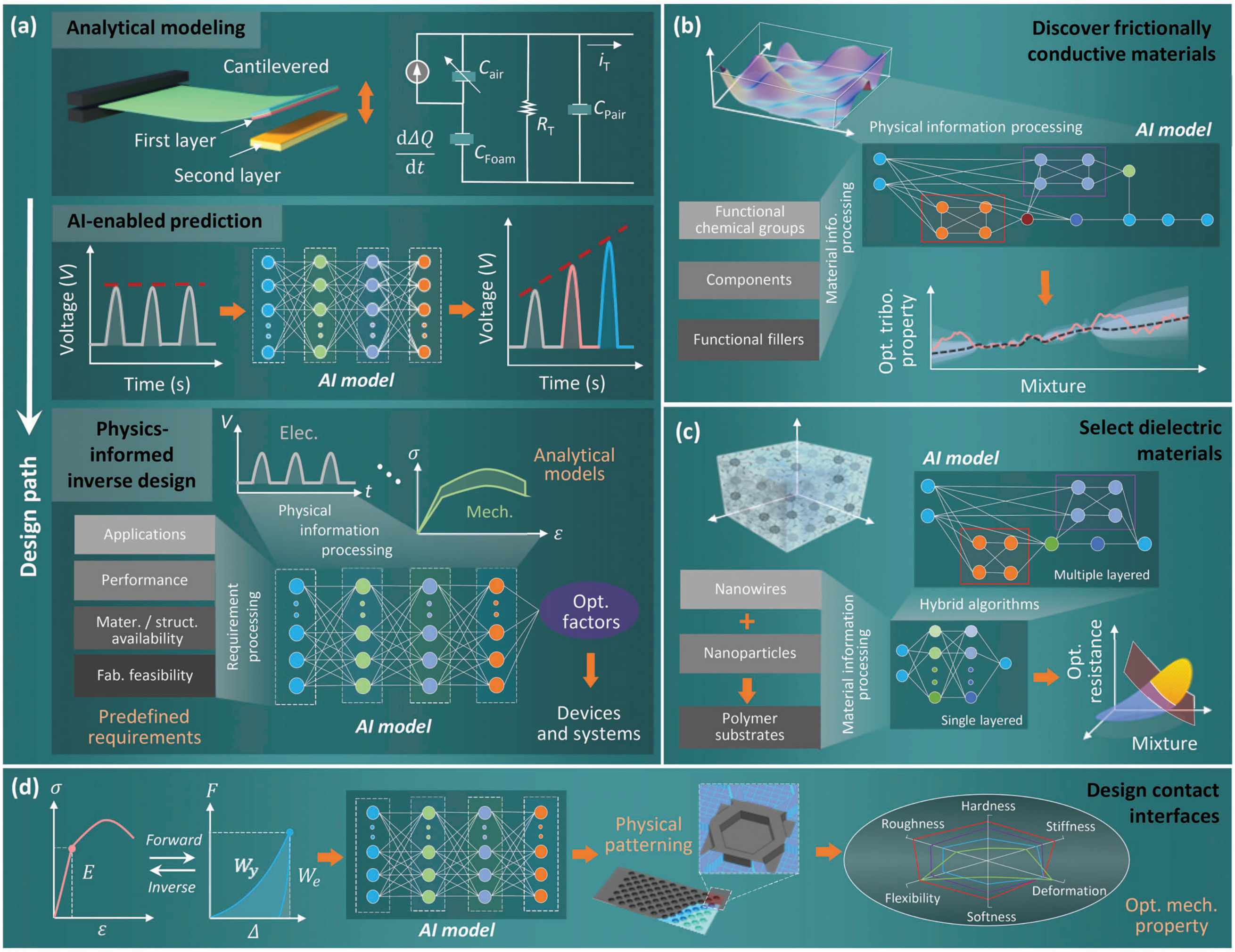

Figure 5. Strategic inverse design of TENGs by physics-informed AI. a) Design path of TENGs from analytical modeling for the triboelectrification effect, AI-enabled prediction for TENG components to physics-informed inverse design for integrated devices and assembled systems. b) Discovery of frictionally conductive materials with programmable triboelectric properties by varying functional chemical groups, material components, and functional fillers, and c) selection of highly dielectric materials by combining nanowires or nanoparticles with well dielectric constants into polymer substrates using strategic inverse design. d) Inverse design on the contact interfaces of TENGs by physical patterning based on mechanical metamaterials from the structural perspective.

and outputs its displacements $u_y(x,y)$. The predicted strains are determined based on the measured and predicted displacements. The predicted stress tensor can then be calculated with the encoded constitutive relations based on the strains and Young's modulus.

4.3. Material Selection for Dielectric Layers

Dielectric materials play a key role in TENGs. Poor dielectric properties in friction layers will severely affect the charge accumulation due to high charge dissipation, which results in the insufficiency of potential difference between two friction layers for certain current output.[99] Recent studies have been conducted to improve the electrical performance of TENGs by obtaining the dielectric materials with ideal properties, for example, mixing high dielectric nanomaterials,[100] changing hydrophilicity,[101] or polarizing dielectric materials.[102]

Strategic inverse design by physics-informed AI can be used to select the materials with ideal dielectric properties. Figure 5c displays highly dielectric materials designed by combining nanowires or nanoparticles with well dielectric constants into polymer substrates. For example, $BaTiO_3$ was reported with predefined dielectric properties based on nanomaterials and silver nanomaterials.[103] Inverse design can also be conducted to eliminate the hydrophilicity of dielectric materials as hydrophilic materials with well water absorption ability are likely to reduce the surface charges due to the conductivity of water molecules. In addition, polarization can be inversely carried out to obtain the dielectric materials with tunable permittivity as electrical insulators can be polarized in electrical fields. For example, interfacial, ion, and molecular polarization can be used to promote the properties of dielectric materials, and thus improve

Table 3. Comparison of the existing physics-informed AI models and AI inverse design models with other AI models on the principle and mechanism, characteristics, application scenario and applicability in TENGs.[12,58–65]

	Principle and mechanism	Characteristics	Application scenario	Applicability in TENGs	Refs.
Physics-informed AI models	• Fundamental AI systems • Introduce appropriate observational, inductive, or learning biases	• Integrate seamlessly data and mathematical physics models • Incomplete models and imperfect data • Strong generalization in small data regime • Uncertainty quantification	• Biophysics • Plasma dynamics • High-dimensional problems • Quantum chemistry • Material sciences • Molecular simulations • Geophysics • Manufacturing systems	• Not yet been applied to TENGs • Use physical relations to address the lack of data • Design and optimization of various structures with complex microstructures or surfaces • Identify and characterize material properties • Improve output performance	[58,59]
AI inverse design models	• Basic NN systems • Evolutionary approaches • Gradient-based approaches	• Data-driven manner for targeted design • Multidimensional design space exploration • High-speed and scalability	• Functional materials • Nano-photonics • Molecular biology • Multiphysics • Robotics and manufacturing • Biomedical engineering	• Not yet been applied to TENGs • Performance-oriented design and optimization • Design structures with complex microstructures or surfaces • Identify and characterize material properties • Improve output performance	[12, 60–62]
Other AI models	• DL • GAN • Reinforcement learning (RL) • Transfer learning (TL) • Bayesian optimization (BO)	• Learn from extensive data volumes • Excellent flexibility and adaptability • Depend on iterative feedback loop • Trade-offs and uncertainty	• Materials design and discovery • Computer graphics • Robotics and autonomous systems • Industrial optimization	• Various AI models in TENGs • Predict and optimize performance • Analyze and address big data from sensing • Improve output performance	[63–65]

the electrical performance of TENGs.[104] Figure 6c shows the flowchart of the physics-informed AI models to predict the nonlinear composition-structure relations of the dielectric materials of oxide glass.[82] The statistical mechanics (SM), multilayer perceptron NN (MLP-NN), and hybrid SM and MLP-NN models were developed, where the SM and MLP-NN models were trained on the experimental data of composition-structure for the glass, and the hybrid model was trained on both the experimental data and statistical mechanics results. Model predictions of Q^n fractions in the glass were presented, where Q^n is the function of Na_2O concentration in the Na_2O-SiO_2 glass system.

4.4. Structural Design and Optimization for Contact Interfaces

Structural design and geometric optimization are important factors for tunning the electrical performance of TENGs.[105] Given the remarkable interest in energy harvesting devices in recent years, various TENGs have been used in the application scenarios with different types of external excitations.[106] Due to the prompt development of additive manufacturing and other fabrication technologies, structural design is likely to provide higher possibility to tailor TENGs compared with the strategies in the material perspective (i.e., design of conductive and dielectric materials). On the other hand, high structural possibility (i.e., structural complexity) results in the difficulty of obtaining the most effective structures of TENGs with the optimal parameters.

The advantages of AI in performance prediction lead to its applications in structural design and geometric optimization of TENGs.[107] Different from the most current studies focused on the overall structures, an emerging direction of strategic inverse design from structural perspective is on the contact interfaces of TENGs. For example, physics-informed NN models were developed to predict the structural instability,[108] design the key structural parameters,[109,110] and optimize the structural response.[111–113] Interfacial inverse design can be conducted on the contact surfaces of TENGs by physical patterning such as designing various artificially localized morphologies. For example, mechanical metamaterials, manmade structural materials assembled by numerous microstructures in a periodic manner, have recently been applied in TENGs to promote the electrical performance due to their structural programmability.[11,114,115] Figure 5d demonstrates the inverse design on the contact interfaces of TENGs by physical patterning based on

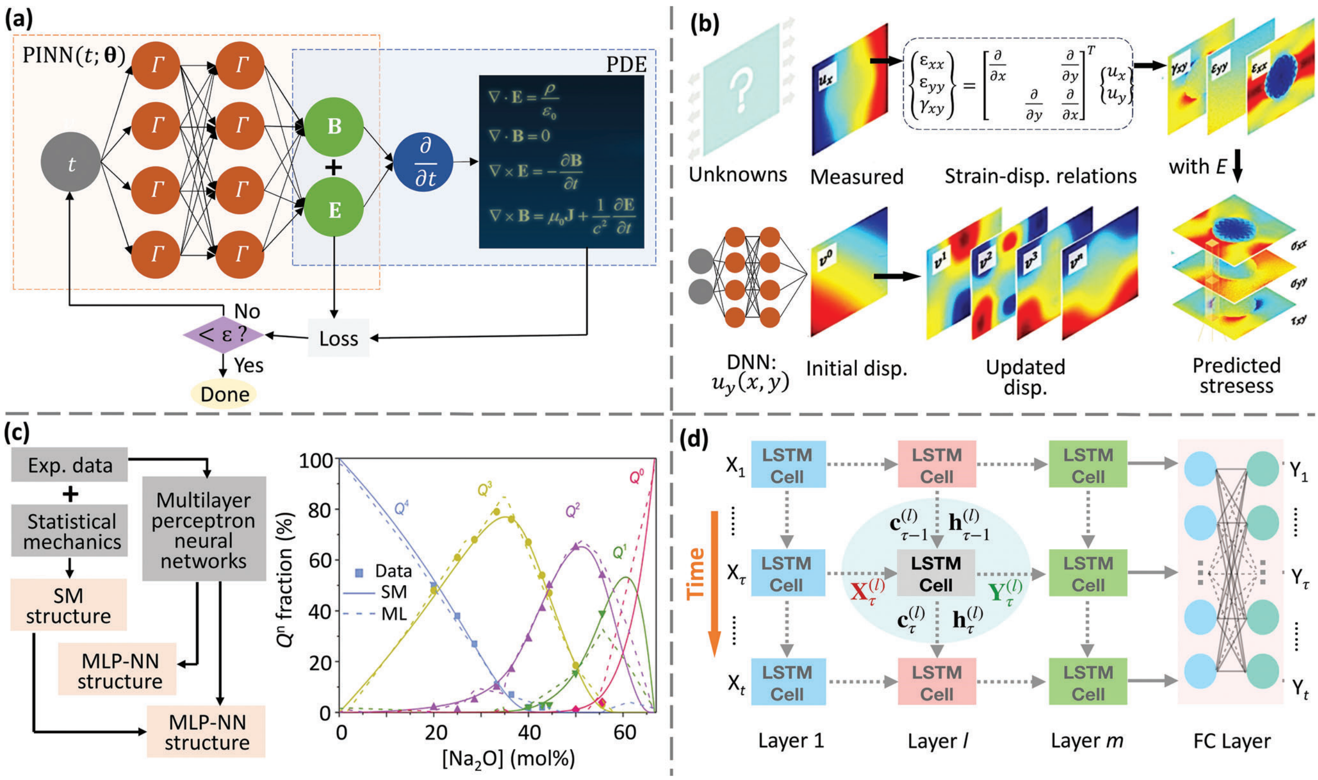

Figure 6. Comparison of the existing physics-informed AI and AI inverse design models. a) Framework of a physics-informed NN (PINN(t;θ)) for Maxwell's equations in theoretical analysis.[58] b) Framework of the physics-informed DL for solving an elasticity problem in conductive materials.[81] c) Flowchart of the physics-informed ML models to predict the nonlinear composition-structure relations of the dielectric materials of oxide glass, and the predictions of Q^n fractions in the glass.[82] d) Framework of the physics-informed multi-LSTM networks model for metamodeling of nonlinear structural systems with scarce data.[83]

mechanical metamaterials. As a consequence, inverse design by physics-informed AI to form the contact interfaces of the conductive and dielectric materials is envisioned as an efficient way to improve the triboelectric effect and maximize the electrical performance of TENGs. Figure 6d shows the framework of the physics-informed multi-long and short-term memory (LSTM) networks model for metamodeling of nonlinear structural systems with scarce data.[83] The physics-informed multi-LSTM networks model was developed with m LSTM layers and multiple fully-connected layers for sequence-to-sequence modeling. Each LSTM layer contained a suite of LSTM cells that were similar to the neural node in classical NNs, containing an independent set of weights and biases shared across the entire temporal space within the layer. **Table** 4 summarizes the existing physics-informed AI and AI inverse design models with respect to the algorithm, advantage and disadvantage of the theoretical analysis, dielectric material selection, and structural design.[11,12,41,42,81–83,90,116–120]

5. Strategic Inverse Design toward Integrated TENG Devices

Benefiting from the rapid development of TENGs during the last decade, the research interest has shifted from unveiling the principles (e.g., four-mode theories) and designing prototypes at the early stage to obtaining TENG devices for various engineering and medical applications. Instead of treating TENGs as the functional parts attached or embedded into devices, studies have been switched to directly integrating devices by the TENG components with different functionalities.[106] These integrated TENG devices are found with the advantages of well reliability, compatibility, and more tunable performance. However, it is difficult to all-in-one design integrated TENG devices that meet specific requirements in applications, especially given the fact that all TENG components need to be considered from the material and structural perspectives simultaneously.[121,122]

Figure 7 illustrates the integrated TENG devices enabled by AI-induced inverse design. Figure 7a displays the three types of technological challenges that are found in strategic inverse design, including 1) insufficiency of data for AI modeling, 2) lack of quantitative specification on performance requirements, and 3) fabrication limitations such as manufacturing precision and performance robustness. Figure 7b presents the potential solutions for addressing the challenges. First of all, GAN algorithms have been reported as a powerful tool to expand data for AI modeling. Second, sensitivity analysis can be used to compare the dominance of material, structural, and excitation factors, and identify the key factors with the contributions exceeding the thresholds of the output voltage and electrical power. Third, multiscale advanced technologies can be used to improve the imperfection in fabrication, especially the technologies that have been rapidly developing such as nanoparticle building blocks or 3D printing.[123]

Table 4. Existing physics-informed AI and AI inverse design models with respect to the algorithm, advantage and disadvantage on the theoretical analysis, dielectric material selection, and structural design.[11,12,41,42,81–83,90,116–120]

	Physics-informed AI models			AI inverse design models		
	Algorithm	Advantage	Disadvantage	Algorithm	Advantage	Disadvantage
Theoretical analysis	• Physics-informed ML[116]	• Self-upgrade without new codes or algorithms • Batch data sorting	• Require big data and storage cost • Calculation error for new data • Unable to recognize multiple choices	• Co-evolutionary particle swarm optimization inverse design (CPSOID)[42]	• High accuracy	• Complex and indigestible solving process
	• Physics-informed genetic programming (GP)[117,118]	• Suitable for complex optimization • Analytical solutions • Optimized results irrelevant to initial conditions • Independent of solution domains • Well robustness	• Low convergence rate and local optimal ability • Substantial control variables	• GWO inverse design (GWOID)[11]	• High accuracy and efficiency • Complex engineering problems with mixed partial differential and integral equations	• Complex and indigestible solving process
Dielectric material selection	• Physics-informed ML[119]	• Self-upgrades without new codes or algorithms • Batch data sorting	• Big data requirements and storage costs • Easy to produce calculation errors for new data • Unable to recognize multiple choices	• DL inverse design[90]	• Well learning ability and portability • Wide coverage • High ceiling	• Rely on computational power • Heavy calculation and inconvenience • Complex algorithm design
	• Physics-informed DL[81]	• Great learning ability and portability • Wide coverage • High ceiling	• Rely on computational power • Heavy calculation and inconvenience • Complex algorithm design	• Recurrent NN inverse design[41]	• Appropriate for processing sequence data	• Gradient explosion and disappearance • Training difficulty due to additional video memory space • Unable to handle long sequences if using tanh and relu
Structural design	• Physics-informed ML[82]	• Self-upgrades without new code or algorithm • Batch data sorting	• Big data requirements and storage costs • Easy to produce calculation errors for new data • Unable to recognize multiple choices	• DL inverse design[120]	• Well learning ability and portability • Wide coverage • High ceiling	• Rely on computational power • Heavy calculation and inconvenience • Complex algorithm design
	• Physics-informed DL[83]	• Well learning ability and portability • Wide coverage • High ceiling	• Rely on computational power • Heavy calculation and inconvenience • Complex algorithm design	• DNN inverse design[12]	• Extract richer features from the data • Diminishing the computational complexity of shallow NN	• Gradient explosion and disappearance • Degradation of weight matrix leads to the reduction of effective flexibility

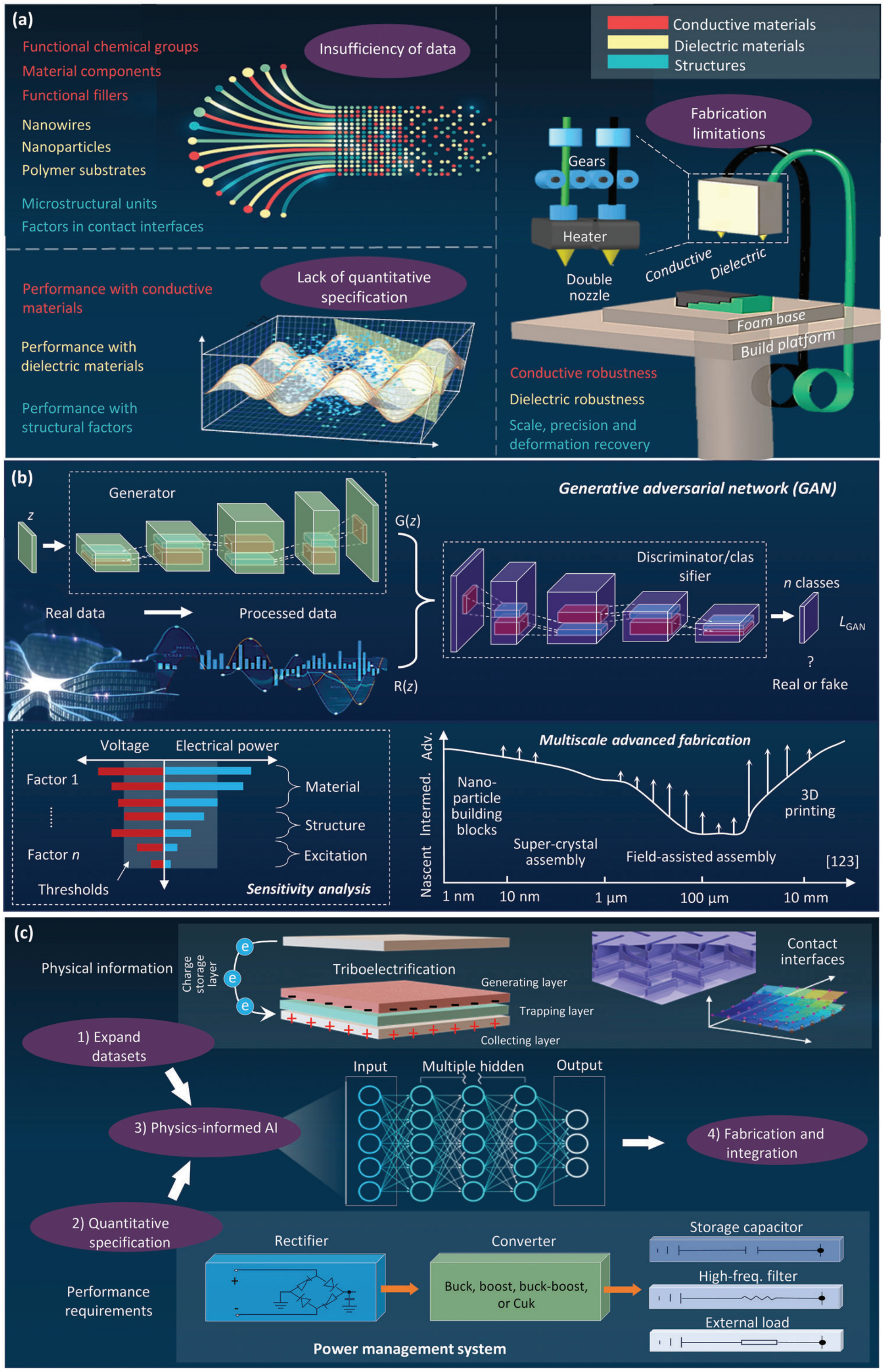

Figure 7. Integrated TENG devices by AI-induced inverse design. a) Three types of challenges in strategic inverse design, that is, insufficiency of data, lack of quantitative specification, and fabrication limitations. b) Potential solutions for addressing the data, quantitation, and fabrication challenges by GAN series algorithms, sensitivity analysis, and multiscale advanced fabrication technologies, respectively. (Reproduced with permission [123], 2023, Wiley)[123] c) Inverse design paradigms of TENGs from characterizing the key physical information, identifying the performance requirements, integrating and developing physics-informed AI models with limited amount of data, to using the AI-based material and structural designs to improve the fabrication and integration.

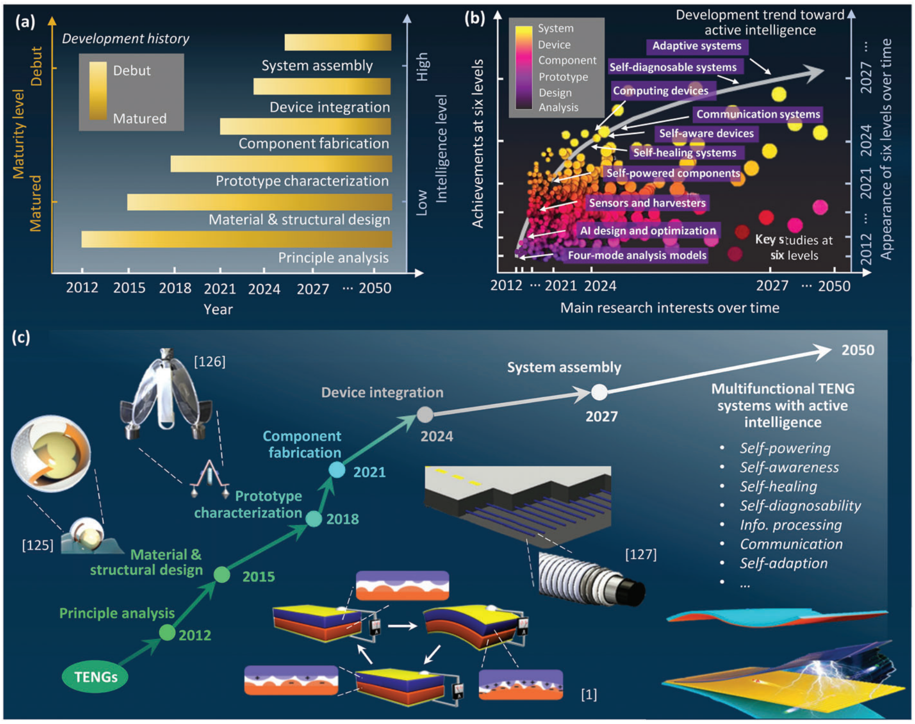

Figure 8. Roadmap of next-generation multifunctional TENG systems. a) Development of TENGs that experience six technology maturity levels of principle, design, prototype, component, device, and system, and b) key achievements and appearance of TENGs at the six levels. c) Roadmap of the next-generation self-powered TENG systems with active intelligence.Reproduced with permission.[1,125–127] Copyright 2023, Wiley-VCH.

Addressing the technological challenges, integrated TENG devices can be achieved, respectively, by principal analysis and theoretical modeling in multidisciplinary fields, expanding to establish numerical and experimental hybrid data pools, and combining different fabrication technologies such as additive manufacturing, photolithography, lasering-cutting, etc. Figure 7c displays the inverse design paradigms that, first of all, characterizing the key physical information (e.g., triboelectrification mechanism and four-mode analytical models) of TENGs; second, identifying the performance requirements (e.g., power supply); third, integrating and developing physics-informed AI models with limited amount of data; and fourthly, using the AI-based material and structural designs to improve the fabrication and integration of TENGs.

6. Roadmap for Next-Generation TENG Systems

Satisfying application requirements with performance orientation, TENGs typically experience six levels of development, that is, principal analysis, material and structural design, prototype characterization, component fabrication, device integration, and system assembly (**Figure 8**a). Current TENGs are technologically mature at the analysis, design, prototype, and component levels. This has led to prosperous research accomplishments including the four-mode analytical models at the analysis level (see Table 1), the inverse design for new materials and optimal structures at the design level (see Figure 5), the specimen fabrication and testing at the prototype level, and the applications at the component level such as energy harvesting and active sensing. Achieving technological maturity demands substantial efforts at the development levels (see Figure 8a). TENGs are undertaking development at the device level while still in infancy at the system level. At the device level, strategic inverse design can be used to achieve predefined functionalities for TENG components and effectively integrate them to form overall devices. Eventually, TENG systems can be formed by assembling different functional devices that are integrated by numerous TENG components at the system level. Figure 8b further displays the key achievements and appearance of TENGs at the six levels. The overall development trend follows a relatively sharp region for the technologically mature levels and, on the contrary, a saturate region for the debut levels. Next-generation multifunctional TENG systems, other than simply satisfying the performance requirements in applications, target the intelligent characteristics of self-powering and self-awareness. Self-awareness refers to the intrinsic self-sensing ability of a system by which it can collect information about the environment and become aware of its condition, for example, self-diagnosability in miniaturized medical implants.[124] It is known as the first step toward achieving a level of intelligence through which the system can acquire and process knowledge, self-heal, compute, communicate, adapt, and respond purposefully. Strategic inverse design at the next stage is expected to realize self-powered multifunctional TENG systems with tunable performance and intrinsic intelligence. Figure 8c demonstrates the path toward realizing self-powered intelligent TENG systems with broad applications ranging from large civil infrastructure systems to miniaturized medical implants.[1,116–119]

7. Conclusions

TENGs have been characterized as high voltage and low current energy harvesting systems. Designing TENGs with desirable output for real-life applications has remained a challenge due to the uncertainties associated with their complex nature in design. Recent research focus has been dedicated to optimizing the electrical output of TENGs from the material and structural perspectives. In this perspective paper, we provided insights into the role and future of AI-enabled inverse design as a powerful tool to realize performance-oriented TENGs (i.e., TENGs with predefined performance). Physics-informed method can be applied in the AI inverse design of TENGs to reduce the dependence on data by using quantitatively physical information. This is an emerging scientific direction that can potentially lead to realizing multifunctional TENG systems with intrinsic intelligence. Physics-informed AI can be obtained by applying the four-mode analytical models to AI inverse design models. This approach can address the challenges of TENGs in design and optimization by discovering new conductive and dielectric materials and optimizing contact interfaces. Physics-informed AI inverse design prompts the six development levels of TENGs in principal analysis, material and structural design, prototype characterization, component fabrication, device integration, and system assembly; especially for the last two development levels that are currently at the early stage. Eventually, physics-informed AI inverse design is expected to assist the significant switch of TENGs from prototypes to multifunctional intelligent systems that can be deployed in real-life applications.

Acknowledgements

Research reported in this work was supported in part by the National Science Foundation (NSF) CAREER award (CMMI-2235494), the National Key Research and Development Program of China (2023YFC3008100), and the Key Research and Development Plan of Zhejiang, China (2021C03180 and 2021C03181). P.J. acknowledges the startup fund of the One-Hundred Talent Program at Zhejiang University, China.

Conflict of Interest

The authors declare no conflict of interest.

Keywords

physics-informed artificial intelligence, strategic inverse design, triboelectric nanogenerators

Received: August 21, 2023
Revised: October 11, 2023
Published online: December 7, 2023

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