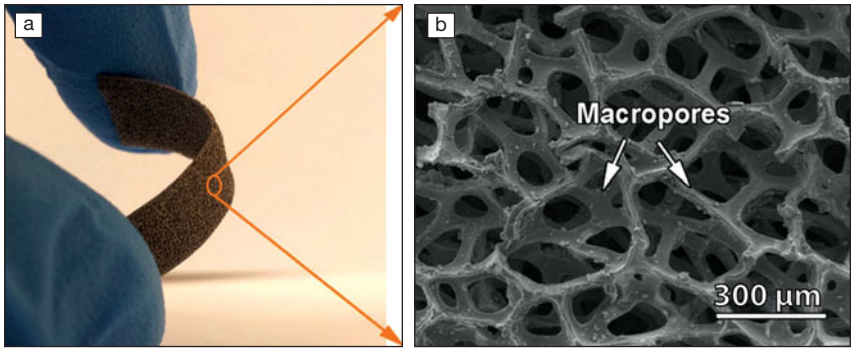
of charge, reactants, and products if these MOFs are to be used as electrocatalysts.

To create a MOF with these properties, Zhao's group devised a novel fabrication method that gave them control over many different factors. According to Sheng Chen, a research fellow in the Zhao group, "Our *bottom-up* growth method enabled us to manipulate the structure and morphology of the MOFs." Because of its 2D nature, more of the metal sites in the ultrathin NiFe-MOF are exposed and available as sites for catalysis during the electrochemical reaction. The NiFe-MOF designed by Zhao's group also has many different types of pores, like the intrinsic micropores and macropores between MOF layers (as seen in the Figure). This diversity in pore size allows electrolytes and gas molecules to diffuse through the MOF during catalysis. Thirdly, growing the NiFe-MOF directly on the electrode gives researchers more control over the final MOF-electrode architecture. This is the first demonstration of a 2D MOF being fabricated directly on a substrate. Lastly, this *bottom-up* approach is much simpler than other methods for creating 2D MOFs. "This synthetic approach is facile, universal, and adaptable for a range of MOFs and substrates," says Zongping Shao of Curtin University in Perth, Australia, who was not connected with the publication.

All of these factors combine to give this 2D NiFe-MOF its versatility and high performance. Electrocatalytic water splitting combines an oxygen evolution reaction at the anode with a hydrogen evolution reaction at the cathode. Zhao and Chen's 2D NiFe-MOF performs both of these reactions efficiently, significantly mitigating the energy losses caused by the slow kinetics of these reactions. Furthermore, an electrochemical cell with the 2D NiFe-MOF as both the cathode and anode showed excellent catalytic activity, producing a current density of 10 mA cm^{-2} at a voltage of 1.55 V. This activity is higher than that of most bifunctional catalysts, and is close to the activity demonstrated in standard precious-metal-based catalysts that are used as a benchmark for performance.

These results are only in their infancy, but researchers are excited about what this could mean for future MOF applications. "This could open up a new avenue for further tailoring and utilizing MOFs as high-performance electrocatalysts," Shao says. He would also like to see a more thorough understanding of how the substrate might affect the catalytic activity of the NiFe-MOF. Looking forward, Zhao says his group hopes to "expand MOF applications beyond water splitting" potentially addressing "challenging problems such as electro-reduction of carbon dioxide to generate liquid fuels."

Lauren Borja



(a) Optical and (b) scanning electron microscope image of the 2D nickel/iron metal–organic framework. Courtesy of Nature Publishing Group.

Universal fragment descriptor predicts materials properties

Luck as a means for scientific discovery is highly inefficient given that the possible number of materials is estimated to be around 10,100. Also, enormous piles of data are currently stored in vast repositories with no meaningful connections to each other. A group of researchers from The University of North Carolina at Chapel Hill (UNC) and Duke University has taken a significant step toward realizing a knowledge-based structure–property relationship that can predict properties given a few fundamental parameters of a material. They do this by applying machine learning techniques to such data, as reported in a recent issue of *Nature Communications* (doi:10.1038/ncomms15679).

At the heart of their approach is what they call a "universal fragment descriptor," which is essentially a labeled graphical representation of the unit cell of an inorganic material. For a given crystal, all the nearest neighbors are identified and a graph is constructed with atoms as the nodes and the bonds as edges. This infinite graph is then broken down to the simplest fragments that capture the local topology in a matrix. Combined with several chemical and physical properties of each atom, these graphs form property-labeled materials fragments (PLMFs) or a "colored graph" in graph theory terminology. The schematic for this construction is given in the Figure.

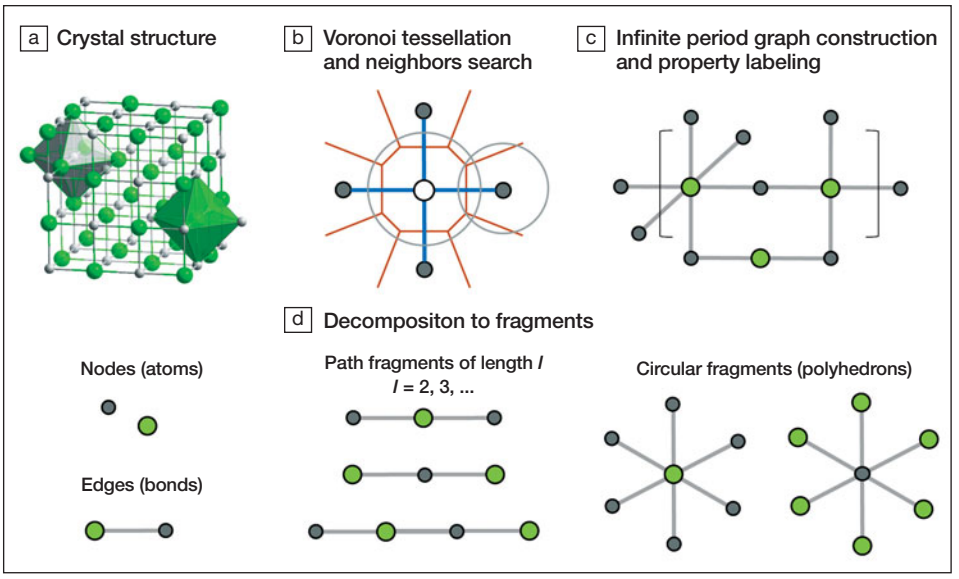
"Methodologically, we could apply this technique to any material, even amorphous solids," Olexandr Isayev of UNC, one of the researchers, told *MRS Bulletin*. "So far we are cautious to limit this method to stoichiometric materials. We are working now to extend this to include vacancies and doping, for example."

To test the predictive power of this new approach, the researchers used rigorous fivefold cross-validation as well as perspective prediction conformation with density functional theory calculations and experiments. In cross-validation, a data set is randomly partitioned into five

https://doi.org/10.1557/mrs.2017.171 Published online by Cambridge University Press

groups. Four of these groups are subjected to machine learning techniques to learn the best relationship or a "rule" that will predict a set of properties (e.g., Debye temperature, metal/nonmetal, and specific heat) from the corresponding fingerprint. This rule is tested on the fifth group to see how well the predictions match the observations. By rotating the five groups, all data get to be in the training set and the testing set.

PLMF was tested on eight predictive models: a binary classification model to predict if a material is metal or nonmetal and seven regression models that predict the band energy, bulk and shear modulus, Debye temperature, heat capacities, and coefficient of thermal expansion. What distinguishes the team's work from other machine learning approaches is the high accuracy of these predictions. For example, the values for bulk and shear modulus are 99% accurate for the data set. The metal/nonmetal classification is 86% accurate for a sample set of 26,674 materials. In other words, only 3621 materials were misclassified in this case.



In property-labeled materials fragments, the crystal structure (a) is analyzed for atomic neighbors through Voronoi tessellation (b). After property labeling, the resulting periodic graph (c) is decomposed into simple subgraphs (d). Credit: *Nature Communications*.

Keith Butler of the University of Bath complimented the team on the novel fingerprint technique: "The work of Isayev et al. presents one of the most convincing approaches for turning the structure and composition of a crystal into a form that is sensible to a machine learning algorithm. It's a big advance and it opens the door for future applications of machine learning for materials design."

Johannes Hachmann of the University at Buffalo, The State University of New York concurs: "One of the key challenges to making machine learning a viable proposition in this application domain is the availability of a suitable numerical representation of compounds in materials space. The proposed universal fragment descriptors offer an exciting new direction on this issue and promise to support easier interpretation of the resulting models and rational design based on these insights."

The research team plans to continue developing better algorithms and perhaps a unified model that will one day work for any materials system.

Vineet Venugopal

Diamond-powered transistor performs in extreme environments

Research is being conducted to employ wide-bandgap semiconductors such as SiC, GaN, and diamond to replace silicon to overcome its inherent limitations of high-frequency switching and power handling. Now researchers at the National Institute for Materials Science (NIMS) in Japan have designed a diamond-powered transistor that can be used in extreme environmental conditions like harsh temperatures and radiation conditions, as reported in a recent issue of *IEEE Electron Device Letters* (doi:10.1109/LED.2017.2702744). Due to their high power frequency, thermal limits, and low power loss at high frequency, diamond-based electronic devices outshine other wide-bandgap semiconducting materials-based devices.

In this study, the researchers used a microwave plasma-enhanced chemical vapor deposition technique to grow a 150-nm-thick epitaxial layer of hydrogenated diamond (H-diamond) at 900–940°C with a chamber pressure of 80 Torr. A 4-nm-thick layer of Al_2O_3 was selected as a buffer (to reduce the effect of lattice mismatch) for the $LaAlO_3$ to utilize H-diamond in enhancement-mode metal oxide semiconductor field-effect transistor (MOSFET) architecture, and a 30.4-nm-thick layer of Al_2O_3 was deposited on H-diamond for the operation of depletion-mode MOSFETs. Both types of devices were completed with Ti/Au metal deposition through e-beam evaporation. The schematic diagram of both circuits is shown in the Figure.

An increase in gain maximum for the NOT logic circuit from 1.2 to 26.1 was recorded when the voltage supplied was changed from –5.0 to –25.0 V. The NOR logic circuit configuration showed immaculate NOR gate characteristics.

https://doi.org/10.1557/mrs.2017.171 Published online by Cambridge University Press