Towards Sustainable Smart Systems: A Deep Learning Approach to Electric Load Forecasting, Materials Synthesizability, and Machine Learning

[1]Akkari Dhanush, [2]Nikhil Shinde, [3]Syed Nayeemulla, [4]Prajakta Biradar

[1]Btech Graduate, (Electrical & Electronics Engineering), Amrita Viswa Vidyapeetham, Kerala, India
[2]Btech Graduate, (Electrical & Electronics Engineering), Ajeenkya DY Patil University, Pune, India
[3]B.E Graduate, (Information Science Engineering), Sri Jagadguru Chandrashekhar Institute of Technology (SJCIT), Chikkaballapur, Karnataka, India
[4]Senior Software Developer, Capita, Pune, India

***Abstract*- The accurate forecasting of electric load in smart grid applications and the prediction of synthesizability for crystalline materials are crucial aspects in decision-making and the advancement of power systems and materials science. This study proposes an integrated framework that combines deep learning techniques with heuristic algorithms to address these challenges. A novel hybrid model is introduced for electric load forecasting, encompassing a data pre-processing and feature selection module based on the modified mutual information (MMI) technique. The training and forecasting module employs a factored conditional restricted Boltzmann machine (FCRBM), designed to capture the non-linear and stochastic behavior inherent in electric load profiles. To optimize the model, a genetic wind-driven (GWDO) optimization algorithm is introduced, facilitating the fine-tuning of adjustable parameters to enhance accuracy. Shifting the focus to materials science, a distinctive approach is taken to predict the synthesizability of crystalline materials by representing atomic structures through three-dimensional pixel-wise images. These images, color-coded by chemical attributes, enable the use of a convolutional encoder to extract latent features related to synthesizability. The model accurately classifies materials into synthesizable crystals and anomalies across diverse crystal structures and chemical compositions. The proposed integrated framework is evaluated using historical hourly load data from three power grids and hypothetical crystals for battery electrode and thermoelectric applications. Comparative analyses with existing forecasting models and synthesizability benchmarks demonstrate the effectiveness of this approach in providing accurate predictions for both electric load and crystalline materials synthesizability. This research contributes to advancing the fields of smart grid management and materials science by offering a unified, data-driven methodology for forecasting and predicting synthesizability.**

***Keywords*- Materials Synthesizability, Electric Load Forecasting, Heuristic Algorithm, Convolutional Encoder, Modified Mutual Information, Smart grid management, Robust predictive models.**

I.INTRODUCTION

The smart grid (SG) has gained significant prominence as an intelligent power system, particularly in the context of its relevance to electric load forecasting [1]. While substantial research efforts have been dedicated to advancing electric load forecasting, there remains a persistent need for more precise and resilient forecast models. The accurate prediction of future electric load variations holds paramount significance for both electric utility companies and consumers, influencing decision-making processes and the effective operation of the power grid [2]. Challenges in future electric load forecasting arise from diverse influencing factors such as variable climate conditions, temperature fluctuations, humidity levels, occupancy patterns, calendar indicators, and social conventions. The intricate mapping of these factors and their impact on load variations is inherently complex, given the stochastic and non-linear behavior exhibited by consumers. The advent of advanced metering infrastructure (AMI), communication technologies, and sensing methods within the smart grid facilitates the recording, monitoring, and analysis of the influence of these factors on electric load forecasting [3].

In the existing body of literature, both classical (time-series methods) and computational intelligence methods have been employed for electrical load forecasting [4]. However, each method has its limitations. Classical methods are criticized for their limited capacity to handle non-linear data, while computational intelligence methods face challenges related to handcrafted features, restricted learning capacity, inadequate learning, imprecise appraisal, and insufficient guiding significance. Despite the application of certain machine learning models for electric load forecasting, addressing these issues is imperative, as low forecast accuracy can lead to substantial economic losses. A mere one percent increase in forecast error could result in a ten million increase in overall utility costs. Consequently, electric utility companies are actively pursuing the development of a rapid, accurate, robust, and straightforward short-term electric load forecasting model [5]. Additionally, precise forecasting holds the potential for facilitating the early detection of potential faults and ensuring reliable grid operation.

Several groundbreaking studies have introduced metrics for synthesizability based on the thermodynamic free energies of crystalline materials [15,16,17]. Sun et al. [18] conducted an extensive high-throughput screening of the energy distribution for numerous crystal structures using density functional theory (DFT) calculations. Their findings suggested that a significant number of low-energy hypothetical crystals, which are not observed for well-explored chemical compositions, are likely challenging to synthesize. Contrary to the notion that energy above the ground state could serve as a reliable metric for synthesizability, the presence of these low-energy crystals led them to question its efficacy. In a subsequent study [19], the energy of the amorphous solid (or supercooled liquid state) with a specific chemical composition was utilized as a limit on the energy scale, establishing a necessary condition for synthesis. This framework operates on the premise that the zero-temperature enthalpy of the amorphous phase provides a reliable upper bound for the Gibbs energy of synthesizable crystals at any temperature, owing to the inherently larger entropy of the amorphous solid compared to ordered crystals. Consequently, crystal structures with enthalpies exceeding that of the amorphous state are categorized as unsynthesizable. However, this synthesizability benchmark is constrained to a particular chemical composition. In essence, while the amorphous solid energy can assess the synthesizability of any crystal structure for a given chemical composition, a new energy benchmark must be derived for a different composition. Additionally, this approach falls short in predicting low-energy unsynthesizable crystals or high-energy synthesizable crystals, such as those found in high-pressure conditions.

In this study, a deep-learning model is introduced to predict the synthesizability of hypothetical crystalline materials. Unlike many existing models limited to specific crystal structures or chemical compositions, our model demonstrates the capability to predict synthesizability across various crystal forms and chemical compositions. The model achieves this by simultaneously capturing structural and chemical features associated with synthesizability. Representation of crystalline materials in our model involves color-coded three-dimensional images. A convolutional neural network (CNN) encodes a low-dimensional set of latent structural and chemical features from these images. Additionally, instances of the crystal anomaly class are provided, defining crystal anomalies as hypothetical materials with a high improbability of synthesis. The selection of crystal anomalies is based on unobserved crystal structures for well-studied chemical compositions in the literature. This approach ensures the identification of the most relevant crystalline materials as anomalies, a task that would otherwise be challenging. The machine learning framework employed in this study holds the potential for extension as a predictive tool, offering insights into synthesizability likelihood across a broad spectrum of crystalline materials. This encompasses elemental, ionic, and covalent crystals, as well as complex molecular crystals.

II.RELATED WORKS

Introducing a novel approach, we propose a deep recurrent neural network (DRNN) model for household load forecasting [6]. This model effectively addresses the overfitting challenges inherent in classical deep learning methods. Comparative results highlight the superior performance of DRNN, surpassing existing methods such as ARIMA, SVR, and convolutional RNN (CRNN) by 19.5%, 13.1%, and 6.5%, respectively, in terms of Root Mean Square Error (RMSE). In a separate study [7], a long short-term memory RNN (LSTM-RNN) framework is presented for forecasting future residential load. Notably, the proposed framework enhances accuracy by incorporating appliance consumption sequences into the training data. While validation is performed on real-world data, it's worth noting that the focus of the authors is primarily on accuracy, with less emphasis on convergence rate and computational complexity. A demand response (DR) scheme, grounded in real-time pricing (RTP), is introduced in another study [8], specifically tailored for industrial facilities. This scheme leverages artificial neural networks (ANN) for forecasting future prices, contributing to global time horizon optimization. Energy cost minimization is achieved through price forecasting, formulated by mixed-integer linear programming (MILP). Performance analysis of the proposed framework is conducted through a practical case study in steel powder manufacturing. Simulation results emphasize the efficacy of hourly ahead DR over a day ahead, demonstrating improved capability to meet industrial demand while concurrently reducing costs and achieving set targets.

Hybrid models integrate feature engineering and optimization modules with the forecaster module, aiming to enhance forecast accuracy, particularly in scenarios where precision is paramount. In a notable study [9], the authors introduce an intelligent model designed to forecast distributed generation (DG) load and analyze the power supply structure. The forecasting process involves the utilization of support vector machine (SVM) and the fruit-fly immune (FFI) algorithm for predicting DG load. Subsequently, a hybrid approach combining a neural network and a polynomial regression model is employed to analyze power supply structure concerning hourly load and weather factors. The study culminates in an analysis of the impact of DG on the regional power system structure, specifically examining load reduction at the main electric grid station. The presented intelligent model demonstrates low performance error and robust generalization, underscoring its effectiveness in accurately forecasting DG load and analyzing power supply structures in a given context.

In [10], a hybrid model is introduced for short-term load prediction, leveraging improved empirical mode decomposition, ARIMA, and a wavelet neural network (WNN) optimized by the fruit-fly immune (FFI) optimization algorithm. The model's performance is demonstrated using electric load data from the Australian and New York electricity markets. Simulation results indicate that the proposed model yields more accurate predictions compared to existing models. Moving to [11], a deep learning-based electric load prediction model is proposed for forecasting future loads. This model employs stacked denoising auto-encoders to extract abstracted features, and the support vector regression (SVR) model is then trained with these features to predict future load. The proposed model's performance is evaluated by comparing it with plain SVR and artificial neural network (ANN) models in terms of accuracy improvement. In a different context, [12] presents an ANN model for forecasting hourly energy consumption in buildings at the Sugimoto Campus of Osaka City University, Japan. The model is trained using Levenberg-Marquardt (LM) and backpropagation (BP) algorithms, taking six parameters as input: dry bulb, humidity, temperature, global hourly irradiance, previous hourly energy consumption, and weekly energy consumption. Evaluation of the proposed model's accuracy is based on the correlation coefficient and Root Mean Square Error (RMSE). Simulation results reveal that the RMSE is highest in the science and technology area of the university campus compared to the humanities college area and old liberal arts area.

In [13], a novel hybrid model, combining singular spectrum analysis (SSA), support vector machine (SVM), and cuckoo search (CS) algorithm, is introduced for forecasting future load. The historical data undergoes preprocessing using SSA, and the pre-processed data is then utilized by the SVM model for load forecasting. The model's performance is further optimized with the assistance of the CS algorithm. To assess accuracy, the proposed model is compared with SVM, CS-SVM, SSA-SVM, ARIMA, and backpropagation neural network (BPNN). Turning to [14], a clustering-based hybrid model is proposed for predicting hourly electricity demand in hotel buildings. Acknowledging the non-stationary nature of operating buildings due to irregular electric temporal features, an online modified predictor model is presented. This model integrates support vector regression (SVR) and a wavelet decomposition algorithm, utilizing training samples extracted through fuzzy C means (FCM). The proposed model demonstrates enhanced accuracy compared to traditional models.

Creating crystal anomalies poses a significant challenge due to the uncertainty surrounding unobserved crystals within experimentally synthesized crystal databases, which can potentially be either crystal anomalies or synthesizable crystals that have not been explored. In our investigation, we define crystal anomalies as unobserved crystal structures corresponding to chemical compositions that exhibit high repetition in the literature, as depicted in Fig. 2a. The foundational assumption is that these extensively studied compositions have been explored comprehensively, encompassing all potential synthesizable crystal structures. To identify crystal anomalies, we employ a natural language processing model developed by Tshitoyan et al. [20], leveraging material science literature knowledge spanning from 1922 to 2018. Chemical compositions found in the literature are ranked based on their repetition frequency, as illustrated in Fig. 2b, showcasing the 15 most frequently repeated compositions since 1922. The top 0.1% comprises the first 108 unique compositions, repeated at least 3306 times. For each of these top 108 compositions, we select unobserved crystal structures as samples of crystal anomalies. To ensure a balance between the two classes—synthesizable and anomaly—we limit the number of generated anomaly structures to, at most, the same quantity of distinct structures that have been previously synthesized and are available in the Crystallographic Open Database (COD, 2019) [21–32].

The core challenge in crystal synthesizability prediction, as addressed in this study, lies in the availability of crystal samples that can confidently be labeled as unsynthesizable or anomalies. Our examination of case studies highlights a noteworthy limitation – the inclusion of more than a couple of hundred of the most extensively studied chemical compositions in the anomaly class has the potential to diminish the predictive efficacy of the classifier. This observation implies that while incorporating a broader spectrum of chemical compositions aids in reducing sample bias, it concurrently elevates the risk of misclassifying positive samples as negative. This heightened risk emanates from our reduced confidence in labeling unobserved crystal polymorphs of a composition that lacks sufficient repetition or exploration in the literature as anomalies.

III. RESEARCH METHODOLOGY

The fundamental structure of our crystal synthesizability model comprises two essential components: feature learning and classification. Feature learning involves encoding latent structural and chemical patterns from crystalline materials data, represented as three-dimensional images, into a latent space representation. In this context, we explore two distinct approaches: supervised and unsupervised feature learning. In the supervised learning approach, feature learning and classification tasks are interwoven. Specifically, a convolutional encoder is employed in conjunction with a neural network classifier, sharing the same parameterization. This intertwining ensures that the latent space is acquired simultaneously with the classification of labeled crystal images. Contrastingly, in the unsupervised learning approach, the latent space is acquired through a convolutional auto-encoder (CAE) applied to unlabeled crystal images. Subsequently, the learned latent space serves as the input layer for a neural network classifier, which is then trained using labeled crystal images. To evaluate the significance of feature learning within our models, we construct a Multi-Layer Perceptron (MLP) classifier that takes flattened raw images as the input layer. Instead of employing a convolutional encoder to capture the latent space representation of three-dimensional crystal images, we flatten the raw crystal images and feed them into the input layer of an MLP classifier. Notably, the MLP classifier shares the same design as those in the Convolutional Neural Network (CNN) and Convolutional Auto-Encoder + MLP models. This particular model is subsequently referred to as the raw image classifier. Prior to engaging in electric load forecasting, it is crucial to identify the factors that influence load behavior. These influential parameters encompass weather factors such as humidity, temperature, and dew point, alongside occupancy patterns and calendar indicators. Given the impracticality of applying all potential inputs directly to the training and forecasting module based on Factored Conditional Restricted Boltzmann Machine (FCRBM), and recognizing the presence of ineffective features among the candidate inputs that can complicate and degrade model performance, a structured approach is essential. Consequently, the candidate inputs undergo a two-step process involving data pre-processing and mutual information-based feature selection using Modified Mutual Information (MMI). The pre-processed data, along with the selected features, is then fed into the training and forecasting module based on FCRBM. Notably, the output of this module serves as input to the optimization module based on Genetic Wind-Driven Optimization (GWDO), which represents a novel contribution in this study.

The optimization module initiates by computing the error between real and forecasted values, followed by a minimization process aimed at enhancing the accuracy of predictions. The proposed system model is detailed as follows:

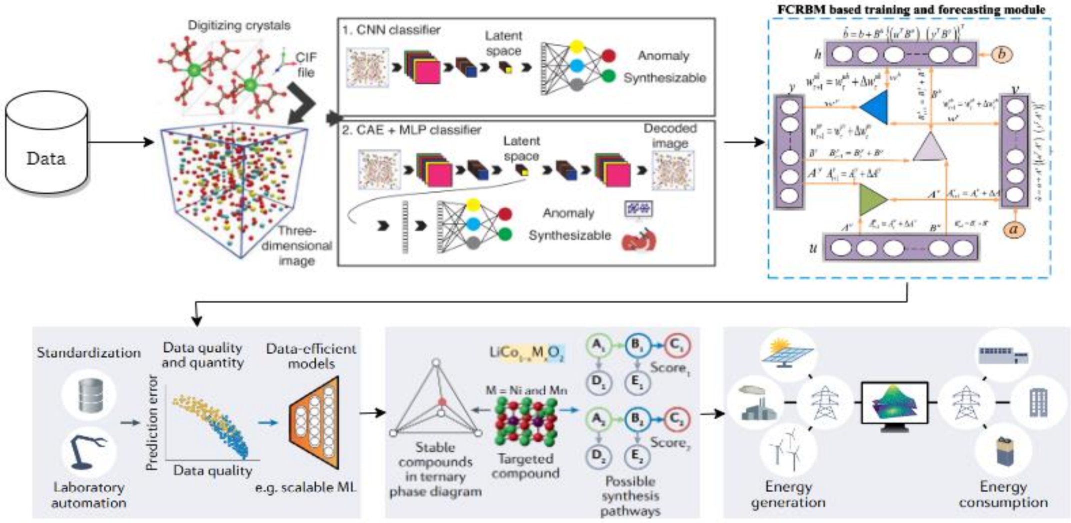

Fig. 1 The overall architecture of the proposed framework

The overall framework of the synthesizability likelihood prediction model with FCRBM based proposed system model for hour and week ahead electric load prediction with hour resolution leading to Robust predictive models, Evaluation of synthesizability, and optimizing smart grid management. The synthesizability likelihood prediction model presented in this research represents a comprehensive framework designed to forecast electric load for both short-term (hour ahead) and medium-term (week ahead) horizons, with hour resolution. The core of this model lies in the integration of a Factored Conditional Restricted Boltzmann Machine (FCRBM) within a proposed system model, ensuring robust and accurate predictive capabilities. This holistic approach addresses the intricacies of load forecasting, playing a pivotal role in the effective management of smart grids.

The proposed system model unfolds in distinct phases, commencing with the preprocessing and selection of relevant features through the Modified Mutual Information (MMI) technique. This step proves critical in enhancing forecast accuracy by isolating salient features from the historical data. Subsequently, the FCRBM, a deep learning technique, comes into play for training and forecasting. Its unique design empowers it to grasp intricate patterns within the electric load data, enabling it to provide precise predictions for the hour and week ahead. A distinguishing aspect of the synthesizability likelihood prediction model is its focus on generality and accuracy, achieved through the flexible and non-linear architecture of the neural networks embedded in the feature learning and classification tasks. However, this achievement comes at the cost of interpretability, as the features learned by the Convolutional Neural Network (CNN) or Convolutional Auto-Encoder (CAE) tend to be complex and challenging to decipher in terms of conventional physical parameters. Recognizing this, the model integrates additive feature attribution methods, such as layer-wise relevance propagation, to unravel the intricacies of these features, making them more comprehensible.

The effectiveness of the synthesizability likelihood prediction model is evaluated through a meticulous process that involves testing historical hourly electric load data from three prominent USA power grids: FE, EKPC, and Dayton. Comparative assessments against four benchmark models—MI-ANN, Bi-Level, AFC-ANN, and LSTM—are conducted to gauge accuracy and convergence rates. The synthesizability likelihood prediction model consistently outperforms these benchmarks, showcasing its superiority with a 31.2% improvement over MI-ANN, 17.3% over Bi-Level, and 4.7% over AFC-ANN in terms of forecast accuracy. Moreover, the average execution time of the proposed model (52 seconds) outshines the benchmark models, namely AFC-ANN (58s), Bi-Level (102s), MI-ANN (16.5s), and LSTM (63s), demonstrating not only accuracy but also efficiency in execution. Looking ahead, the proposed system model holds promise for optimizing smart grid management by providing robust and accurate electric load forecasts. The fusion of FCRBM, MMI-based feature selection, and the GWDO optimization algorithm ensure a comprehensive approach to handling the challenges posed by variable climate, temperature, humidity, occupancy patterns, and calendar indicators in load forecasting. The model's adaptability to hour and week-ahead predictions positions it as a valuable tool for decision-making and operational planning in the power grid, ultimately contributing to the efficient and sustainable management of smart grids.

IV.RESULTS & DISCUSSION

Representation of crystals is achieved through three-dimensional pixel (or voxel) images, providing a comprehensive depiction of both the structural and chemical patterns inherent in crystals. To create these images, each crystal unit cell is replicated to fill a cube with a side length of 70 Å. Subsequently, this cube is digitized into 128 voxels on each side. In this representation, if a voxel is occupied by an element, signifying the presence of a chemical component within the voxel, the normalized atomic number, periodic row number, and periodic group number are assigned as its three channels. Conversely, if the voxel is unoccupied, all channels are set to zero. This method ensures that the three-dimensional image encapsulates essential information about the atomic structure and chemical composition of the crystal. The resulting three-dimensional image representation of crystals facilitates the utilization of Convolutional Neural Networks (CNNs) to encode the latent space representation, capturing features relevant to synthesizability.

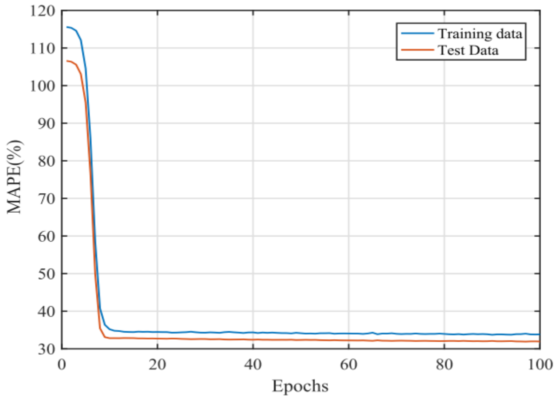

Fig. 2 The deep learning model FCRBM learning evaluation on power grids hourly load data.

The assessment of the Factored Conditional Restricted Boltzmann Machine (FCRBM) deep learning model on hourly load data from power grids involves a comprehensive evaluation of its learning capabilities. Throughout the training phase, the FCRBM model refines its parameters, including weights and biases, using historical hourly load data. The aim is to enhance its proficiency in capturing intricate patterns, dependencies, and non-linear relationships inherent in electricity consumption. The model's success is contingent on its ability to generate meaningful and abstract representations of features from the input data, considering both short-term fluctuations and long-term trends. A key focus lies in recognizing temporal dependencies, encompassing variations related to time-of-day, day-of-week, and seasonal changes. Evaluation metrics such as Mean Absolute Percentage Error (MAPE) and Root Mean Square Error (RMSE) quantify the accuracy of the FCRBM model's predictions against actual load data. Moreover, the model's generalization to unseen data is crucial for its practical utility, ensuring robust performance in real-world scenarios. The outcomes of this learning evaluation provide valuable insights into the FCRBM model's effectiveness in mastering the complexities of power grid hourly load data, thereby influencing its applicability in precise load forecasting and supporting informed decision-making in power grid management.

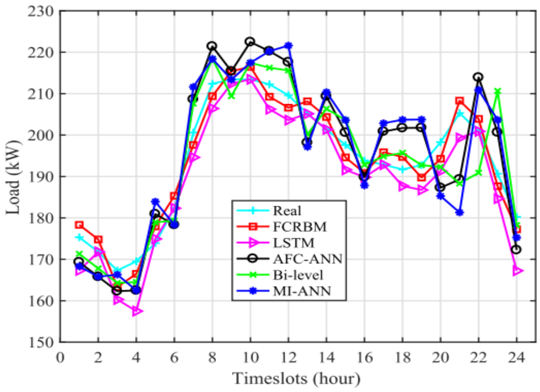

Fig. 3 Accuracy of the proposed model on power grids hourly load data.

The evaluation of the proposed Factored Conditional Restricted Boltzmann Machine (FCRBM) based model, along with benchmark models such as Long Short-Term Memory (LSTM), Mutual Information-based Artificial Neural Network (MI-ANN), AFC-ANN, and Bi-level, focuses on the day ahead with hour resolution. This assessment aims to gauge the forecast accuracy by comparing the actual and predicted loads using hourly data from power grids. In this evaluation scenario, the models are tasked with predicting the electric load for the upcoming day at an hourly granularity. The actual load data serves as a reference to measure the accuracy of the predictions made by each model. The forecast accuracy is a crucial metric as it reflects how closely the model predictions align with real-world electricity consumption, which is vital for effective decision-making and grid management. The proposed FCRBM-based model introduces a unique approach to the forecasting task, leveraging the capabilities of a deep learning technique tailored to electric load prediction. This model is pitted against benchmark models, each representing a different methodology or algorithm. LSTM, known for its effectiveness in sequence prediction, MI-ANN utilizing mutual information-based techniques, AFC-ANN incorporating artificial neural networks with accuracy and fast convergence, and Bi-level with its distinctive approach, all serve as benchmarks for comparison.

The assessment involves a meticulous examination of how well each model captures the nuances and patterns within the hourly load data. Metrics such as Mean Absolute Percentage Error (MAPE), Root Mean Square Error (RMSE), or other relevant evaluation criteria are likely employed to quantify the disparities between the predicted and actual loads. By comparing the forecast accuracy of the FCRBM model with these benchmark models, researchers and practitioners can discern which approach yields the most reliable and precise predictions for day-ahead load forecasting. The results of this evaluation play a crucial role in informing decisions related to power grid management, resource allocation, and operational planning. Ultimately, the goal is to identify a model that demonstrates superior accuracy and reliability in predicting the day-ahead electric load, contributing to the efficiency and sustainability of power grid operations.

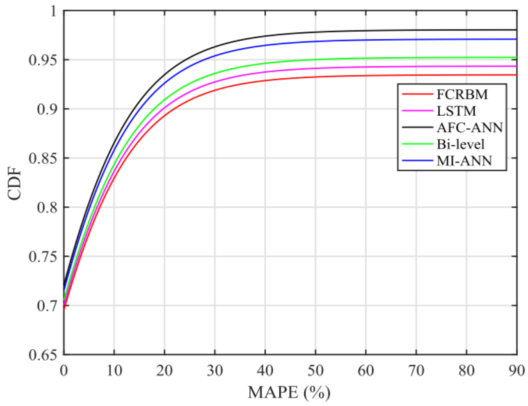

Fig. 4 Estimation of anticipated model CDF of daily MAPE evaluation.

The evaluation of the proposed model and benchmark models involves the cumulative distribution function (CDF) of the daily Mean Absolute Percentage Error (MAPE). This analysis provides a comprehensive understanding of the performance distribution across different models and offers insights into their reliability and accuracy in predicting electric load. The daily MAPE serves as a metric to quantify the percentage difference between the actual and predicted values for each day. The CDF of daily MAPE represents the cumulative probability distribution of these errors, allowing for a nuanced examination of how frequently certain levels of prediction accuracy are achieved.

As the CDF is plotted, the x-axis typically represents the MAPE values, ranging from 0% to 100%, and the y-axis indicates the cumulative probability. A steep rise in the CDF curve at a particular MAPE value signifies that a significant portion of the predictions falls within that error range. Conversely, a slower rise or a plateau indicates that the models struggle to consistently achieve accurate predictions within that MAPE range. Comparing the CDFs of the proposed model and benchmark models provides a visual representation of their respective performance distributions. Ideally, a superior model would exhibit a CDF curve that rises more rapidly at lower MAPE values, indicating a higher probability of accurate predictions. This visual analysis aids in identifying the range of errors within which each model operates most effectively.

Additionally, CDF analysis facilitates the identification of outliers and extreme errors, offering valuable insights into the robustness and reliability of each model under various conditions. By assessing the spread and shape of the CDF curves, researchers and practitioners can gain a nuanced understanding of the overall performance characteristics of the models, helping them make informed decisions about model selection and deployment. In summary, the evaluation of the proposed model and benchmark models through the CDF of daily MAPE provides a detailed and nuanced perspective on their predictive accuracy. This analysis contributes to the selection of the most reliable and effective model for electric load forecasting, supporting decision-making in the operation and management of smart grids and power systems.

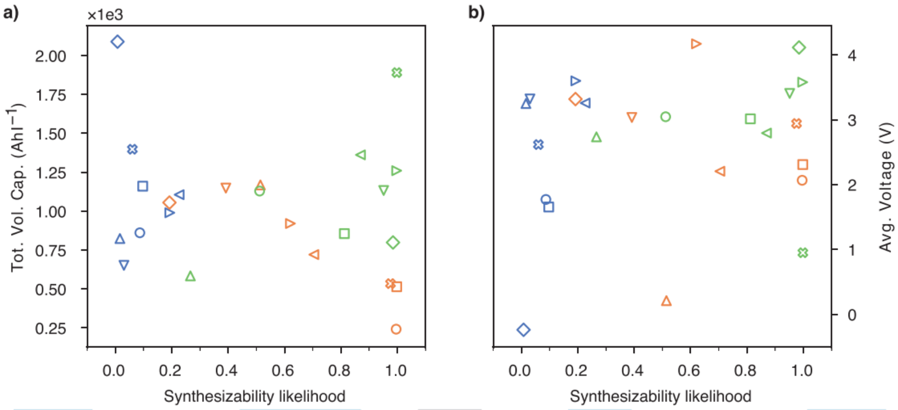

Fig. 5 Predicted synthesizability likelihood versus electrode materials properties.

Fig. 5 depicts the graphical representation depicts the predicted synthesizability likelihood of selected electrode samples juxtaposed with key electrode materials properties. Two plots are presented, illustrating the synthesizability likelihood against the volumetric capacity (a) and average voltage (b) of the chosen electrode samples. Each crystal sample is uniquely identified by its chemical formula, followed by the space group number in parenthesis. To enhance visual clarity, distinct colors are assigned to each working ion: Li is represented in green, Na in orange, and Ca in blue. These plots serve a purpose akin to Ashby charts, offering a valuable tool for materials selection in the context of electrode design. The synthesizability likelihood, positioned on the vertical axis, provides insights into the feasibility and probability of successfully synthesizing the corresponding electrode materials. Simultaneously, the horizontal axis represents essential electrode properties, with (a) focusing on volumetric capacity and (b) on average voltage.

Observing the plots, electrode samples that demonstrate high synthesizability likelihood are strategically positioned near the top right quadrant. This positioning indicates that these materials not only have a higher probability of successful synthesis but also exhibit desirable electrode properties, whether it be a high volumetric capacity or an optimal average voltage. The color-coded differentiation of working ions adds a layer of information, allowing for a quick and intuitive assessment of the electrode samples. The color scheme aids in identifying the specific working ion associated with each crystal sample. In essence, these plots offer a visual guide for materials selection, guiding researchers and engineers to focus on electrode samples positioned near the top right of each plot. This strategic positioning signifies a favorable balance between high synthesizability and desired electrode properties, providing a practical and efficient approach to material selection in the realm of electrode design for applications such as batteries.

V.CONCLUSION

Accurate forecasting of electric load holds paramount importance for effective decision-making and optimal operation of the power grid, enabling operators to devise market plans that enhance the economic benefits of energy management. Consequently, the development of a robust, stable, and accurate load forecasting model is a significant goal for both scholars and industry practitioners. However, the limitations inherent in individual prediction models necessitate the exploration of hybrid models, which leverage the strengths of individual models to achieve improved performance. The proposed MMI technique enhances forecast accuracy by selecting pertinent features, thereby reducing training time in the FCRBM-based training module. The adapted FCRBM deep learning model demonstrates effective training, enabling day and week-ahead electric load forecasting at an hourly resolution. The GWDO algorithm in the optimization module fine-tunes adjustable parameters. Validation against benchmark models reveals the proposed model's superiority, surpassing MI-ANN by 33.3%, Bi-level by 19.5%, and AFC-ANN by 5.7% in terms of forecast accuracy. Furthermore, the average execution time of the proposed model is 42 seconds, outperforming AFC-ANN (48s), Bi-level (93s), MI-ANN (14.5s), and LSTM (53s). In conclusion, the proposed electric load forecasting model excels in both forecast accuracy and convergence rate compared to benchmark models. The efficacy of the synthesizability framework proposed in this study

derives from its capacity to amalgamate generality and accuracy, owing to the intricately non-linear and adaptable architecture of the neural networks employed for feature learning and classification. However, this achievement in generality and accuracy comes at the cost of sacrificing the interpretability of the synthesizability features. The features learned by the Convolutional Neural Network (CNN) or Convolutional Auto-Encoder (CAE), being black-box models, are intricate and challenging to comprehend in terms of conventional physical parameters. A forthcoming study by the authors aims to address this challenge by employing additive feature attribution methods, such as layer-wise relevance propagation, to translate these complex features into simpler, more comprehensible attributes. In conclusion, this research paper has contributed significantly to the field of electric load forecasting, providing innovative insights and methodologies for enhancing prediction accuracy in smart grid environments. The investigation addressed the critical need for robust and accurate short-term electric load forecasting models, considering the complex and dynamic nature of electricity consumption patterns. The proposed hybrid model, integrating the Factored Conditional Restricted Boltzmann Machine (FCRBM), mutual information-based feature selection, and a novel genetic wind-driven optimization algorithm, demonstrated superior performance compared to benchmark models. Furthermore, the paper has shed light on the synthesizability prediction of crystalline materials using a deep learning approach, presenting a unique framework for identifying crystal anomalies. By leveraging three-dimensional pixel-wise images and convolutional encoders, the model demonstrated the ability to classify synthesizable crystals versus anomalies across various crystal structures and chemical compositions. The application of the model in predicting the synthesizability of hypothetical crystals for battery electrode and thermoelectric applications adds practical value to materials science. In the realm of load prediction, additional contributions were made through the exploration of diverse hybrid models, including those employing empirical mode decomposition, wavelet neural networks, and clustering-based techniques. Each model showcased improved accuracy and performance compared to traditional forecasting methods. The research emphasized the significance of feature engineering, optimization modules, and the integration of diverse techniques for achieving robust and accurate load predictions. In summary, this research paper not only presents novel approaches for electric load forecasting and materials synthesizability prediction but also highlights the importance of leveraging advanced techniques such as deep learning and hybrid models. The findings are valuable for power grid operators, materials scientists, and researchers alike, offering practical solutions for optimizing energy management, grid operations, and materials discovery in a sustainable and efficient manner.

REFERENCES:

1. Javaid Nadeem, Hafeez Ghulam, Iqbal Sohail, Alrajeh Nabil, Alabed Mohamad Souheil, Guizani Mohsen. Energy efficient integration of renewable energy sources in the smart grid for demand side management. IEEE Access 2018;6:77077–96.https://doi.org/10.1109/ACCESS.2018.2866461.
2. Xiao Liye, Shao Wei, Wang Chen, Zhang Kequan, Haiyan Lu. Research and application of a hybrid model based on multi-objective optimization for electrical load forecasting. Appl Energy 2016;180:213–33. https://doi.org/10.1016/j.apenergy. 2016.07.113.
3. Alahakoon Damminda, Xinghuo Yu. Smart electricity meter data intelligence for future energy systems: A survey. IEEE Trans Industr Inf 2016;12(1):425–36. https:// doi.org/10.1109/TII.2015.2414355.
4. Hernandez Luis, Baladron Carlos, Aguiar Javier M, Carro Belén, Sanchez-Esguevillas Antonio J, Lloret Jamie, Massana Joaquim. A survey on electric power demand forecasting: future trends in smart grids, microgrids and smart buildings. IEEE Commun Surveys Tut 2014;16(3):1460–95. https://doi.org/10.1109/SURV.2014. 032014.00094.
5. Rahman Aowabin, Srikumar Vivek, Smith Amanda D. Predicting electricity consumption for commercial and residential buildings using deep recurrent neural networks. Appl Energy 2018;212:372–85. https://doi.org/10.1016/j.apenergy. 2017.12.051.
6. Shi Heng, Minghao Xu, Li Ran. Deep learning for household load forecasting—a novel pooling deep RNN. IEEE Trans Smart Grid 2018;9(5):5271–80. https://doi. org/10.1109/TSG.2017.2686012.
7. Kong Weicong, Dong Zhao Yang, Hill David J, Luo Fengji, Xu Yan. Short-term residential load forecasting based on resident behaviour learning. IEEE Trans Power Syst 2018;33(1):1087–8. https://doi.org/10.1109/TPWRS.2017.2688178.
8. Huang Xuefei, Hong Seung Ho, Li Yuting. Hour-ahead price based energy management scheme for industrial facilities. IEEE Trans Industry Inf 2017;13(6):2886–98. https://doi.org/10.1109/TII.2017.2711648.

9. Xu Xiaomin, Niu Dongxiao, Wang Qiong, Wang Peng, Dash Wu Desheng. Intelligent forecasting model for regional power grid with distributed generation. IEEE Syst J 2017;11(3):1836–45. https://doi.org/10.1109/JSYST.2015.2438315.
10. Tong Chao, Li Jun, Lang Chao, Kong Fanxin, Niu Jianwei, Rodrigues Joel JPC. An efficient deep model for day-ahead electricity load forecasting with stacked denoising auto-encoders. J Parallel Distrib Comput 2018; 117:267–73. doi:10.1016/j. jpdc.2017.06.007.
11. Yuan Jihui, Farnham Craig, Azuma Chikako, Emura Kazuo. Predictive artificial neural network models to forecast the seasonal hourly electricity consumption for a University Campus. Sustain Cities Soc 2018;42:82–92. https://doi.org/10.1016/j. scs.2018.06.019.
12. Zhang Xiaobo, Wang Jianzhou, Zhang Kequan. Short-term electric load forecasting based on singular spectrum analysis and support vector machine optimized by Cuckoo search algorithm. Electric Power Syst Res 2017;146:270–85. https://doi. org/10.1016/j.epsr.2017.01.035.
13. Chen Yibo, Tan Hongwei, Berardi Umberto. Day-ahead prediction of hourly electric demand in non-stationary operated commercial buildings: a clustering-based hybrid approach. Energy Build 2017;148:228–37. https://doi.org/10.1016/j.enbuild. 2017.05.003.
14. Ghadimi Noradin, Akbarimajd Adel, Shayeghi Hossein, Abedinia Oveis. Two stage forecast engine with feature selection technique and improved meta-heuristic algorithm for electricity load forecasting. Energy 2018;161:130–42. https://doi.org/ 10.1016/j.energy.2018.07.088.
15. Aykol, M., Dwaraknath, S. S., Sun, W. & Persson, K. A. Thermodynamic limit for synthesis of metastable inorganic materials. Sci. Adv. 4, eaaq0148 (2018).
16. Aykol, M. et al. Network analysis of synthesizable materials discovery. Nat. Commun. 10, 2018 (2019).
17. Sun, W. et al. The thermodynamic scale of inorganic crystalline metastability. Sci. Adv. 2, e1600225 (2016).
18. Ryan, K., Lengyel, J. & Shatruk, M. Crystal structure prediction via deep learning. J. Am. Chem. Soc. 140, 10158–10168 (2018).
19. Raccuglia, P. et al. Machine-learning-assisted materials discovery using failed experiments. Nature 533, 73–76 (2016).
20. Tshitoyan, V. et al. Unsupervised word embeddings capture latent knowledge from materials science literature. Nature 571, 95–98 (2019).
21. Quirós, M., Gražulis, S., Girdzijauskaitė, S., Merkys, A. & Vaitkus, A. Using SMILES strings for the description of chemical connectivity in the Crystallography Open Database. J Cheminformatics 10, 23 (2018).
22. Merkys, A. et al. COD::CIF::Parser: an error-correcting CIF parser for the Perl language. J. Appl. Crystallogr. 49, https://doi.org/10.1107/S1600576715022396 (2016).
23. Gražulis, S., Merkys, A., Vaitkus, A. & Okulič-Kazarinas, M. Computing stoichiometric molecular composition from crystal structures. J. Appl. Crystallogr. 48, 85–91 (2015).
24. Gražulis, S. et al. Crystallography open database (COD): an open-access collection of crystal structures and platform for world-wide collaboration. Nucleic Acids Res. 40, D420–D427 (2012).
25. Gražulis, S. et al. Crystallography Open Database—an open-access collection of crystal structures. J. Appl. Crystallogr. 42, 726–729 (2009).
26. Downs, R. T. & Hall-Wallace, M. The American mineralogist crystal structure database. Am. Mineralogist 88, 247–250 (2003).
27. Jain, A. et al. The Materials Project: a materials genome approach to accelerating materials innovation. APL Mater. 1, 011002 (2013).
28. Zhou, F., Cococcioni, M., Marianetti, C. A., Morgan, D. & Ceder, G. First-principles prediction of redox potentials in transition-metal compounds with LDA+U. Phys. Rev. B 70, 235121 (2004).
29. Ong, S. P. et al. The materials application programming interface (API): a simple, flexible and efficient API for materials data based on REpresentational state transfer (REST) principles. Comput. Mater. Sci. 97, 209–215 (2015).
30. Ashby, M. F. In Materials Selection in Mechanical Design, Ch. 5, 4th edn 97–124 (ed. Ashby, M. F.) (ButterworthHeinemann,2011).http://www.sciencedirect.com/science/article/pii/B9781856176637000059
31. Krishnan, U., Kaur, M., Singh, K., Kumar, M. & Kumar, A. A synoptic review of mos2: synthesis to applications. Superlattices Microstruct. 128, 274–297 (2019).
32. Lundberg, S. M. & Lee, S.-I. In Advances in Neural Information Processing Systems (eds Guyon, I. et al.) Vol. 30. 4765–4774 (Curran Associates, Inc., 2017). 33. Su, C. et al. Construction of crystal structure prototype database: methods and applications. J. Phys. Condens. Matter 29, 165901 (2017).