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Editorial

Forum on Artificial Intelligence/Machine Learning for Design and Development of Applied Materials

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Machine learning (ML) and other artificial intelligence (AI) methods are bound to transform science and technology, as this is already happening in many other areas of human activity. The use of machine learning in chemistry, materials sciences, and their applications has grown enormously. More than 60% of all articles on these topics have been published since 2019. Recent research has been focused mostly on materials design and discovery, in addition to the analysis of images, sensing, and biosensing data for various types of diagnosis. A boost has been observed as a result of materials genome initiatives and the availability of large databases of materials properties made possible, in some cases, with high-throughput experimental and theoretical methods. Not surprisingly, applications of these procedures have been carried out for a wide variety of materials, as the underlying principles are entirely generic.

This forum on Artificial Intelligence/Machine Learning for Design and Development of Applied Materials reflects this diversity. The collection of 15+ papers covers artificial intelligence (AI)/machine learning (ML) applied to research on electrocaloric ceramics and piezoceramics, glasses, thermoelectric materials, electrode materials for batteries, dielectric and semiconducting polymers, polymer nanocomposites, copper-based catalysts, metal−organic frameworks, molten salts, and 2D materials. Despite the diversity in materials and intended applications, the studies reported share an overall thematic approach: pattern recognition strategies with ML algorithms are applied to classify materials (or materials properties) using large databases generated from experimental results and/or computer simulations. The papers in the forum highlight the capabillity of AI/ML to enable the prediction, screening, and optimization of properties and/or materials. Examples include prediction of adiabatic temperature changes, high thermal conductivity, sulfur solubility in glasses, new 2D materials, conducting polymers, thermoelectric materials, and materials for Li−S batteries. Moreover, screening has been performed on battery electrode materials and metal−organic frameworks, and ink writing conditions were optimized for 3D printing.

The results and applications showcased in the forum are illustrative of the strengths and limitations of ML. Specifically, it is being used to address either long-standing scientific issues or to facilitate data acquisition and interpretation that otherwise would be tedious, cumbersome, or unmanageable altogether. As discussed in some of the papers in the forum, and in the literature, the predictive power in discovering and designing new materials or properties depends on the breadth and coverage of the data sets employed. In other words, the effectiveness and usefulness of ML are dependent upon the intrinsic quality and scope of the data sets. If sufficient quality data is available for training, supervised ML is suitable for classification tasks, where it can already outperform humans in many applications. Archetypical examples are facial recognition and diagnosis based on image analysis, in which a high accuracy, sometimes bordering on 100%, may be obtained provided that the data set is sufficiently comprehensive and the necessary computational power is available. However, present technology does not render ML efficient for tasks that require a considerable degree of interpretation. This limitation applies to any application of ML or AI; in the context of materials discovery and design, it means that precise scientific or technological questions must be identified, whose response can be inferred from patterns in the data under analysis. For instance, today it may be possible to optimize conditions for achieving high-performance materials, but developing ML-based strategies to learn the fundamental laws of physics and the underlying functioning mechanisms of such materials is by far a more ambitious challenge.

The impact of AI on chemistry and materials science has been mostly associated with ML. Little has been done in other subareas of AI, e.g., neural networks, expert systems, evolutionary computation, robotics, computer vision, speech and natural language processing, and planning. The exceptions involve the use of genetic algorithms and neural networks within deep learning and other ML approaches, and natural language processing in knowledge discovery, where the literature in specific classes of materials was mined. Though knowledge discovery is believed to be central for AI applications, the results so far have been limited, because of the inability of machines to interpret text. For ML-related applications in the short term future, we believe in the strengthening of initiatives to generate and curate large databases with materials properties. In particular, large, accurate, and inclusive databases are still lacking in fields such as—but not limited to—catalysis, energy storage and conversion, sensing, and biosensing. These advances can be

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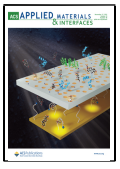

achieved in conjunction with recent progress made with the materials genomics projects and the databases for medical images already available. The establishment of reliable, comprehensive databases will make it possible to extend ML to an even broader range of applications.

The topics covered in the forum are all related to using ML to assist in solving particular problems of materials and their associated applications. However, there is a whole developing field in which the focus is exactly the opposite, i.e., using materials to enable AI applications. Indeed, virtual reality environments and the Internet of Things rely on various kinds of wearable devices, from sensors and biosensors to actuators and instruments with embedded electronic circuits. Furthermore, robotics (especially with soft robots) requires another set of nanotech-based devices, e.g., for artificial vision and in mimicking human senses. Speech processing and voice recognition may be revolutionized once wearable devices with strain sensing capability reach a sufficient performance. Tailored materials with memory effects are already used in "proof-of-principle" experiments for evolutionary computation, and one may envisage machine learning via hardware. Though seldom mentioned, all of the ML applications today are performed with software. When ML is effectively done with hardware, which may take decades, AI will be transformed entirely such that it can be used successfully in designing innovative classes of materials not only to tackle targeted needs but also address nuances associated with developing, understanding, and optimizing specific applications. Such breakthrough advances will, however, only be possible with correspondingly significant developments in computational and materials sciences.

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