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Journal of Materials Chemistry A and *Materials Advances* Editor's choice web collection: "Machine learning for materials innovation"

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Today, many urgent challenges are mainly materials-related issues. Novel materials with desirable physical and chemical properties are urgently needed; however, the disadvantages of the typical "trial-and-error" method, such as high cost and long period, make it difficult to meet the requirement for more advanced materials. With the development of high-performance computations and experimental technologies, high-throughput materials design has come true and the era of big materials data is coming. As a result, effectively analyzing big materials data to find hidden rules, which could be used to rationally design desirable materials, provides a chance to bring about breakthroughs in materials innovation.

Machine learning is undergoing a renaissance, influencing many scientific fields, especially materials science. Usually, the relationship between the descriptors (or features) and the desired information is extremely complex and non-linear; therefore, it is difficult to discover the statistical law by only relying on physical insight and principles. Machine learning technology could develop flexible models, which are trained by the input data to predict the desired information based on various algorithms. Currently, machine learning is widely used in materials science with the gradual spread of machine learning toolkits, the process of algorithms and the development of materials databases.

In order to highlight recent advances of machine learning in materials innovation, this online collection summarizes recently published research articles and reviews on machine learning. Lithium based batteries are one of the most commercially successful energy storage devices. However, further improvement is urgently needed to enhance safety and capacity. Huang *et al.* investigated the intercalation of alkali metal atoms in "hard" carbon systems over a range of densities and degrees of disorder by combining density functional theory (DFT) and machine learning methods (DOI: 10.1039/c9ta05453g). Besides electrode materials, electrolytes are also important for batteries. Liu *et al.* developed an approach to assess the possible reactions and thermodynamic stability of $Li|Li_7La_3Zr_2O_{12}$ interfaces under various chemical conditions and proposed that some dopants in $Li_7La_3Zr_2O_{12}$ could stabilize lithium metal anodes (DOI: 10.1039/c9ta06748e). Moreover, machine learning methods could also be used to explore novel lithium ion conductors. Suzuki *et al.* used machine learning methods to obtain unknown chemically relevant compositions of Li_2O–GeO_2–P_2O_5 and Li_2O–ZnO–GeO_2 systems. Two kinds of materials, $Li_6Ge_2P_4O_{17}$ and $Li_3Zn_{0.65}Ge_{4.35}O_{10.85}$, with high ionic conductivity were discovered (DOI: 10.1039/d0ta02556a).

Electrocatalysis provides a promising pathway to achieve sustainable development. Machine learning has been widely used to explore novel electrocatalysts. Lin *et al.* built machine learning models to predict the limiting potentials based on easily obtainable physical properties of graphene-supported single atom catalysts (SACs) for the oxygen reduction reaction (ORR), oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) (DOI: 10.1039/c9ta13404b). Similarly, Wu *et al.* used machine learning

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methods to reveal an intrinsic descriptor to identify the ORR catalytic activity of graphene-supported SACs (DOI: 10.1039/d0ta06207c). Besides SACs, alloys are promising electrocatalysts for HER. Li *et al.* used DFT computations to explore the catalytic activity of bimetallic alloy (100) surfaces for HER and then built a machine learning model to predict the HER activities of other, different bimetallic alloys (DOI: 10.1039/d0ta04615a). Additionally, the nitrogen reduction reaction (NRR) has attracted wide attention. Zafari *et al.* applied a deep neural network algorithm to predict the electrocatalytic activity of B-doped graphene SACs for NRR (DOI: 10.1039/c9ta12608b). The effective cyclic utilization of CO_2 plays a key role in low-carbon economies and sustainable development. Kim *et al.* used Gaussian process based Bayesian optimizations to obtain the optimum operating conditions to maximize CO production *via* CO_2 reduction on Ag electrodes (DOI: 10.1039/d0ta05607c). Yang *et al.* built a machine learning model based on the intrinsic properties of substrates and adsorbates to rapidly screen alloy catalysts for the CO_2 reduction reaction with the usual DFT accuracy (DOI: 10.1039/d0ta06203k). Catalysts for other reactions could also be identified by machine learning methods. Saxena *et al.* developed machine learning models to predict the binding energies of oxygen and carbon on bimetallic alloys and Cu-based single atom alloys and then the binding energies were further used in an *ab initio* microkinetic model to evaluate the turn over frequency for ethanol decomposition and non-oxidative dehydrogenation reactions (DOI: 10.1039/c9ta07651d). The highlight by Tomboc *et al.* demonstrates that computational studies and machine learning assisted tools could be used to find the optimum catalyst composition and structure of high entropy alloy nanoparticles, which is important for improving the catalytic performance of high entropy alloy based electrocatalysts and for gauging the relevance of structural factors (DOI: 10.1039/d0ta05176d).

Organic photovoltaics (OPVs) have attracted great attention; however, the performance can be further improved. Sahu *et al.* performed high-throughput screening of 10 170 candidate molecules with machine learning models (DOI: 10.1039/c9ta04097h). Lin *et al.* used a machine learning method to predict the power conversion efficiency of OPVs and the results are consistent with the experiments (DOI: 10.1039/c8ta11059j). The review ''Machine learning for renewable energy materials'' by Gu *et al.* summarized the applications of machine learning methods in theoretical approaches for renewable energy technologies such as catalysis, batteries, solar cells and crystal discovery (DOI: 10.1039/c9ta02356a).

Thermoelectric materials can convert heat into electricity, and have attracted considerable interest as power generation devices. Ricci *et al.* used machine learning models to predict unavailable values in materials project databases and then screened gapped metals with attractive thermoelectric properties based on high-throughput computations (DOI: 10.1039/d0ta05197g). To reveal the connection between the electronic and thermal transport, Juneja *et al.* established a machine learning model to predict the lattice thermal conductivity based on bonding characteristics (DOI: 10.1039/d0ta02364g).

Adsorbent materials are important for storage and removal. Lin *et al.* screened 50 959 hypothetical pure silica zeolites and identified 230 zeolites with good adsorption performances for linear siloxanes and derivates by means of Grand Canonical Monte Carlo simulations and machine learning (DOI: 10.1039/c9ta11909d). Lee *et al.* used an artificial neural network to generate energy shapes of crystalline nanoporous materials to obtain accurate performance limits for methane storage (DOI: 10.1039/c8ta12208c).

Membranes are widely used in materials science. Liu *et al.* established machine learning models to predict the proton conductivity, methanol permeability, tensile modulus and degradation temperature of hydrocarbon-based proton exchange membranes (DOI: 10.1039/c9ta00688e). Liu *et al.* built machine learning models to predict the performance of polyvinylidene fluoride, polyethersulfone and polysulfone filtration membranes in the separation of macromolecules and salts from water based on a comprehensive dataset with 1895 vectors (DOI: 10.1039/d0ta07607d).

In addition, machine learning methods can be used in many other fields of materials science. Bagheri and Cremona evaluated the application of machine learning in the formulation of construction materials (DOI: 10.1039/d0ma00036a). Li *et al.* employed a multiscale computational approach to evaluate the cooling performance of over three million cascaded adsorption heat pumps and demonstrated that machine learning could be successfully implemented to predict the overall cooling performance of cascaded adsorption heat pumps (DOI: 10.1039/c9ta09227g). Bokka *et al.* used machine learning techniques to accurately predict the stimuli of a sensor (DOI: 10.1039/d0ma00573h).

We hope that this special collection of articles published in *Journal of Materials Chemistry A* and *Materials Advances* on the topic of machine learning for materials innovation is of considerable interest to a wide range of groups.

Sincerely yours,

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