Chapter 6

Artificial Intelligence for Energy Conversion

Tapasi Ghosh1*, Bhargavi Koneru2, and Prasun Banerjee2
1 Ramaiah University of Applied Sciences, Bengaluru, Karnataka, India
2 Multiferroic and Magnetic Material Research Laboratory (MMMRL), GITAM School of Sciences, Gandhi Institute of Technology and Management (GITAM) University, Bengaluru, Karnataka, India
* tapasi03@gmail.com

Abstract
Many aspects of modern life are dependent on energy of various forms, which has already created strain on natural energy reserves and affected our environment adversely. Scientists and researchers are searching for alternative sources of energy that are sustainable, environment friendly, and renewable. However, any developmental work to invent a material or technique as a new source of energy involves a lengthy and complex experimental process to produce in scale. The last decade has seen remarkable progress in the field of Artificial Intelligence (AI) due to advancements of many new computer hardware, software’s, algorithms, technologies, and availability of a large amount of raw input data. We have started harnessing the power of AI to facilitate the process of discovering new materials as alternative energy sources and exploring the different advanced methodologies over the traditional approaches to utilize natural and eco-friendly sources for energy conversion. This book chapter will highlight some of the advancements in Machine Learning and Deep Learning techniques to explore new material resources and methodologies for energy conversion.

Keywords
AI, ML, ANN, Energy Conversion, Catalysts, Microbial Fuel Cell

Contents

Artificial Intelligence for Energy Conversion .........................................................123
1. Introduction .........................................................................................................124
1. Introduction

Energy is a physical quantity which appears in different forms. Energy cannot be created nor destroyed; instead, it can only be moved from one form to another. During this conversion, the total amount of energy remains conserved. The primary forms of energy stored in objects are either kinetic energy or potential energy. When a ball is thrown upwards, it gains potential energy due to the change in its position and simultaneously falls due to the influence of gravitational force. The potential energy held in the ball is transformed into kinetic energy as a result of the ball's mass and speed. This is a simple example of energy conversion from one form to another. When we rub our palms, the mechanical energy of our body transforms into heat and sound energy. Similarly, a hydroelectric dam turns the kinetic energy of moving water into electric power. Our daily life activities are fulfilled by turning around energies of different forms, and with the ease of modern life, these dependencies are ever-increasing and indispensable.

Though the total amount of energy around us is conserved, we constantly transfer readily available chemical energy (solar electromagnetic energy stored from sunlight) into thermal energy. Energy conversion occurs spontaneously in nature through natural events. However, energy conversion devices initiate the process artificially, e.g., thermocouples convert solar energy into electricity. Solar cells are direct energy conversion devices that produce electricity from optical and electromagnetic radiation. Similarly, other energy conversion devices such as thermoelectric devices and fuel cells are used in power
satellites, aerospace systems, power plants, automotive industries, and consumer companies to build a better product for batteries, antennas, etc. Since the average energy consumption of a person has increased in modern life, energy conversion is required to satisfy specific demands of heat or light.

Researchers are working for efficient, effective, reliable, and economically viable energy conversion systems to fulfill the needs of electricity, heating, and cooling for houses, buildings, industrial plants, etc. The R&D work on technological development for various energy conversion systems is ongoing [1] to produce renewable, sustainable, environment-friendly materials and devices, e.g., hydrogen energy conversion systems. Nonrenewable resources (e.g., coal, oil) will deplete quickly over time, and excessive fossil fuel combustion pumps up harmful greenhouse gases to the environment (a potential cause of global warming). On the contrary, the impact of the consumption of renewable energy sources (e.g., sunlight, wind) is benign to the atmosphere. The efficient production of solar and wind energies depends on climate conditions. Whereas safety concerns still undermine the harnessing of nuclear fuel from the controlled fission or fusion process of the nuclear power plant. The discovery of clean energy materials is critical for our modern society's growth.

Artificial Intelligence (AI) has emerged as an essential technology for sustainable, cost-effective renewable energy. AI facilitates communication between air turbines, predicts unscheduled maintenance, reduces costs, regulates power generation flow in smart power plants, and forecasts the weather in advance for solar and wind power plants. For example, Google's Deep Mind [2] is applied for weather forecasts at U.S. wind power facilities to overcome the intermittency challenge. AI is also used to invent new elements and explore critical material properties for energy transformation [3]. AI can accelerate the entire process of discovering new materials through R&D in a laboratory to the commercialization for mass production, which usually takes years.

In this book chapter, we organized the text in the following way: we briefly introduce energy conversion and the mechanism of AI, how models are trained and tested to gain reasoning, which is essential for any Machine Learning algorithm to acquire intelligence. In the next section, we intend to highlight some of the used cases of AI for material science applications such as photonics materials, electrochemical catalysis, electrolysis, and fuel cells technologies, and finally we conclude.

2. **Alternative sources of energy and artificial intelligence**

Artificial Intelligence is an area of study which allows the computer/machine to acquire the ability to reason artificially, which is in analogy with the cognitive ability of the human
brain. It allows a computer system to mimic human cognitive skills such as decision-making and problem-solving. However, the neuron in Artificial Neural Network (ANN) model architecture is a much simplified representation of the structure and synaptic functions of neurons in the human brain. Usually, an AI system is built using machine learning and other techniques. Machine Learning is a sub-branch of AI involving the process through which the computer learns to make decisions without any direct human intervention when trained with large amounts of data. ML is a combination of mathematical logic and model architecture to gain insight into input data, find the hidden pattern, and simultaneously make decisions for unknown and unseen information based upon acquired intelligence.

Frank Rosenblatt designed the deep learning model, among the most basic ANN designs, in 1957 [4]. The Perceptron, also known as the Threshold Logic Unit (TLU), computes a weighted sum of the given inputs, and the output is the outcome of the step function applied over the weighted sum. The training mechanism of Perceptron follows Hebb's Rule, "Cells that fire together, wire together" [5], i.e., the connection between two neurons gets more potent when they fire simultaneously. Modern day ANN refers to the Multilayer Perceptron (MLP) designed by stacking multiple Perceptrons. An MLP architecture usually consists of one input layer, one or more layers of TLUs known as hidden layers, and a final output layer. Until 1986, it was a challenging task to train an MLP, but the invention of back propagation techniques [6] to tune the model parameters automatically has been a breakthrough in the field of AI.

There are multiple reasons for the recent popularity of application of AI in the field of material sciences, e.g., access to open-source machine learning tools and a significant quantum of labeled data to train the algorithms Application Programming Interface (API) resulted in applying the latest developed models and algorithms in a short time. At the same time, recent invention, and advancement of new hardware technologies, e.g., Graphics Processing Unit (GPU) to store and process a large amount of data required to train complex algorithms, is influencing it. The same reasoning is applicable for fostering ML adoption in other research areas as well [7]. ML is replacing some of the traditional research methodologies of inventing new materials or material properties, which were time-consuming involving rigorous processes. In contrast, AI delves into the data, can find the latent representation, and can draw inferences from the unseen data based on the reasoning gained during the training of the models. The Deep Neural Network (DNN) [8] is a model architecture consisting of multiple layers. Each layer holding many neurons can uncover the most relevant features representative of the output to be used in the entire ML job. These characteristics are generated in the first set of layers in the DNN, by providing more weights to the attributes representative of the output. For example, in the case of face
recognition tasks, it gives relatively more weightage to the lower-level features related to eye or facial expression. DNN can bypass some of the tedious jobs of feature engineering. Some of the limitations of DNN are the necessity of enough training data for such an extensive network; the training can be prolonged. Generative models, e.g., Generative Adversarial Networks (GAN) depend upon the use of a deep learning process to learn the lower geometrical feature representations from testing phase data in order to predict the result for fresh unseen data based on the learnt distribution. GAN is used to produce realistic simulated data in data-limited situations [9].

3. Machine learning and its application in material sciences

Machine Learning models learn to argue using the following methods: training data, reinforcement classification, moderately supervised learning, and recurrent neural networks [10]. In training data learning, the datasets for which the algorithms are trained are "labeled" data, i.e., a set of output-input pairs. During the data training stage, the algorithm learns the weights, which map the input features to the given output. Most importantly, the model puts more weight on the segments having the most significant impact on the given output. Once the model parameters (weights) are updated, it can make inferences for unseen data. The assumption is much less computation expensive than the training stage. K-Nearest Neighbors, Regression Analysis, Support Vector Machines, and Judgment Trees are examples of key supervised learning algorithms. The training data in unsupervised learning is unlabeled, and the models learn to categories the input data using Clustering, Principal Component Analysis, etc., methods [11].

When developing a Machine learning model, the accessible information is often divided into learning, verification, and testing sets. As explained before, the training dataset is used for training the models to gain insight into the hidden pattern in the data. The validation set helps to choose the best among many trained models. More specifically, one introduces multiple models with various hyper parameters (training rates, variety of hiding layers, neurons in each hidden unit, and so on) and selects the model whose performance is best for the holdout set. Finally, the test set was used to determine how effectively the trained model extrapolates to new scenarios that it has not encountered previously [12].

4. Limitation of principled method and how ML can intervene

Traditionally the electronic structure computational method such as Kohn-Sham density functional theory (DFT) is practiced extensively, which led to the creation of several computational materials databases and subsequently to the discoveries of numerous materials. However, the high predictive accuracy of these methodologies relies on
correlation energy functional, which is constructed based on heuristic approaches [13]. ML can fill up this space by enforcing its ability to extract the concise pattern from the trained data and then apply that data-driven knowledge to predict the properties of previously unseen data with minimal computing resources (inference). ML may help to identify complications and create innovative materials with crucial features. For example, a machine learning trained functional on a few molecules can be applied to hundreds of molecules [14]. This is an active research area in the material science community to look for suitable representations of material properties to use the latest ML models [15]. Different material databases, e.g., Resources Group [16] as well as the Experimental Atomic Substances Collection [17], have been designed to cater to the need for a large dataset for training ML models. Even new super hard materials have been discovered by training ML models using computational databases, and other illustrative examples have been reported in [18].

5. Applications of AI in the domain of energy conversions

5.1 AI in photonics

Artificial intelligence has lately been hailed as a critical tool for gaining information and evaluating cause-and-effect links in complicated processes in a massive data environment, notably for operational parameter management and factory automation. When it comes to the application of optoelectronic materials, we find the different aspects of using those materials like sensors, light-absorbing materials, electronic sensors, automatic lights, and LED screens etc., whereas the most and more explored applications come with artificial intelligence, optoelectronic materials can be made from different compounds and compositions [19]. The most produced and used optoelectronic materials in AI are perovskite structured materials. Because of their tailored perovskite structural features, materials such as F, Cl, Br, I, and an alkaline or alkali-earth element are used. J.I. Gomez-Peralta et al. performed a DFT simulation on 136 materials to find their application for AI and better understand their perovskite structure; out of 136 compounds, 96 showed the perovskite compound properties. Artificial neural networking plays a significant role in optoelectronic compounds production. As a result of an analysis process in which they examined the sustainability of the ANN-predicted perovskite structures after experimental and theoretical computations, the molecules predicted by the ANN have been shown to be strong enough to form the perovskite structure. The corner-shared octahedral structure that distinguishes the perovskite structure remained intact after recurrent refinement simulations [20].
ANN has been applied to the maximum number of compounds, and properties have been studied following two different static and dynamic methods. In the static approach, the compounds are synthesized with greater crystal growth and the pros and cons of the compounds are identified as the optimal conditions, temperature dependency, and crystal growth morphologies. With this, the material is created with minimal structural defects [21]. Researchers have derived 81 stimulations from ANN with few inputs and a smaller number of layers. These ANN-derived simulations were used to study the crystal growth structure, the rotational rate of the crystal, temperature dependency of the sample, and the temperature holding capability of the sample containers or crucibles. To describe the complex nonlinear relationship between crystal growth process parameters and interface form, researchers have employed two statistical artificial neural network methods and Gaussian process (G.P.) models [22].

The process involving two statistical approaches was mainly used to identify and optimize magnetic parameters for temperature field control. From this, it is more apparent than in a static method that when both artificial neural networking and Gaussian processes are involved in showing functional group identity and external factor influence, we observe better results compared to ANN alone. Coming to the Dynamic method, it is crucial to inhibit turbulent motion in the melt and manage temperature differences in the crystal, which are responsible for producing harmful crystal defects and unwanted fluctuation in crystal diameter [23].

The dynamic ANN method has been applied to overcome these crystal diffusions, and crystal structure studies were made in the static feed dynamic crystal growth approach, the researchers evaluated the process parameters of two warmers as well as the velocities of the thermal barrier throughout the particles generated. Precise temperature control is required for the Metal-Organic Chemical Vapor Deposition (MOCVD) of GaN for micro-scale and absorption spectra. Preserve wavelength homogeneity and manage wafer bow and decrease wafer slide. NAXR neural networks have proven successful for numerous time-series modeling jobs, notably in control applications, by learning long-term data analysis applications using open-source massive crystallization process data will eliminate the final barrier for ANN applications and considerably expedite the development of new novel crystal substance products. [24]

5.2 AI in electrochemical catalyst

On the basis of evidence of the start spinning DFT computational and dynamic modeling, comprehensive knowledge of an implementation of empirically achievable single-atom electrochemical catalyst for \( \text{H}_2\text{O}_2 \) creation has been described. When the electrode potential reaches equilibrium, the \( \Delta g^\circ \) changes in each fundamental step are equal,
permitting all interaction free energies to be zero. The Gibbs energy diagram of oxygen gas conversion to $\text{H}_2\text{O}_2$, where the computer initially evaluated the sustainability and selectivity of 31 single-atom catalysts, is one of the examples [25]. By considering the seven single-atom catalysts with different combinations of single crystal atoms, the DFT simulations are to make under the effect on $\text{H}_2\text{O}_2$ and then identify six among the top 7 highly potential catalysts have macro cyclic structures, implying that in this study, macro cyclic structures surpass graphene and other materials [26]. Metals having a weaker oxygen affinity, such as Ag, Au, and Pd, can significantly reduce band recombination between the metal and oxygen, resulting in greater preference favoring $\text{H}_2\text{O}_2$ production. This explains how such materials are widely utilized in ORR full form? as electro catalysts with a two-electron $\text{O}_2$ reduction ratio [27].

Analyzing a single-atom catalyst (SAC) and utilizing Machine learning techniques to investigate the affinity and specificity of a single atom catalyst the proportional connections between the Gibbs free energy and the proportionality connections in between the (OOH) and carboxylic group illustrate the variations in $G(\text{O})$ and $G(\text{OOH})$ on the 31 studied SACs ML explains why SAC selectivity and functionality differ and how the development of a more effective and reliable SAC for hydrogen peroxide generation. As can be shown, ML may significantly aid in establishing the link between material structure and attributes [28]. The technique was utilized to pick distinctive variables and provided the catalytic efficiency prediction equation. Combining two separate transverse magnetization decay curves (TMDCs) while altering the rotary orientation, bonding duration, spacing among layers, and band gap proportion of two different materials, performance may be significantly improved. In terms of creating a very sophisticated and highly specialized electro catalytic activity for oxygen reductions and release, researchers have summarized the process of developing precise descriptors and discovered different types of Descriptive tags that can increase the capacity to forecast material characteristics by applying machine learning and increased transmission processing to produce new as well as other catalysts compounds.[29].

5.3 **AI in electrolysis**

The most efficient technique for producing hydrogen is water electrolysis. However, the cathode materials are primarily costly metals that are inappropriate for large-scale usage. In such situations, computational methods play a role in identifying the different techniques for producing hydrogen-like materials [30]. Support Vector Machine methods and Artificial Neural Networks were used to explore the atomic characteristics, which demonstrated a significant relationship among both the catalytic site and bond angles parameters at the atomic level [31]. Changes beyond the original input set's prediction may
indeed be attributed to a reduced amount of low performance samples in the original database. SVR’s effectiveness is confirmed by the defined metrics. Over-fitting of all algorithms is possible, although it is dependent on the quantum of data used for training. As a result, as is customary, the facts determine the forecast rather than the other way around. To find a superior neural network approach, different numbers of neurons in the hidden layer were placed behind the four input neurons and in front of the one-bit output neuron [32]. Neuron densities in a simple linear plane range from 2 to 30 were tested, with modest networks with hidden layers of 6 or 8 neurons surpassing the rest. Decreased neuron quantities resulted in far more inaccuracy, but increased neuron quantities risked overfitting the network.[33]. Adding extra dropout layers to avoid overfitting had little impact. The network was trained across 500 epochs to avoid overfitting, with the option of quitting early if the metrics did not change. For validation, a 20% partition of something like the training dataset was used. Scientists picked a 46661 configuration of neurons and functioned as an input signal for this confirmation, as seen in the Fig: 1 [34].

![ANN input and output nodes](image.png)

**Fig: 1. ANN input and output nodes [34]**

The combined use of artificial neural networks, other types of AI technologies, and the Machine learning approach to assess performance and forecast atomic qualities projected more stable crystal structures. The researchers then trained and predicted the electro-chemical data set using three different ML models, organizing, and modifying the
data, overseeing the learning process, and assessing the three strategies using test data. Their empirical investigation shows that use of highly complex patterns does not necessarily result in more accurate prediction results, and that model accuracy is linked to the data itself [34].

5.4 AI in fuel cell technology

Although computational equations could be used to characterize the Microbial Fuel Cells (M.F.C.) biofilm formation mechanism and the physicochemical consequences, they cannot attain the desired results when simulating complex settings such as varied and combined microbial populations. To create mathematical correlations between wastewater/solution parameters, biofilm populations, and reactor efficiency, Artificial Neural Networks (ANNs) were applied. ANN simulations that included biotic interactions projected reactor efficiency better than those that did not. Because of the intricate interactions that take place in mixed species in bio electrochemical reactors such as microbial fuel cells (MFCs), as shown in Fig. 2, it is challenging to anticipate performance outcomes under experimental situations.

![Image](image_url)

*Fig: 2. MFCs interaction in the mixed-phase system [35]*

It was challenging to construct thorough probabilistic models for different and dynamic microbial communities; nevertheless, at this time, the ANN-based simulations made it simple to reliably assess a variety of reactor output and biofilm compositions throughout
water treatment. The algorithms that link community composition, wastewater parameters, and reactor function have the ability to find the previously unknown and unverified waste waters that result in high MFC productivity. The effectiveness of data mining techniques is determined by the integrity of the data set. Several factors, including reactor architecture, operating parameters, and starting biofilm communities, were regulated in the current study to ensure that results correctly reflected connections between the parameter estimates [35].

**Table 1: Simulation Process**

<table>
<thead>
<tr>
<th>Domain of Energy Conversions</th>
<th>First Generation</th>
<th>Second Generation</th>
<th>Third Generation</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>AI in Photonics</strong></td>
<td>Structural properties calculation</td>
<td>Crystal structure prediction</td>
<td>Statically driven design</td>
</tr>
<tr>
<td><strong>AI in electrochemical Catalyst</strong></td>
<td>Local optimization algorithm</td>
<td>Global optimization algorithm</td>
<td>Chemical and physical data computation</td>
</tr>
<tr>
<td><strong>AI in Electrolysis</strong></td>
<td>Data collection</td>
<td>Experimental analysis</td>
<td>Simulated data comparisons</td>
</tr>
<tr>
<td><strong>AI in Fuel Cell Technology</strong></td>
<td>ANN Model Development</td>
<td>Multivariate Polynomial Regression (MPR) Method</td>
<td>Comparison of the ANN and M-ANN [36, 37]</td>
</tr>
</tbody>
</table>

**Conclusions**

AI is playing a pivotal role in empowering sustainable and economic forms of power generation. The energy sector has already deployed AI and machine learning for various functionalities, e.g., smart grids to balance electricity demand and supply, sensor-connected power plants, and windmills to mitigate the effects of low airflow in some regions. Still, wind and solar renewable energy suffer from intermittency problems. Catalyst is a crucial ingredient in sustainable energy conversion systems. The invention of suitable materials for catalysts is time-consuming, requiring theoretical domain knowledge and a rigorous experimental process. Deploying different modern machine learning algorithms and architectures and combining different hyper-parameters and optimization techniques, researchers can discover several catalysts for energy conversion systems. ML algorithms can virtually scan the existing databases and identify materials' novel characteristics and properties using a data-driven approach. It compensates for the said
limitations of the current conceptual framework. It can immediately analyze and anticipate material properties and crystal structures, as well as build new materials. AI can overcome human shortcomings in temporal analysis and processing. Secondly, AI can bring the reduction in time necessary for commercialization by reducing the material development cycle. Previously, to adjust and improve experimental circumstances, researchers had to read hundreds of thousands of relevant publications. They can only rely on human classification and summarization to select items for required characteristics, which are significant and time consuming. Using AI techniques increase efficiency through modeling and optimization without raising costs can be achieved. Finally, AI shows promise in material prediction. Nonetheless, there are several obstacles to overcome.

Acknowledgments

T. Ghosh acknowledges the DST Grant WOS-A/PM-42/2018 to support the research activities. PM P. Banerjee thanks SERB, India, for a TAR/2021/000032 research grant. B Koneru thanks GITAM University for Dr M. V.V. S Murthi research fellowship.

References


https://doi.org/10.3390/app11146348

https://doi.org/10.3389/fenrg.2020.00167