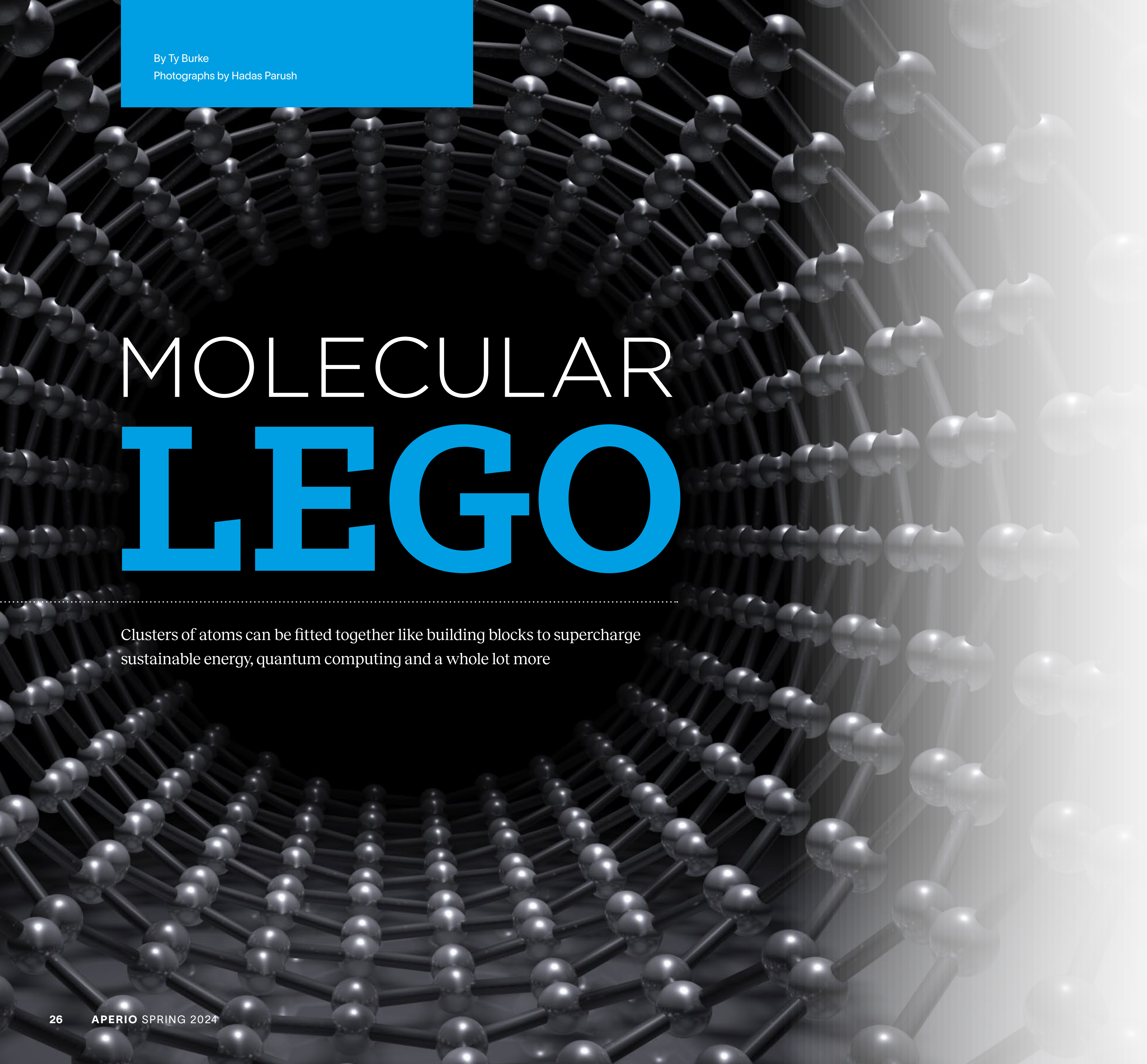
By Ty Burke
Photographs by Hadas Parush



MOLECULAR LEGO

Clusters of atoms can be fitted together like building blocks to supercharge sustainable energy, quantum computing and a whole lot more

A green energy revolution is well underway, but the speed bumps are formidable. Consider the challenge of energy storage. Wind turbines only generate electricity when the wind blows, and solar panels when the sun shines. This intermittency makes large-scale energy storage a necessity, but current technologies have significant limitations.

Today, the batteries used for this type of storage rely on metals such as lithium and cobalt, which are energy intensive to mine and have a relatively limited lifespan. The same materials are used in electric vehicle batteries and have not been able to match the range of their petroleum-powered counterparts.

Advanced nanostructured materials could flip the script. Through a process called solid-state synthesis, nanotechnologists are creating purpose-built crystals, manipulating their structure to achieve specific properties. One of the leading lights in this emerging field is Elena Meirzadeh, an assistant professor at the Weizmann Institute of Science and Azrieli Early Career Faculty Fellow.

Meirzadeh was born in Tehran and moved to Israel when she was 11 years old. But she did not have a strong command of either Hebrew or English, and it took time for her to adjust to life in Israel. She didn't even take to science right away, and almost gave up on chemistry in high school. But in her final year, she was inspired by the hands-on scientific approach of her chemistry teacher, who taught science as a process of experimentation rather than a theoretical endeavour. That captured Meirzadeh's imagination and remains central to her research approach.

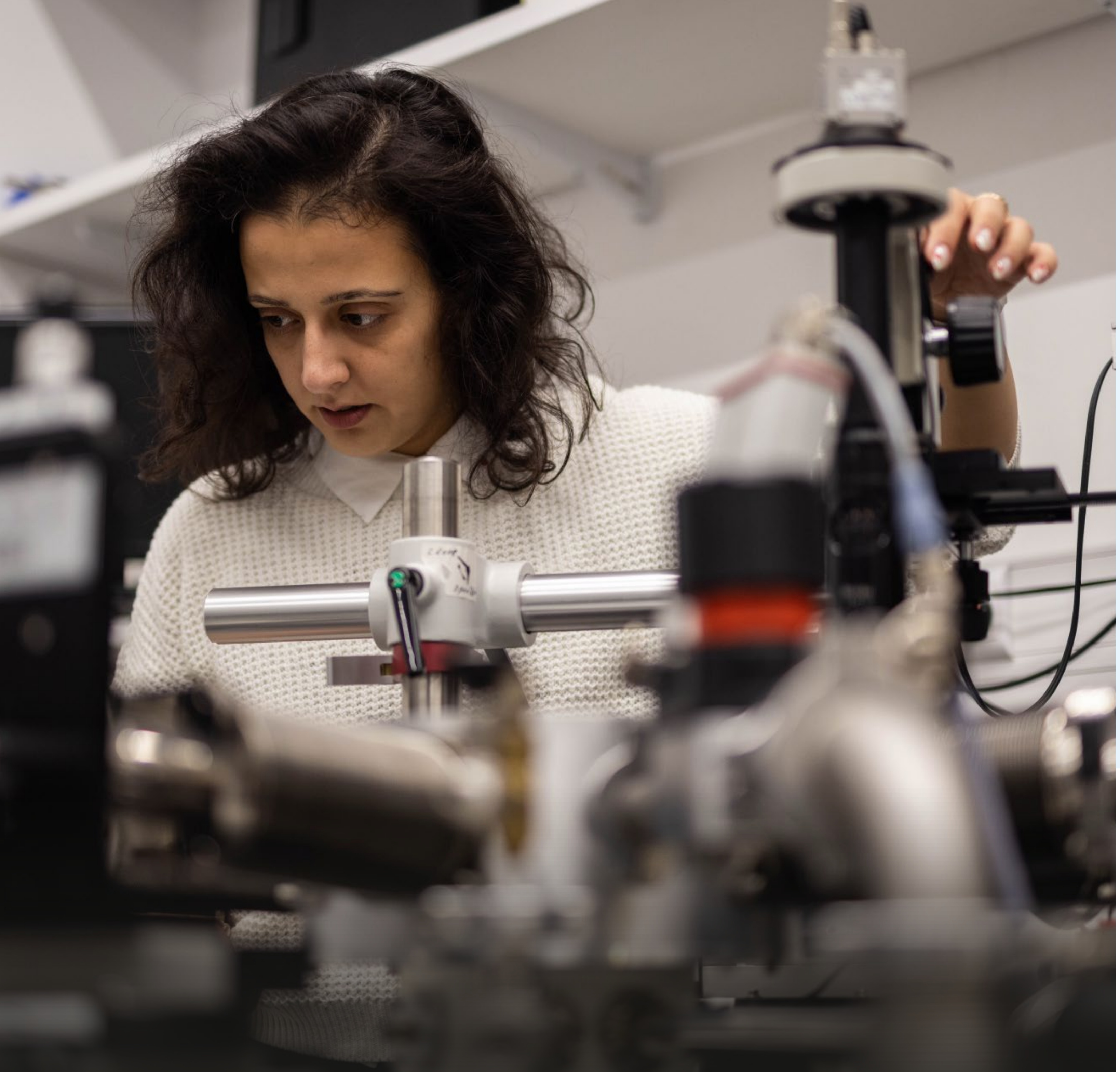
Working in her lab, Meirzadeh synthesizes crystals composed of atomically precise molecular structures known as superatoms that could be deployed in a variety of applications. One day, these carbon-based molecules could vastly improve energy transport and storage. The optoelectronic properties of superatoms could also make them useful for quantum computing transistors. Some are even superconductors, and this could have all kinds of potential applications if technical challenges can be overcome.

"I'm fascinated by the mechanisms of the formation of crystals — how to make them and incorporate interesting properties into their design," says Meirzadeh.

It's easy to get caught up in her enthusiasm. By controlling the parameters of solid-state synthesis and exposing materials to various external stimuli, Meirzadeh can "tune" her crystals to achieve specific magnetic or electrical properties. She does this using a synthetic approach she developed called pyrolytic vapour polymerization reaction. The technique seals the molecular precursors for a new crystal inside a vacuum tube made of quartz, which is then baked in a specialized oven. The precursors vaporize and react, and as they cool, they solidify into a new crystal.

It's a powerful technique that allows scientists to grow large, high-quality single crystals, Meirzadeh says. Using a combination of experience and intuition, she can manipulate various parameters to achieve specific goals. "If we can grow single crystals, determine their structure and measure their properties, then we can know that a specific structure results in a specific property," says Meirzadeh. "And we can change a structure to get that property and basically design whatever we want. But that's really hard to do."

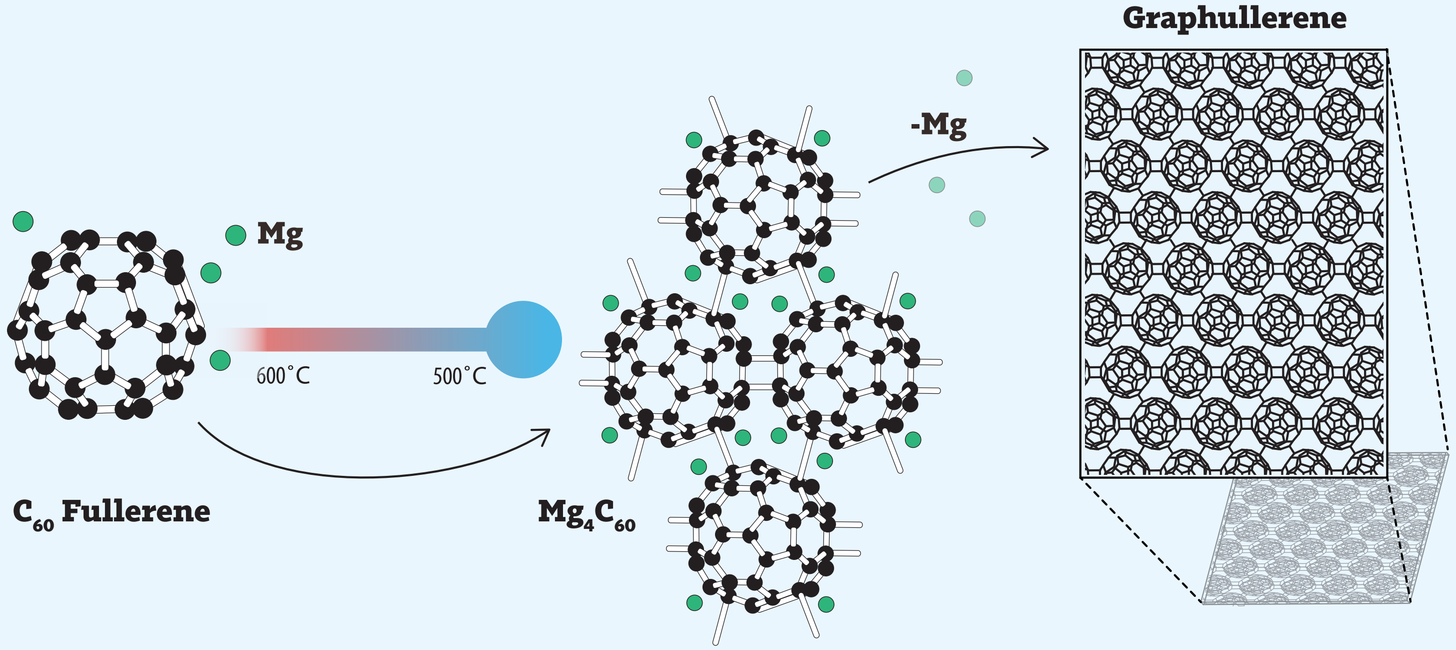
The oven Meirzadeh uses to cook new materials has zones for heating and cooling that can be precisely controlled. And even after the molecular precursors crystallize into a unified material, its exact identity is still a mystery. It could be something already known to science, and most of the time it is. But the process can also create something entirely novel, and Meirzadeh needs to characterize the new crystal to determine whether it is. During her postdoctoral research at Columbia University, Meirzadeh created a superatomic two-dimensional material called graphullerene — by happenstance — that exhibits promising thermal conductivity properties (see related story).



Meirzadeh synthesizes crystals composed of atomically precise molecular structures known as superatoms that can be deployed in a variety of applications, notably energy transport and storage

An assistant professor at the Weizmann Institute of Science and Azrieli Early Career Faculty Fellow, Elena Meirzadeh can "tune" her crystals to achieve specific properties.

A CARBON COPY THAT IS TOTALLY UNIQUE



Graphullerene is a new form of carbon that can withstand very high currents and heat. The material is synthesized by reacting fullerenes — lattice-like spheres linking many carbon atoms in geometric patterns — with magnesium in a quartz tube at elevated temperatures (left). Negatively charged molecular sheets of fullerenes with magnesium counter ions grow at the colder end of the tube (centre). Pure graphullerene is obtained by removing magnesium using acidic solutions. The resulting crystal (right) can be peeled into thin, two-dimensional sheets that can be manipulated to tune the optoelectronic properties.

To determine the crystal structure, Meirzadeh uses an X-ray diffractometer. When an X-ray hits a crystal, it forms a diffraction pattern that reveals the position of the atoms within the crystal. Placed inside a diffractometer, a crystal is bombarded with electromagnetic radiation from different angles. This creates a pattern of waves that reflects both the atoms that compose it and the way they fit together. Each crystal has a unique signature that can be determined by analyzing the pattern these waves form. This information is then compared to known crystal structures to determine whether the crystal is something entirely new.

Solid-state synthesis has been long been used to produce inorganic materials from atomic precursors, but Meirzadeh uses organic molecules to create crystals, and their organic chemistry presents additional challenges.

Carbon is the basis for all life on earth and, like most life forms, carbon-based molecules tend to be sensitive to extremely high temperatures. This means that the possible parameters for synthesizing carbon molecules are more limited than with inorganic precursors. While inorganic precursors can be baked at temperatures that exceed 1000°C, the materials Meirzadeh produces are cooked at temperatures around 600°C.

Working with carbon offers advantages as well. It is a shape-shifting element that can take many different forms. This is because of its valency — the number of ways it can combine with other atoms. Carbon has six electrons, and four of them are available to form bonds. There are, therefore, many different configurations in which carbon atoms can bond with each other and other molecules. That is why there are several different types of this single element.

Elements that can take different forms are known as allotropic; naturally occurring carbon allotropes include diamonds and graphite. Fullerenes, another carbon allotrope, are an important focus of Meirzadeh's research. Fullerenes were first identified in the 1980s and are characterized by their unusual shape. They are hollow, lattice-like spheres that link together many carbon atoms in adjacent pentagonal and hexagonal shapes.

Using solid-state synthesis, Meirzadeh can link fullerenes into two-dimensional molecular sheets that can be measured and structurally manipulated. This gives fullerene unusual potential as a nanomaterial. "Fullerenes are not called superatoms only because they're big," she says. "This is a fancy word for an atomically precise molecular cluster. There are atoms and there are nanoparticles, and somewhere in between you have superatoms."

The superatom edge: "Imagine you have a set of Lego, and then I bring you a bunch of new Lego bricks with different geometries. You can build different things."

A LAB EXPERIMENT THAT WENT DELIGHTFULLY WRONG

Elena Meirzadeh created a form of carbon called graphullerene, but the first synthesis of the material was the result of a happy accident. While undertaking her postdoctoral research at Columbia University, Meirzadeh attempted to synthesize a crystal in her lab, one whose structure was already known to science. But it didn't come out as she anticipated.

When Meirzadeh analyzed the new crystal in the lab, she realized she had failed at what she was trying to do — and done something far more interesting instead. The crystal she had created did not match the characteristics of the one she'd aimed to, or those of any other known material. "It was unexpected," she says, "but you need to be open-minded about what you might find. I realized right away I had hit the jackpot."

Meirzadeh was thrilled that she had created something new, but suddenly her research into its properties was forced to shut down. It was early 2020, and COVID-19 lockdowns meant her lab at Columbia had to close. Meirzadeh knew she had something big, but she had to halt her research into the new material. Six months later, the lab reopened and Meirzadeh resumed her research into graphullerene. The findings were published in the journal *Nature* in January 2023, with Meirzadeh as the lead author. ▲●■

With nanoparticles, it is difficult to determine precisely how many atoms are involved, but with superatoms this can be measured.

Meirzadeh compares the ability to control this process to building with Lego on a molecular scale. "Imagine that you have a set of Lego, and then I bring you a bunch of new Lego bricks with different geometries. You can build different things," she says.

"Working with fullerene molecules is like this. You can manipulate the system using synthetic tools. If we change the conditions, we can get hexagonal or rectangular structures, or even other shapes. It's a much more diverse building block than single atoms. By changing these geometries, we can also change the thermal conductivity and the electronic and magnetic properties. That's the beauty of using these molecules as your Lego pieces."

In practice, this does not involve any plastic bricks. Rather, Meirzadeh controls the parameters of the pyrolytic vapour polymerization reaction to achieve different geometries — changing vapour pressure, adjusting the amount of material loaded into the quartz tube, setting a higher or lower temperature, or adjusting the cool-down rate, among other parameters. This allows Meirzadeh to build molecules made with the component parts she wants to include.

But the Lego analogy doesn't end there. Another advantage of working with layered materials is that they can fit together in ways that other nanomaterials cannot.

When Meirzadeh removes a crystal from the oven, it is macroscopic and far larger than a single molecule. To obtain molecular sheets from the larger crystal, Meirzadeh uses a process called mechanical exfoliation. This applies friction to flake off ultra-thin layers of the superatoms. These are potential building blocks for heterostructures that could open additional frontiers in nanotechnology, including new types of semiconductors.

"Many of the materials I make are two-dimensional," says Meirzadeh. "These have very strong bonds in two dimensions but a weak interaction in the third dimension. When you confine electron movement to two dimensions, you get new physics. Conduction changes and magnetic properties change. But the most common technique to make these materials is growing thin films, and these have a lot of defects. When you exfoliate crystalline sheets, it can give you much better performance."

Because these crystalline sheets are composed of clusters of atoms — and not simply a two-dimensional sheet — they are better able to form chemical bonds in the third dimension. This makes a material such as graphullerene suitable to bond with other materials in various configurations and heterostructures. Heterostructures combine multiple nanomaterials into a single device, which makes it possible to unlock the potential of both materials simultaneously, and even achieve sought-after properties that neither one has its own.

When materials are stacked on top of each other and the angles of the layers are rotated, it can change the optoelectronic structure, and specific combinations can yield desirable properties. With the two-dimensional material graphene, stacking layers in a heterostructure is how superconductivity is achieved.

Similar to the superatoms that can be used to build them, heterostructures are still in an early stage of development. It will take decades to realize their full potential, though Meirzadeh's research could play an important role in getting there, according to Milko van der Boom, head of the molecular chemistry and materials science department at the Weizmann Institute.

"Elena's chemistry bridges the gap between traditional organic chemistry and solid-state synthesis of 2D atomic crystals," says van der Boom. "Making new materials by using superatomic building blocks, as Elena does, allows a whole new library of materials with more diverse and complex structures to be created beyond what's available today."

For Meirzadeh, it was the wealth of possibilities in nanotechnology that drew her to the field. "My goal is to make functional materials that have applications in the future. In the beginning, it was hard to choose a direction for my research," she says.

"I tried to imagine what the future work would be. I didn't just want to do something that would be published in a big journal. I wanted to do something that opens an entirely new field." ▲●■