

Image-based machine learning for materials science

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ABSTRACT

Materials research studies are dealing with a large number of images, which can now be facilitated via image-based machine learning techniques. In this article, we review recent progress of machine learning-driven image recognition and analysis for the materials and chemical domains. First, the image-based machine learning that facilitates the property prediction of chemicals or materials is discussed. Second, the analysis of nanoscale images including those from a scanning electron microscope and a transmission electron microscope is discussed, which is followed by the discussion about the identification of molecular structures via image recognition. Subsequently, the image-based machine learning works to identify and classify various practical materials such as metal, ceramics, and polymers are provided, and the image recognition for a range of real-scenario device applications such as solar cells is provided in detail. Finally, suggestions and future outlook for image-based machine learning for classification and prediction tasks in the materials and chemical science are presented. This article highlights the importance of the integration of the image-based machine learning method into materials and chemical science and calls for a large-scale deployment of image-based machine learning methods for prediction and classification of images in materials and chemical science.

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I. INTRODUCTION

The structure–property relationship is critical in materials science. Morphology, phase, atomic structure, surface structure, and interfacial structure are all examples of structures that are of interest to materials scientists.¹ In addition, it is viable to tailor synthetic parameters to regulate material structures and their applications in an effort to address the fundamental questions in materials science such as those related to the four essential elements in materials science: composition/structure, synthesis, property, and performance. This is a key paradigm for many materials’ research areas, such as metallic materials, semiconductors, and functional materials for catalysis, optoelectronics, and batteries. Microscopic imaging is one example of the structure characterization techniques to provide real-time information on the structure of materials over a wide scale range. The recent development of the materials’ genome calls for the fundamental understanding on structure–property relationships of materials based on the materials and chemical genes, which can be realized by the data-driven method. This is a new research paradigm

that helps us comprehensively understand the structure–property relationships from a global picture and avoids the typical trial-and-error process required in traditional methods.^{2,3}

Three major types of data are universally available in the materials and chemical databases, including numerical, textual, and image data. The numerical data, such as the boiling points, structural geometries, molecular weight, bandgap, and power conversion efficiencies, correspond to the traditional data source that is widely employed for machine learning applications in materials and molecular science. In addition, structure and property databases such as materials project, Open Quantum Materials Database (OQMD), Joint Automated Repository for Various Integrated Simulations (JARVIS), Automatic FLOW for Materials Discovery (AFLOW), Cambridge Structural Database (CSD), and Inorganic Crystal Structure Database (ICSD) are prepared via the long-term curation of small (single data-point) datasets to provide quantitative information on all aspects of the materials and chemicals. In contrast, the latter two types of data are less understood and are

receiving attention in recent years owing to their ubiquity in the publications and databases. Since a larger number of textual data^{4–7} associated with materials' composition, structure, synthesis, property, and performance exist in the materials and chemical literature, several natural language processing (NLP)-based material studies have been carried out to extract the hidden relationships and predict new materials or chemical candidates.^{8–12} In most cases, the word embedding method such as word2vec is leveraged to establish the relationships between various materials and applications via the calculation of cosine similarity between the word vectors.^{4,12–16}

In materials and chemical sciences, various types of images such as those obtained from atomic force microscopy (AFM), the scanning electron microscope (SEM), the transmission electron microscope (TEM), scanning probe microscopy (SPM), x-ray diffraction (XRD), UV-vis spectroscopy, and infrared spectroscopy (IR) are available,¹⁷ which serve as the natural choice for the database preparation, model training and information extraction, and calls for machine learning-driven image techniques to analyze the materials and chemicals as well as uncover the underpinning physics.^{18–22} In addition, materials and chemical sciences are associated with a number of images ranging from macroscale to nanoscale sizes; for example, extensive failure and defect recognition is often required for metal, ceramic, polymer, and composites materials industries. The nanoscale images consist of molecular and morphological images from the optical and electron microscope for a detailed analysis. In particular, the images obtained from SEM, TEM, and SPM provide rich information on nanoscopic structures for the materials analysis, and the patterns in the images should be analyzed in detail via machine learning techniques to provide latent information.

In this article, we review recent progress on image-based machine learning works for materials and chemical science. Note that our focus is set on the explicit application of image recognition techniques to images only. The numerous attempts to apply image-related algorithms to more abstract, not picture-related data are not covered in this review. The information extraction from the macro-, micro-, nano-, and molecular-scale images using data-driven and machine learning approaches are discussed in detail. More importantly, the property prediction of chemicals and materials, including the infrared spectra and the band structure, can be facilitated via image-based machine learning methods. Case studies of image recognition and analysis for devices and advanced materials such as solar cells, batteries and catalysts, as well as the defects and failure detection are provided. We argue the effectiveness of machine learning for various materials and chemical images, including the nanomaterials' images, macromaterials' images, device images, and molecular images [Fig. 1(a)], while the image-based machine learning technique is particularly viable to predict the spectroscopic data in the form of images of the chemicals and materials, which complements traditional experimental characterizations and the first-principles calculations. We also provide recommendations on future research regarding the interdisciplinary research area combining the image recognition and materials/chemical science. The image-based data driven studies are beneficial for the accelerated development of chemical and materials science.

II. GENERAL WORKFLOW

The typical workflow of the AI-driven analysis on materials and chemical images consist of task analysis, data preparation, model

construction and validation, feature analysis, and result visualization [Fig. 1(b)], representing the typical machine learning processes in the literature.¹ However, image-based data types require advanced machine learning algorithms to abstract more information and establish the hidden relationships. In the starting point, the specific task types, whether regression or classification, should be identified. Second, the comprehensive image dataset should be prepared either from the structured database or the publications, with the labeled data ranging from experiments to simulations. For example, the SEM images, almost ubiquitous in nanomaterials research studies, should be manually classified and clearly annotated for improved accuracy. The data augmentation process is recommended if the image data are scarce and sparse, and the dataset is then split to prepare training, testing, and validating datasets. Third, the structured data are trained to build accurate machine learning models via image-based machine learning algorithms. Various algorithms and toolkits are available for the image-based machine learning analysis, including ResNet,²³ UNet,²⁴ PixelNet,²⁵ AlexNet,²⁶ DefectSegNet,²⁷ Variational AutoEncoder,²⁸ Inception,²⁹ and Densenet,³⁰ with variable convolution and pooling processes. Various frameworks incorporating the image-based machine learning functions are available, including TensorFlow,³¹ Keras,³² PyTorch,³³ Caffe,³⁴ Theano,³⁵ MXNET,³⁶ CNTK,³⁷ DeepLearning4J,³⁸ Chainer,³⁹ and FastAI.⁴⁰

A convolutional neural network (CNN) is a deep learning neural network that uses the architecture of a multi-layered feed-forward neural network to handle organized arrays of data such as images, which is built by stacking multiple hidden layers on top of each other in succession. CNN and its derivatives are the most popular deep learning algorithms for materials image analyses, such as materials categorization, phase identification, locations of atomic species, defect detection in scanning electron and transmission electron microscopy, and crack recognition. In a broader sense, one of the many advantages of utilizing a neural network is the considerably faster calculation time, which is important for analyzing the complex image data. For classification, the data inputs are classified into groups (e.g., which material type) based on a supervised learning process (learning with labeled data). There are binary classifiers with only two outcomes and multi-class classifiers in machine learning. A decision tree is a representative classification algorithm, in which repeated inquiries leading to exact classifications can be used to create a "if-then" framework for decreasing the pool of possibilities over time. In contrast, regressions establish connections and correlations between various types of data, and the statistical regression has long been used to forecast future output based on current data. With continuous variables, linear regression produces outputs with any value within a range. Logistic regression, polynomial regression, support vector regression, decision tree regression, and random forest regression are also common regression algorithms.⁴¹ In many cases, the inputs for the image-based machine learning techniques are the direct inputs of images. For example, the inputs can be drawn from a material dataset of SEM photos that are divided into several material categories. The outputs are material types, structures and attributes, etc., depending on research objectives. In addition, the identification of geometric descriptors is important for the spectra image prediction process. For instance, the molecular conformations act as inputs in the training set, while the vibrational frequency, transition dipole, and adjacent coupling

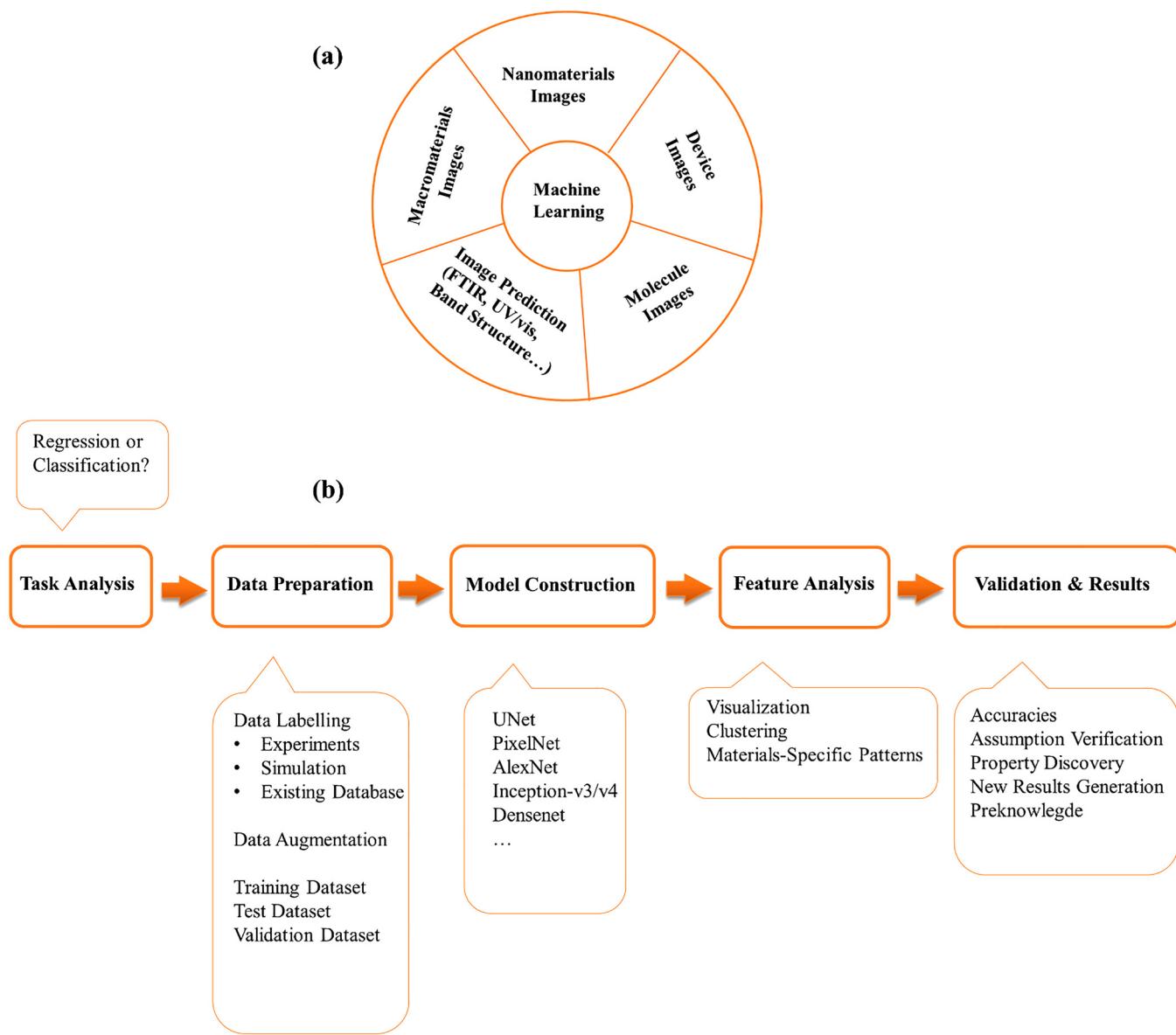


FIG. 1. (a) Image-based machine learning for analyzing various materials and chemical images, including nanomaterial images, macromaterial images, device images, molecular images, and spectra image prediction. (b) Typical workflow of the machine learning-driven analysis on chemical and material images, consisting of a task analysis, data preparation, model construction, feature analysis, and validation.

parameters are the outputs.⁴² In some other cases, the inputs include the unit-cell geometry while the output is the tight-binding Hamiltonian, which helps band structure prediction.⁴³

A. A few words on feature extraction

In the machine learning process, the image-related features or descriptors are often analyzed to help visualize and cluster the

materials- or chemical-specific patterns. The domain-specific results are generated and visualized based on assumption verification, properties discovery, and comparison with preknowledge. The convolution layer performs a convolution operation on the original image and a specific filter is applied to extract the feature map;⁴⁴ combining multiple convolution layers enables CNNs to recognize more complex structures and objects in images. However, the convolutional layers produce a feature map that is location-dependent,

and pooling is applied to generalize the features extracted by convolutional filters and help the network recognize features independent of their locations. The pooling operation also reduces the amount of data in the picture and speedup the model training process. Max pooling⁴⁵ and average pooling⁴⁶ are the two common approaches to pooling; max pooling is associated with the selection of the maximum pixel value in the receptive field while average pooling is associated with the employment of the average value of pixel values in the receptive field. The descriptions of selected jargons and acronyms in machine learning are listed in **Table I**.

B. Data quality

Poor data quality, such as missing entries, low resolution, duplicate data inputs, the presence of noise, small dynamic range, and broken formats, significantly limits the image-based machine learning ability to make predictions and provide scientific insights. Unfortunately, we are frequently confronted with images of poor quality in daily research studies, and the data scarcity and data sparsity issue are particularly well-known in the materials science domain. In order to address the data quality issue, researchers should well document the reproducible and reliable data online

TABLE I. Descriptions of selected jargons and acronyms in machine learning.

Jargon/acronyms	Full name/description
CNN	A convolutional neural network (CNN) is a deep learning neural network that uses the architecture of a multi-layered feed-forward neural network to handle organized arrays of data such as images.
Deep learning	A type of machine learning that uses artificial neural networks and representation learning to learn.
Neural network	A network or a circuit made up of artificial neurons or nodes.
Regression	A statistical process for evaluating the relationships between a dependent variable and several independent variables. The most common one is linear regression.
Clustering	Splitting a set of data points into groups so that data points in each group possess similar characteristics.
Classification	Determining which categories an observation belongs to.
Supervised learning	Using labeled datasets to train algorithms that accurately classify data or predict outcomes.
Unsupervised learning	A machine learning technique that does not require people to supervise the model. Instead, the model works independently to identify previously unnoticed patterns. It is mostly concerned with unlabeled data.
Human–materials perception	Human material perception depends on the image features related to the material properties in the natural visual environment. Human observers effortlessly recognize materials and infer their physical, functional, and multisensory properties at a glance without touching materials.
Machine vision	Machine vision, or computer vision, is the process by which machines can capture and analyze images.
NLP	Natural language processing (NLP) is a branch of artificial intelligence that helps computers understand, interpret, and manipulate human language.
OCR	Optical character recognition (OCR) translates pictures of typed, handwritten, or printed text into machine-encoded text by electrical or mechanical means.
ResNet	An architecture presented by Microsoft in 2015 that establishes a new architecture called the residual network. ²³
UNet	A convolutional neural network for biological picture segmentation that works well with fewer training photos and provide more exact segmentations. ²⁴
PixelNet	A segmentation approach using a pixel-level convolutional neural network. ²⁵
AlexNet	A high-performance convolutional neural network architecture containing eight layers utilizing GPU during training. ²⁶
Inception	A convolutional neural network assisting image analysis and object detection. ²⁹
DenseNet	A convolutional neural network making use of dense connections between layers via Dense Blocks that connect all layers with matching feature-map sizes directly. ³⁰
SVM	Support vector machine (SVM) is a supervised machine learning model that finds a hyperplane in an N-dimensional feature space that distinguishes between data points.
k-means clustering	A vector quantization method seeking to partition n observations into k clusters, with each observation belonging to the cluster with the nearest mean.
TensorFlow	A machine learning and artificial intelligence software library created by Google Brain team that is free and open-source, focusing on the deep neural network. ³¹
Keras	An open-source software library for artificial neural networks that provides a Python interface, serving as a user interface for TensorFlow. ³²
Pytorch	An open source machine learning framework based on the Torch library created by Facebook. ³³
Caffe	A deep learning framework made developed by Berkeley AI Research. ³⁴
ImageDataExtractor	A tool extracting and quantifying data from microscopy images developed by a Cambridge group. ⁵³

and augment the dataset if possible when they publish the results. In addition, several alternative neural architectures have been developed, such as those applying resolution correction prior to classification.⁴⁷ The problem of the small dataset in materials science has been addressed by several machine learning studies considering alternative algorithms.^{48,49} For example, an ensemble-averaged model is introduced via averaging the model coefficients over an ensemble of subset trained model instances.⁵⁰ Sufficient accuracies should be achieved when constructing a neural network, which are usually evaluated using the Pearson coefficient and mean absolute deviation and the robustness should be verified using cross-validation. The predictive power of image-based machine learning is demonstrated to be comparable to traditional materials' prediction methods such as quantum chemical approaches^{42,43} or experienced human researchers^{51,52} in terms of material perception and prediction, if not more accurate. Nevertheless, it should be noted that in the current stage, the major advantage of the machine learning approach for science corresponds to the faster calculation time rather than accuracy once the model is successfully built when compared with traditional quantum chemistry methodologies, and the neural network can be deployed for more accessible and low-cost computing hardware (e.g., laptops) with improved automation.

III. PREDICTION OF PROPERTY IMAGES

The materials and chemical science is associated with numerous spectra and properties images, such as the UV-vis absorption spectra, band structure, Fourier Transform infrared (FTIR) spectra, phonon spectra, and spatial distributions of molecular orbitals. These images are typically obtained via experimental characterizations or quantum mechanical calculations, which can be especially expensive and cumbersome in some cases where large-size chemicals and materials and repetitive calculations are involved. Interestingly, the machine learning has been adopted to rapidly predict the structural and property images of chemicals and materials, enabling the exploration of a much wider design space. For example, an effective machine learning protocol for predicting the protein infrared (IR) spectra image is proposed by Ye *et al.* [Fig. 2(a)], which is suggested to complement repeated expensive quantum-mechanical calculations in a fluctuating environment for determination of the secondary structure of the macromolecule. In particular, the establishment of the machine learning protocol for the IR spectra prediction depends on several key structural descriptors.⁴² Specifically, the inputs in the training set are molecular conformations while the outputs are the vibrational frequency, transition dipole, and neighboring coupling parameters. For molecular excitation spectra prediction,⁵⁴ the inputs are the coordinates and charges of the atoms of the molecule while the outputs are the excitation energies or the molecular excitation spectrum. Tsymbalov *et al.* employ machine learning to engineer the electronic band structure of semiconductors,⁵⁵ while Peano *et al.* use deep learning to rapidly explore the topological band structures of materials [Fig. 2(b)], and the neural network is feasible to design the band inversion for topological transport and symmetry predictions as well as the prediction of the band structures from unit-cell geometries or potentials.⁴³ In this case, the input image is the unit cell of the potential (the unit-cell geometry, i.e., a potential or a material

distribution) while the output is the tight-binding (TB) Hamiltonian, the vector that contains the energies and hopping matrix elements of the TB model. The degeneracy is a critical problem; however, the neural network is suggested to perform well to identify the degeneracies despite the lack of the training on potentials with smaller unit cells. The deep learning process for spectra prediction and analysis is different from that for the microscopy analysis in terms of inputs and outputs. In the machine learning process, the careful selection of features/descriptors and variables is critical. One of the drawbacks is the resolution in some cases, and several important characters are lost; in order to establish the valid neural network, *a priori* knowledge is needed. It is expected that the image-based machine learning techniques are capable of efficiently predicting more structural and property images of materials and chemicals in a cost-effective manner beyond the FTIR spectra and band structures, provided that a large database of materials or chemical images are available in a consistent format, and proper descriptors can be formulated to expedite the machine learning process.

IV. NANO-SCALE IMAGES

CNN and its neural network derivatives that are common for analyzing images in the social media are also popular deep learning algorithms for materials' image analyses, such as materials' categorization, phase identification, locations of atomic species, defect detection in scanning electron and transmission electron microscopy, and crack recognition. One of the many advantages of utilizing a neural network is the considerably faster calculation time, which is important for analyzing the complex image data. In addition, the performance evaluation metrics of the model, including accuracy, precision, and recall, are generally used in most of the tasks. In the modeling process, simple but non-linear mathematic operations are often involved, such as convolutions, normalization, and activations to match the input image with the proper output label.⁴⁴ Machine learning has been extensively applied for the analysis of electron microscopy images, particularly classifying the SEM images and information extraction from these images.^{56–60} Advanced statistical analysis and machine learning techniques can be used for extracting relevant physical and chemical information from microscope data on multiple functional materials.^{61–63} Aversa *et al.* annotate 22 000 SEM images and classify them into ten categories, including 0D particles, 1D nanowires and fibers, 2D films and surfaces, and 3D devices and pillars [Fig. 3(a)],⁶⁴ while Modarres *et al.* employ neural networks including Inception-v3, Inception-v4, and ResNet for SEM image recognition.⁶⁵ In the process, the correct manual labeling and annotation of the SEM images for model training is a key step toward accuracy classification. Apart from classifying dimensionalities of SEM images, more detailed information can be extracted via the machine learning approached from SEM images;⁶⁶ for example, an automated recognition tool is developed by Li *et al.* to automatically detect and analyze defects (closed circular/elliptical solid loops, open ellipse loops, open circular loops, and line dislocation segments) in electron microscopic images [Fig. 3(b)],⁶⁷ where the inputs are the micrographic images (the CNN training set had 60 000 images of 64×64 pixels) while the outputs are the quantitative image/defect analysis metrics associated with the defect contour and the size

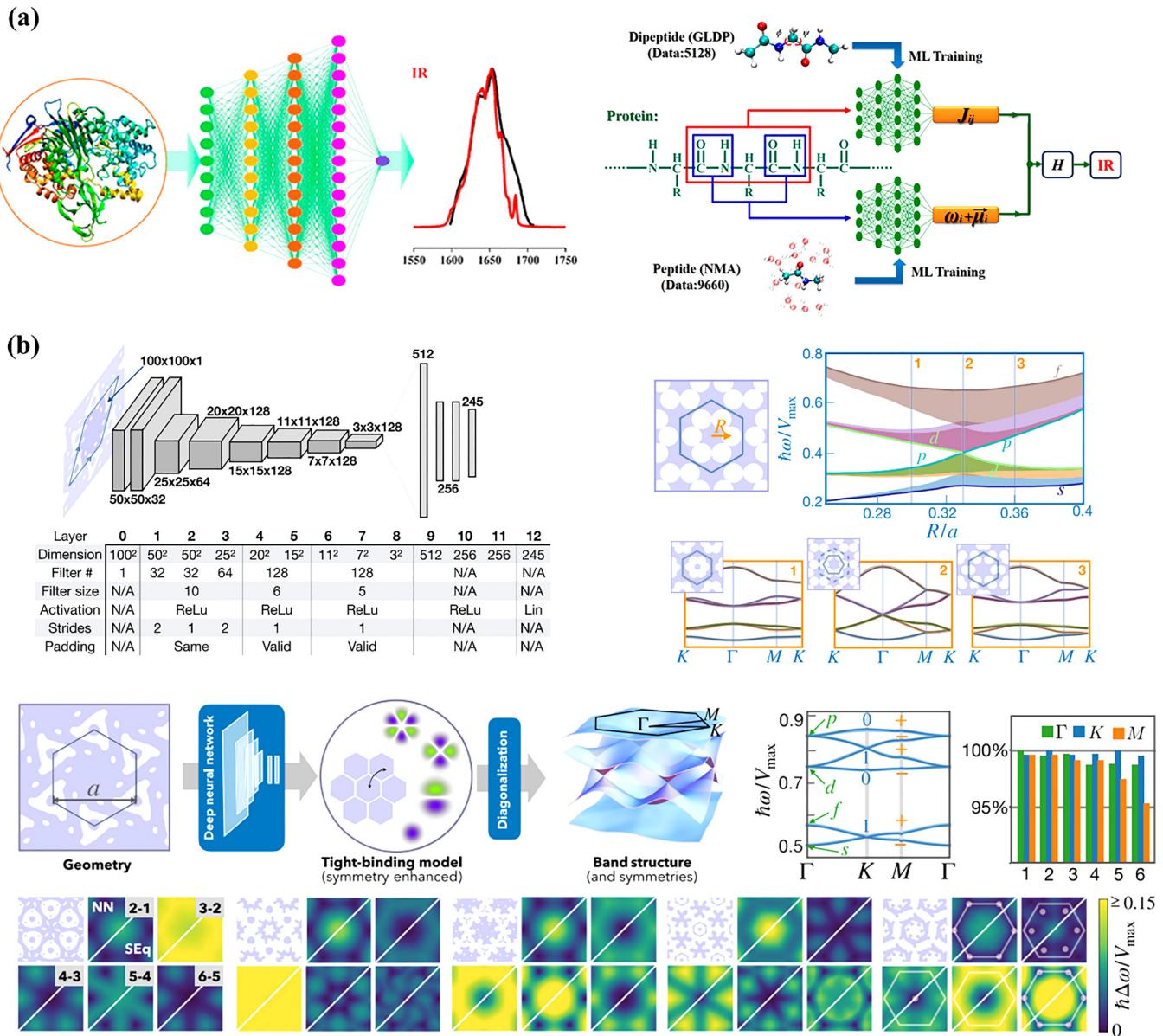


FIG. 2. (a) A machine learning protocol for predicting protein infrared spectra based on structural descriptors; the machine-learning-based parameters are employed to construct the amide I band Hamiltonian.⁴² Reproduced with permission from Ye *et al.*, J. Am. Chem. Soc. **142**, 19073 (2020). Copyright 2020 American Chemical Society. (b) Image-based neural networks for topological band structures, including the design of a band inversion for topological transport and symmetry predictions as well as the prediction of band structures from unit-cell geometries or potentials. The geometry is fed into a multilayer convolution network to generate the coefficients of a symmetry-enhanced tight binding model and then diagonalized to construct the band structure. The k -resolved bandgap for five validation geometries are compared.⁴³ Reproduced with permission from Peano *et al.*, Phys. Rev. X **11**, 021052 (2021). Copyright 2021 American Physical Society.

information for the defect contour. Apart from that, Kim *et al.* propose automatic pipelines⁶⁸ for extensive information extraction of nanomaterials from SEM images via machine vision, especially the particle size distribution, shapes, core–shell structures and morphology details [Fig. 3(c)]. The data science has been employed to

facilitate the development of nanoscopic images for accuracy improvement and information extraction, such as denoising, drift and distortion correction, spectral unmixing and those including the non-local patch-based methods, component analysis, clustering, optimization, and compressed sensing.⁶⁹ Clustering approaches are

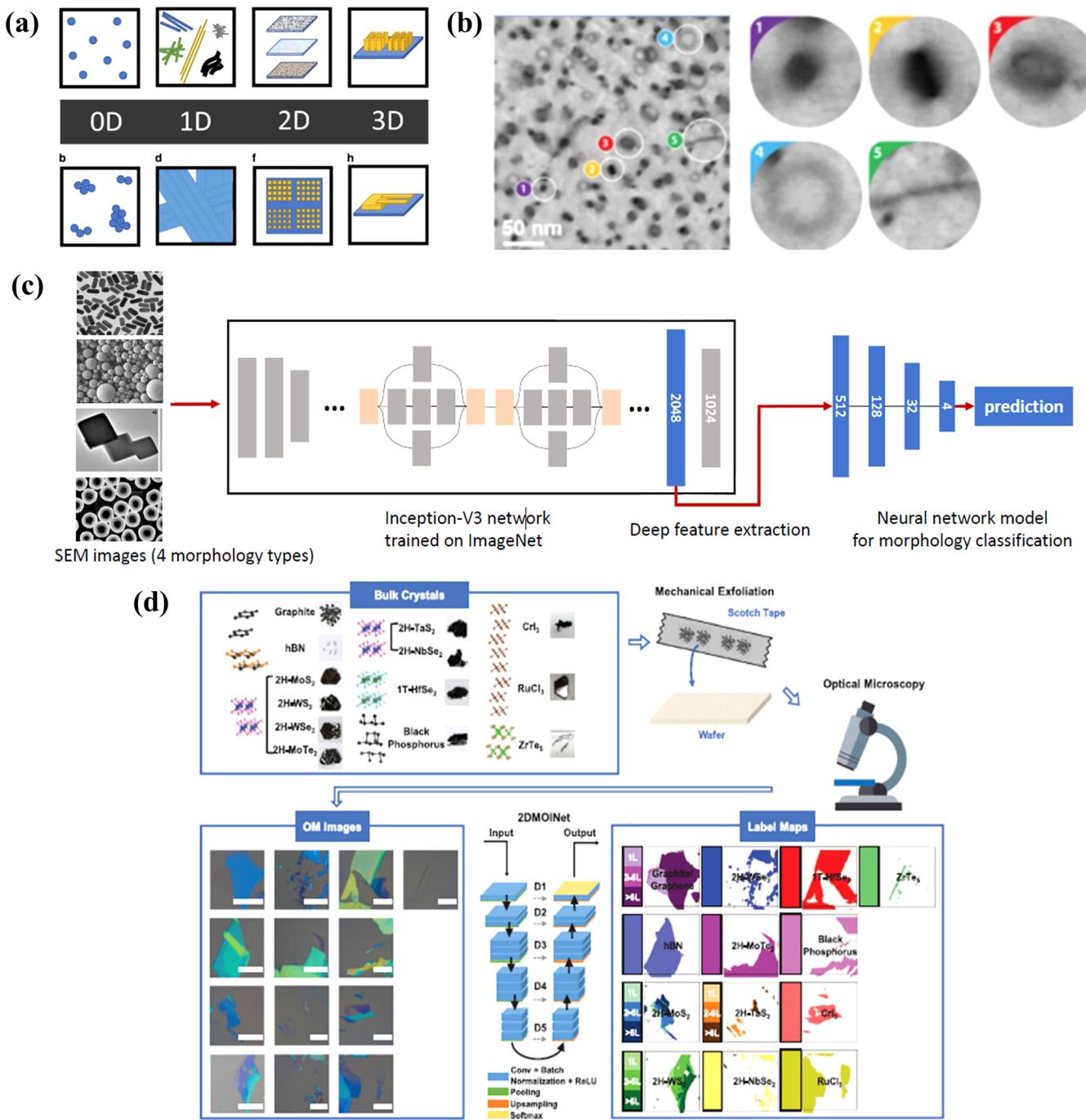


FIG. 3. (a) Nanostructure classification of SEM images based on dimensionality from 0D to 3D, including tips, particles, patterned surfaces, mems devices and electrodes, nanowires, porous sponge, biological, powder, films, coated surfaces, and fibers.⁶⁴ Reproduced with permission from Aversa *et al.*, *Sci. Data* **5**, 180172 (2018). Copyright 2018 Springer Nature. (b) Automated machine learning program for defect detection in the STEM image. The common defect types including closed circular/elliptical solid loops, open ellipse loops, open circular loops, and line dislocation segments are identified.⁶⁷ Reproduced with permission from Li *et al.*, *npj Comput. Mater.* **4**, 36 (2018). Copyright 2018 Springer Nature. (c) The overall pipeline of the proposed algorithm and the deep CNN-based morphology classification of SEM images.⁶⁸ Reproduced with permission from Kim *et al.*, *Nanoscale* **12**, 19461–19469 (2020). Copyright 2020 Royal Society of Chemistry. (d) The flowchart of a deep learning method using trained 2DMOINet to identify 2D materials based on properties measured via optical microscopes.⁶⁴ Reproduced with permission from Han *et al.*, *Adv. Mater.* **32**, 2000953 (2020). Copyright 2020 Wiley.

used for extracting relationships between the microstructure and stiffness of composite materials,⁷⁰ the segmentation of metallurgical images,⁷¹ as well as the prediction of the effective diffusion coefficient in porous materials.⁷² Moreover, McCue *et al.* have employed data mining and automated image mining to gather information of nanoporous gold from published papers,⁷³ and Chowdhury *et al.* employ computer vision and machine learning to study dendritic morphologies.⁷⁴ Several image processing toolkits such as ImageDataExtractor are developed, which helps extract and quantify data from microscopy images for data-driven studies.⁵³ In total, the image-based machine learning approaches are widely deployed for the SEM image analysis and image categorization, and such analysis is beyond the capabilities of traditional methods.

The machine learning analysis is important to obtain morphology, size, distribution, and intensity information beyond SEM.^{1,75–78} For example, Förster *et al.* develop a CNN model to determine the chirality of carbon nanotubes from high-resolution TEM images, and accurate assignment of the chiral index is achieved.⁷⁹ Yao *et al.* apply the U-Net neural network, a convolutional neural network architecture previously designed for biomedical image segmentation²⁴ to obtain nanoparticle dynamics (diffusion and interaction, reaction kinetics, and assembly dynamics) from liquid-phase TEM videos, which is suggested to demonstrate a superior capability to predict the position and shape boundary of nanoparticles from highly noisy and fluctuating background.⁸⁰ The microscopic image and spectral intensities from scanning transmission electron microscopy (STEM) are rich sources to provide information for materials,⁸¹ and the structural information including the atomic defects in STEM are handled by the computer vision and machine learning techniques.⁸² Based on STEM and energy-dispersive x-ray spectroscopy, the multivariate statistical analysis is employed to obtain the detailed composition of halide perovskite materials.⁸³ Practically, Jesse *et al.* apply big-data methods to process the high-dimension microscopy data from STEM in the domain of BiFeO₃, revealing domain differentiation by k-means clustering.⁸⁴ Machine learning is employed to help develop scanning probe microscopy (SPM) techniques by extracting information from the tip-surface junction.^{85,86} The automation of the image recognition process with minimal human intervention is important, and Krull *et al.* design DeepSPM to help automatically find good sample regions, assess image quality, and acquire and classify data of the scanning probe microscope without human supervision.⁸⁷ AFM provides valuable information on the morphologies of materials,^{88,89} while the electrical and chemical heterogeneity, ferroelectricity and ferroelasticity, surface passivation and chemical modification, ionic migration, as well as the material/device stability of the halide perovskite materials are revealed by the combination of multimodal and machine learning approaches.^{90–92} Apart from that, Laanait *et al.* reconstruct 3D atomic distortions of the perovskite structure based on CaTiO₃ epitaxial thin film on a single crystal substrate (LaAlO₃)_{0.3}(Sr₂AlTaO₆)_{0.7} and output the octahedral rotation symmetry from electron microscopy with deep learning.⁹³ The feature extraction is critical to realize improved interpretability and helps build more accurate machine learning models; features such as contrast, color, edges, shapes, flake sizes, and their distributions are extracted efficiently by the deep-learning method [Fig. 3(d)].⁹⁴ Deep neural networks have also accelerated the XRD analysis for hybrid perovskite materials⁹⁵ and the oxide systems,⁹⁶

while important descriptors are extracted to predict **crystallographic** structures.⁹⁷ The image recognition process is closely related to well-established machine vision techniques, which has been employed to detect nanoparticles that achieve high accuracies with less than a second.⁹⁸ As a result, the employment of machine learning methods significantly accelerates the analysis and classification of electron and optical microscope images of microscopic and nanoscopic materials.

The microscopy images are fundamentally different from natural images such as those taken from a cell phone or professional camera. Scientific data of materials science should be accessible, interoperable, and reusable, according to FAIR guiding principles.^{99,100} Microscopy images in materials science contain properties that make the microscopic imaging analysis exceedingly diverse and demanding when compared to natural images. For instance, high-level noises and distortions, existence of gray-scaled pictures, inclusion of experimental details, association with dynamic datasets, label intensive labeling process, ill-defined tasks, and lack of prior knowledge make the microscope image analysis distinctive with natural images. These issues can be addressed via efforts such as incorporating suitable physical and chemical parameters using spatial-temporal neural networks or data augmentation such as geometrical transformations in the deep learning process.

V. MOLECULAR IMAGES

The image-based machine learning methods have been applied for efficiently recognizing molecular structures and chemical information, either from the paper schematics to help prepare a formatted dataset or from nanoscopic microscope images to offer more scientific insights.¹⁰¹ For instance, Beard *et al.* develop the ChemSchematicResolver toolkit to identify the chemical schematic diagrams such as molecular structure images within the figure of a document, resolve any R-group substituents, and convert the diagrams to machine-readable format in a high-throughput and autonomous manner [Fig. 4(a)].¹⁰² In this case, the inputs are the direct input of images that comprise chemical schematic diagrams or the document input with figures scraped from articles while the outputs are the chemical records/SMILES and label data (image). In order to understand the ultimate molecular scale structure of chemicals and materials, Ziatdinov *et al.* combine a Markov random field model and CNNs to classify structural and rotational states of individual building blocks in a molecular assembly on the metallic surface in high-resolution scanning tunneling microscope (STM) measurements, thereby reading and recognizing the complex molecular assemblies on the surfaces [Fig. 4(b)].¹⁰³ Alldritt *et al.* automate the structure discovery process in AFM using a deep learning structure with a unique descriptor characterizing the molecular configuration [Fig. 4(c)], which is employed to resolve adsorption structures of 1S-camphor on Cu (111).⁸⁶

VI. MACRO-SCALE IMAGES

From the industrial and engineering point-of-view, accurate recognition and classification of materials and chemicals in the daily life is critical for the Internet of Things (IoTs) and industrial automation. The materials and chemical attributes in the macro-scale can be local, i.e., without shape, which is in vast contrast to other traditional image recognition studies such as facial

recognition where the shape is the major target. The restrictions in the shapes and geometries provide barriers for the efficient **human-materials perception** and the automatic chemical detection that are related to the materials and chemical sciences. Several apparent visual material attributes include fuzziness, texture, and color, while the materials can be classified as metal, ceramics, polymer, and composites, including the subcategories of metal that include iron, copper, steel, aluminum, and various types of glasses. Schwartz *et al.* achieve weak supervision to acquire classifiers to efficiently recognize materials and their visual attributes by simply asking yes/no questions, identifying the learned attributes for traits

such as fuzzy, shiny, smooth, soft, striped, metallic, organic, translucent, transparent, rough, liquid, woven, and manmade [Fig. 5(a)].⁵² For example, several attributes (0 and 8) are grouped together to point to the metal as the material trait. In this process, the annotation of materials before the training and test step is important to segment the images, and the workflow leads to the grouping of similar materials in the attribute space while others distribute in separate regions. The inputs are based on a local material recognition dataset consisting of 4745 images of 16 materials categories (at least 200 images per category) while the outputs are materials' classification (wood, foliage, fabric, food, water, metal,

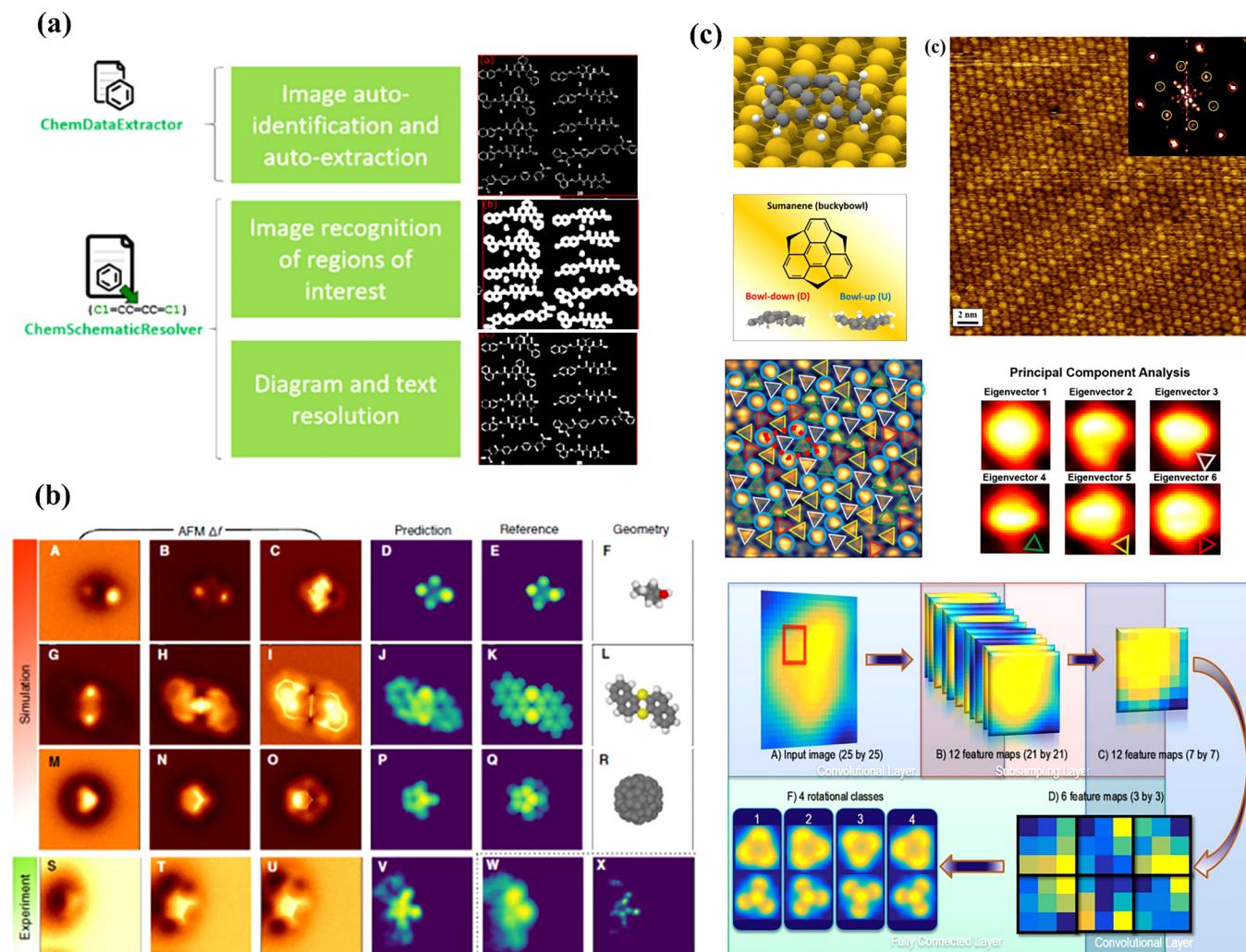


FIG. 4. (a) ChemSchematicResolver to decode molecular with labels and R-groups into annotated chemical named entities. Various morphological transformations of the molecular images include binarization, subsequent dilation, and subsequent erosion.¹⁰² Reproduced with permission from Beard and Cole, J. Chem. Inf. Model. **60**, 2059–2072 (2020). Copyright 2020 American Chemical Society. (b) A CNN process to predict the adsorption structure of a molecule on Cu (111) from AFM.⁸⁶ Reproduced with permission from Alldritt *et al.*, Sci. Adv. **6**, 1–10 (2020). Copyright 2020 AAAS. (c) Machine learning-assisted recognition of sumanene molecules on a gold (111) substrate from the STM image.¹⁰³ Reproduced with permission from Ziatdinov *et al.*, npj Comput. Mater. **3**, 31 (2017). Copyright 2017 Springer Nature.

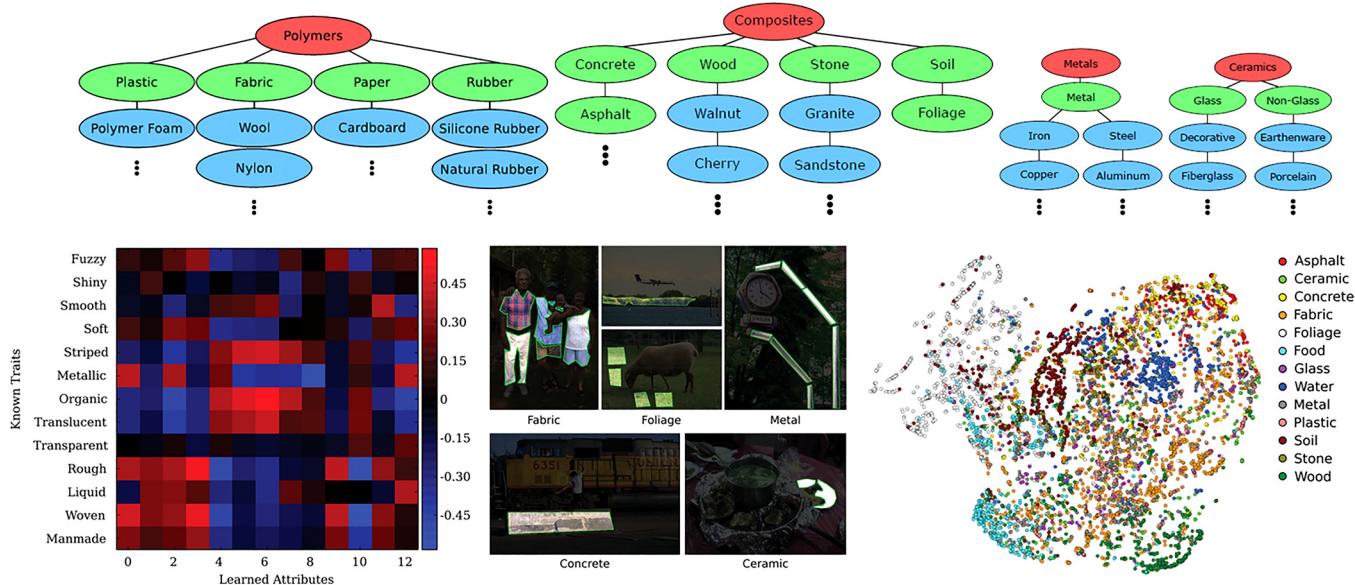


FIG. 5. Examples of classifications of materials in the daily life based on the image-based machine learning method, which correlates known traits of materials (fuzzy, shiny, smooth, soft, striped, metallic, organic, translucent, transparent, rough, liquid, woven, and manmade) and learned attributes. The attribute space for different materials in separate regions are visualized.⁵² Reproduced with permission from Schwartz and Nishino, IEEE Trans. Pattern Anal. Mach. Intell. **42**, 1981–1995. Copyright 2020 IEEE.

plastic, stone, wood, concrete, ceramic, asphalt, glass, soil, etc.). In addition, the global context helps accurate material recognition, suggesting that the local appearance analysis followed by global texture identification improves the accuracy of material recognition in the presence of limited training data.¹⁰⁴ Well-annotated materials database is critical to construct the machine learned model to recognize materials. An annotated surface database OpenSurfaces¹⁰⁵ is prepared to supply rich information of material names, reflectance, textures, and scene category and object names and can help the construction of machine learning models to recognize materials. A large scale dataset of materials in the wide “Materials in Context Database” (MINC) is available, with the developed CNN model achieving 85% accuracy for materials’ classification.¹⁰⁶ Combined features are proposed to recognize materials using the support vector machine (SVM) algorithm,⁵¹ and a Vector-LabPics dataset consisting of 2187 annotated images is prepared, with the chemistry-specific materials such as liquid, solid, foam, suspension, and powder properly assigned; this helps the training of a neural network for liquid and solid classification.¹⁰⁷

The development of the interdisciplinary study relies on joint efforts from scientists in materials/chemical science, computer science, and brain studies.^{108–122} The development of vision science is critical to disentangle the sophisticated interactions between lighting, shape, and materials; for example, the understanding of the reflectance of materials at different orientations and processes of light–matter interactions is helpful to build an accurate model.¹²³ A material recognition method has been proposed for robotic tactile sensing based on 144 000 tactile images, with materials classified into four categories, achieving 90% in 37 ms for

material recognition.¹²⁴ Material attributes are discovered with semi-supervision based on crowd-sourced perceptual material distances.¹²⁵ SpeCam¹²⁶ is developed to detect hidden materials underneath the camera using mobile devices. It is proposed that statistical appearance models are efficient and facile to perform the material recognition task than the computation of physical parameters; the material category and statistical appearance are highly related in the case of viscous liquids.¹²⁷ It is expected that the successful automatic recognition of more detailed materials and chemical information can be achieved for machine vision, and the development of the Internet of Things (IoTs) can be contributed by the knowledge obtained from materials and chemical scientists such as the formulation of molecular and materials features that underlies the materials and chemical properties.

VII. DEVICE IMAGES

A number of machine learning studies are carried out for higher-level electrode and device images such as solar cells, batteries, and fuel cells to facilitate proper operation and defect identification. Sun *et al.* predict the solar cell output from video streams using CNNs, where the images of the sky provide valuable information on the current and future cloud and, thus, the photovoltaic output [Fig. 6(a)].¹²⁸ Functional microscopy provides quantitative information about relevant parameters associated with figures-of-merit and nanoscale spatial resolution of solar cell materials, such as hybrid perovskites, CdTe, CIGS, CZTS, and pc-GaAs, and should be analyzed in a more automatic way.¹²⁹ For example, Collins *et al.* develop unsupervised clustering methods to

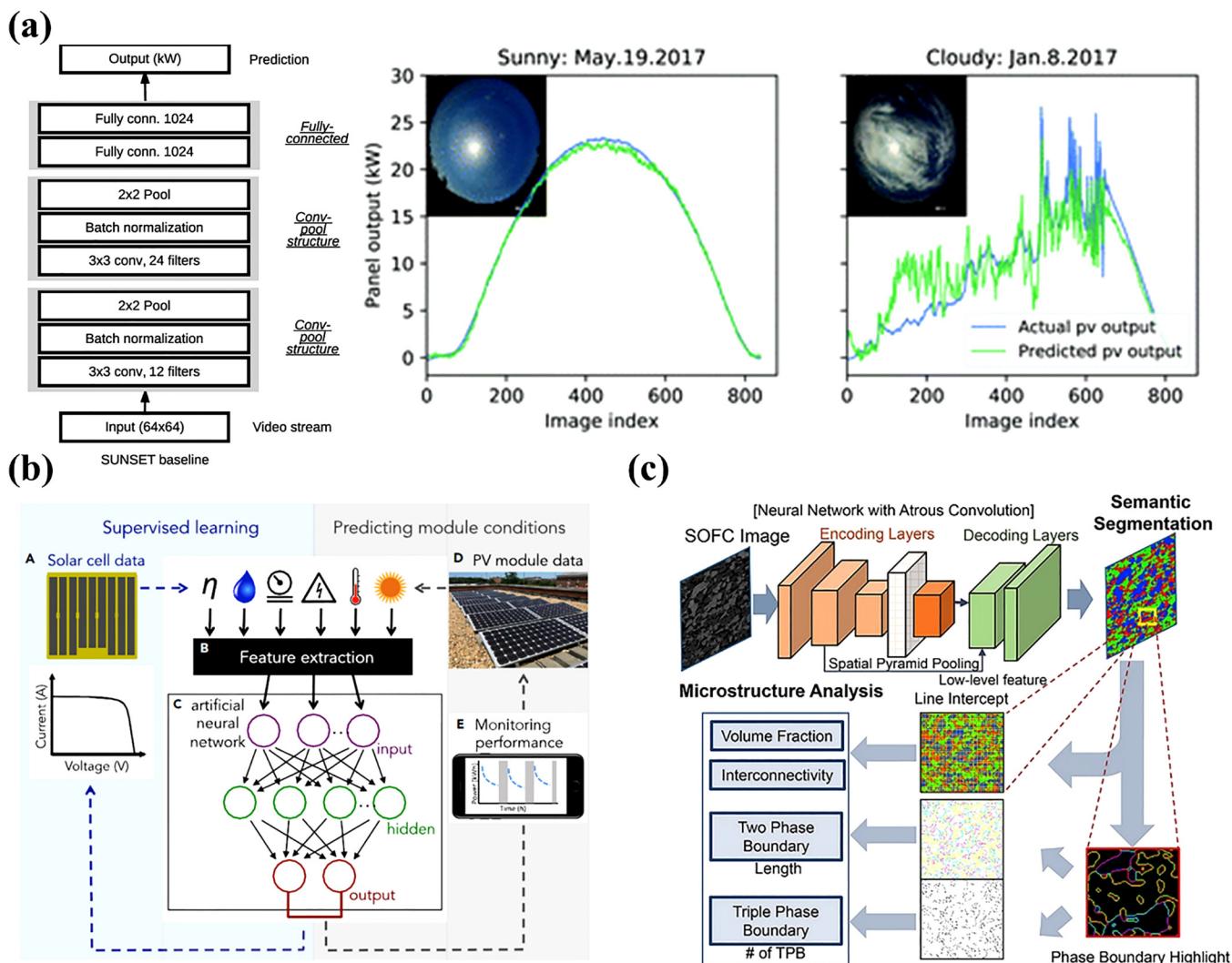


FIG. 6. (a) Process of predicting solar cell output from video streams in the presence of the sky images using CNNs.¹²⁸ Reproduced with permission from Sun *et al.*, Energy Environ. Sci. 11, 1811–1818 (2018). Copyright 2018 Royal Society of Chemistry. (b) A machine learning framework to monitor the re-ap–rest–recovery cycle of perovskite solar cells and predict the module conditions.⁸⁸ Reproduced with permission from Howard *et al.*, Joule 3, 325–337 (2019). Copyright 2019 Elsevier. (c) Semantic segmentation-assisted deep learning for analyzing cathode composite materials of solid oxide fuel cells.¹³¹ Reproduced with permission from Hwang *et al.*, J. Power Sources 471, 228458 (2020). Copyright 2020 Elsevier.

distinguish spatial variability and interpret multidimensional data-sets from Kelvin probe force microscopy data.¹³⁰ In addition, there is evidence that the recent image recognition progress benefits the perovskite solar cells: the machine learning framework considering the operating parameter benefits the image analysis of perovskite solar cells [Fig. 6(b)], and the machine learning frameworks are developed to monitor the perovskite solar cells and predict module conditions.⁸⁸ Last but not least, Hwang *et al.* integrate semantic segmentation with image processing-assisted stereography tools for three-phase composite cathode materials of solid oxide fuel cells based on Gd_2O_3 -doped CeO_2 and $\text{La}_{0.6}\text{Sr}_{0.4}\text{CoO}_{3-\delta}$, automatically

extracting detailed microstructural features (size distribution, surface fraction, volume fraction, lengths of two-phase boundaries, and density of triple-phase boundaries) based on two-dimensional images [Fig. 6(c)].¹³¹

VIII. SUGGESTIONS AND OUTLOOK

Despite significant progress of image-based machine learning for materials science, several issues should be addressed. Apart from the algorithm development to reduce the computation cost, the following suggestions are provided to facilitate the future

development in this area, including application for image prediction; application for image classification; bridging the science gaps; improvement in database preparation; improvement in automation and annotation; comparison with texts, images, and videos; and the development of an image search engine.

Application for image prediction: One of the most intriguing prospects of the image-based machine learning method for materials and chemical science is their capability to fast and efficiently predict the property images of materials and molecules, which are especially expensive for traditional quantum mechanical simulations when large-scale repetitive calculations are involved. Importantly, Ye *et al.* have already successfully demonstrated an image-based machine learning protocol for IR spectra prediction of large-size molecules that can potentially substitute the widely deployed first-principles calculations.⁴² However, this depends on the establishment of suitable structural descriptors and the availability of large databases, and so far, only FTIR and band structure predictions by image-based machine learning methods have been attempted, and such predictions are based on limited types of materials and chemicals. More types of scientific images are suggested to be readily predicted beyond the FTIR and band structure images; these include UV-vis spectra, molecular orbital distributions, phonon spectra, etc. The image-based machine learning techniques should be further optimized to rapidly predict the structural and property images of chemicals and materials to explore a much wider design space. The materials and chemical scientists and engineers are suggested to address the property prediction issues for advanced and sophisticated solids and molecules considering the rapid developments of image-based machine learning algorithms that have been achieved in computer vision and medical communities, especially in the cases where the traditional quantum chemical calculations introduce inaccessible cost and even fail. Sufficient predictive accuracies of the neural network for spectra images have been obtained, which are evaluated via the Pearson coefficient and mean absolute deviation, and the robustness is verified via cross-validation.¹³² For example, an average error below 0.19 eV and the spectral weight within 3% are achieved by a neural network for peak predictions of molecular ionization spectra.⁵⁴ However, high accuracies are often obtained at the expense of the selection of a large broadening value, which may detriment the resolution of the spectra. As a result, more studies should be carried out to optimize the neural networks that address the broadening issue in the image learning process.

Application for image classification: Apart from spectra image prediction, the machine learning is especially viable for image and materials/chemical classifications, particularly the recognition of materials and chemicals from an industrial and commercial point of view. Schwartz *et al.* have already demonstrated an excellent example to efficiently recognize the materials' categories (metals, polymers, and ceramic materials) and their visual attributes beyond geometries.⁵² Nevertheless, the accuracies on the subcategories of these materials that can be commercially critical are relatively poor at the moment, and this is associated with the limited number of suitable material features. It is of equal importance to apply the image recognition techniques for both macro- and nano-scale images, and the knowledge obtained from human-material-perception research studies is transferable for chemical and materials' domains. As a result, more

appropriate material attributes beyond geometries, textures, and fuzziness that facilitate the recognition of materials images should be designed and well-understood; for example, the attributes related to optical properties (absorption, reflection, transparency, etc.) that are well-recognized in materials science can be particularly helpful. Future image-based machine learning techniques can be employed to identify defects in the modules and explosives in the laboratory given the model is properly trained, and the defects' identification and the real-time device condition monitoring for the solar cell and battery device performance evaluation and optimization are especially pertinent to the image-based machine learning process. Materials scientists and data scientists should collaborate to analyze the microscopy data and different types of images in materials science. More user-friendly software and platforms specializing into materials subjects should be developed. In addition, model and loss function should be tailored to make it compatible with fundamental physical and chemical principles, and *a priori* knowledge is necessary when analyzing the materials' images. Moreover, the neural network should be carefully tested and adapted to real scenario experiments, while control experiments should be available.

Science gaps: It should be noted that future data-driven studies should pay more attention to the knowledge and science gaps, despite the fact that the interpretability of the machine learning process is almost a universal problem in materials science that makes this method quite controversial. Several studies have been devoted to address the interpretability and scientific insight issues via the careful design of descriptors and chemical visualization of the predicted database.^{133–135} In the current stage, the major advantage of the machine learning approach corresponds to the faster calculation time and deployment for more accessible and low-cost computing hardware rather than accuracy, and the domain-specific knowledge can be extracted from the design of more relevant molecular descriptors for the vibrational and excitation and band spectra. The neural network has been demonstrated to be reliable to reproduce the domain specific features.⁴³ It is desirable if the neural network is able to make trustworthy and robust predictions even when insufficient training examples are available, which is suggested to be achievable using the concept of adversarial approaches where the input is changed in a deliberately disadvantageous way to maximize the deviation from the correct output.¹³⁶

Improvement in database preparation: In the light of the big-data era and the materials informatics, data mining and optical character recognition (OCR) can be applied to extract a large number of useful images from the materials and chemical image databases, in a way analogous to the information extraction from the medical images. For example, a large amount of images and associated texts are stored in the online databases and publications while the formats can be troublesome for the information extraction, while the OCR techniques and data mining techniques can be readily available to extract useful caption and embedding information and convert them into readable formats.

Improvement in automation and annotation: Although improved automation of image recognition processes for materials has been achieved,¹³⁷ the full automation of this process is unavailable. Fully automated materials recognition tools should be developed, and an uttermost important task is to prepare sharable and exchangeable image data and metadata with unified format. Better

annotation on pictures and images in a publication should be addressed by the article authors, and it would be helpful that the open accessible materials' image databases are more easily and freely accessible.

Comparison with texts, images, and videos: The machine learning techniques combining both NLP and image recognition capabilities should be developed, since both texts and images provide valuable information on materials,^{138,139} and this can facilitate digitization^{4,11,140} in the materials and chemical domains that may deal with the extraction of textual information from images and the text-to-image synthesis. The integration of the voice recognition and sense of touch into the image recognition is another promising method to characterize materials.^{141,142} A video system that promptly gives information on materials' structures and properties should be designed for commercial and industrial applications. The development of the image-based machine learning methods for the materials and chemical sciences can also benefit the progress of devices for the vision purpose, such as the artificial retina where the materials are capable of bionic and machine vision.^{143–145}

Suggestions on image search engine: Last but not least, it is expected that an image search engine can be provided in the near future to help the researchers successfully find the desired materials and chemical information by a simple "click" button based on the image inputs, in a way similar to the Google image search. Such databases can be designed via the manual annotation or an automatic process that auto-generate databases,¹⁴⁶ which has been demonstrated in the biomedical areas where the accurate mining of images is critical to retrieve valuable information.¹⁴⁷ The search engine has already applied for the search of molecular structures; nevertheless, significantly more types of materials and chemical images should be better handled by the computer. The Google-type image search engine depends on the development of comprehensive databases storing materials images and knowledge transfer between the materials/chemical scientists and the image-processing computer scientists.

IX. CONCLUSIONS

Image-based machine learning methods are receiving attention and have found successful applications for materials and chemical science to complement the traditional computational methods. There are numerous images in the published papers and in materials science databases such as spectral images and SEM/TEM images, which act as a potential data source for materials prediction and analysis. However, image-based machine learning is associated with larger computational cost, and more GPU resources are often required for accurate model construction and detailed analysis. In addition, the materials-specific algorithms are not well developed, and more user-friendly software should be designed to help the materials scientists. One of the promising applications of image-based machine learning for materials science is the classification of the SEM images and the automated information extraction from these microscopic images. Another direction is the prediction of spectra and device performance based on existing spectra images of materials and chemicals. In this process, the feature selection is key to realizing accurate spectra prediction while the broadening issue severely hampers the progress. As a result, more efforts

should be made to extract hidden scientific information from features and address the broadening issue in the image learning process. Although the image-based machine learning studies are relatively new for materials and chemical scientists, we suggest this new data-driven approach can act as an effective alternative to obtain the structural and property information to supplement the traditional artificial intelligence and first-principles calculations in materials and chemical sciences, and this can also provide an important step for the advancement of materials informatics.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Lei Zhang: Conceptualization (equal); Data curation (equal); Formal analysis (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Project administration (equal); Resources (equal); Software (equal); Supervision (equal); Validation (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal). **Shaofeng Shao:** Formal analysis (equal).

DATA AVAILABILITY

The data that support the findings of this study are available within the article.

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