Game changers

Fresh perspectives are essential if new materials are to help solve the world's big challenges.

Global issues, such as climate change and improving sustainability in manufacturing, and technological opportunities, including artificial intelligence and quantum computing, are driving forward the frontiers of research in materials science. These four scientists are among a new generation of researchers helping to push forward these boundaries while also bringing diverse skills to the field, ensuring a broader range of views are included in tomorrow's solutions.

Composite creator
Grace Gu

Grace Gu is taking inspiration from a wide range of places when she comes up with designs for composite materials that are more robust, adaptable and cheaper to produce than current forms. Turning to "the hidden gems of the mathematical world" to inform her designs has been especially rewarding, says Gu, who works as a mechanical engineer at the University of California, Berkeley (UC Berkeley).

Earlier this year, she co-authored a paper[1] on composite material designs based on aperiodic monotiles – unique shapes, discovered just last year[2] – that can cover a surface without ever repeating pattern. The materials were shown to be stronger, stiffer and tougher than conventional honeycomb tile structures because the non-repeating pattern creates a tightly packed network with a high tolerance of defects due to how the patterns distribute stress throughout the material. Lightweight composite materials with these characteristics are highly sought after in spacecraft and satellite manufacturing.

"Our experiments show that the designs not only absorb energy efficiently, but also exhibit unique interlocking behaviours where the tiles actually interact with and reinforce each other," says Gu.

She says that she is excited by the simplicity of these designs that use a single shape because they have "immense potential for engineering applications, as they could reduce manufacturing complexity and costs".

"There's actually an entire family of monotiles, which gives us a wide range of design possibilities, so far more flexibility than traditional honeycomb structures," Gu says of the potential for these designs in creating stronger and more efficient materials.

ILLUSTRATIONS BY PADDY MILLS FOR NATURE INDEX

Grace Gu is using techniques such as machine learning to design composite materials.

Gu's ability to recognize patterns has been key to her success as a researcher. She recalls a lightbulb moment she had in 2016 when AlphaGo, an artificial-intelligence (AI) system created by London-based company Google DeepMind, defeated the world's best player at the board game Go. Gu noticed that the grid used in Go – on which two players move stones to control territory – was similar to the pixelated 2D composite-design problem she was working on at the time.

"We have different types of materials that can occupy different positions" on a grid, and "design strategies that are like boardgame strategies", she says. Gu considered that if machine learning could be used to train a system to play Go — known for its immense complexity and astronomical number of possible moves — it could help her find new composite designs more efficiently.

Gu found that AI could predict the properties of materials at a vastly accelerated pace[3], and it changed how she approached this kind of work in the future. Initially applying machine learning to pixelated designs inspired by AlphaGo, Gu and colleagues have since explored graph-based and Bezier curve approaches to this work, which can capture other types of structures and geometries more effectively.

As a woman in a male-dominated field, Gu is passionate about mentoring young women in research. She says she realized the importance of representation when, during the first class she taught at UC Berkeley, a female student raised her hand to say that she was excited for the semester because Gu was the first female professor she had been taught by at the university. "I think back at these moments and remind myself that this is the best part about being a professor; mentoring and teaching the next generation to fulfil their potential and beyond," she says.

Gu has received numerous accolades for her work, including a 2020 Outstanding Young Manufacturing Engineer Award from US industry body SME and The American Society of Mechanical Engineers Early Career Award in 2023. **Esme Hedley**

Decarbonization designer
Marcileia Zanatta

Marcileia Zanatta's research harnesses decarbonization to create sustainable materials.

Marcileia Zanatta's desire to design new products to overcome challenges began as early as age eight, when she dreamed of inventing something that could dissolve the hair trapped in her shower drain. "I used to observe everyday problems and say: 'When I grow up, I'm going to create something that solves this'," she recalls.

She went on to study industrial chemistry at university in her native Brazil and, while doing a master's at the Federal University of Rio Grande do Sul in Porto Alegre in 2012, she began working on decarbonization — a field she finds "incredibly rewarding because of its direct impact on people's lives".

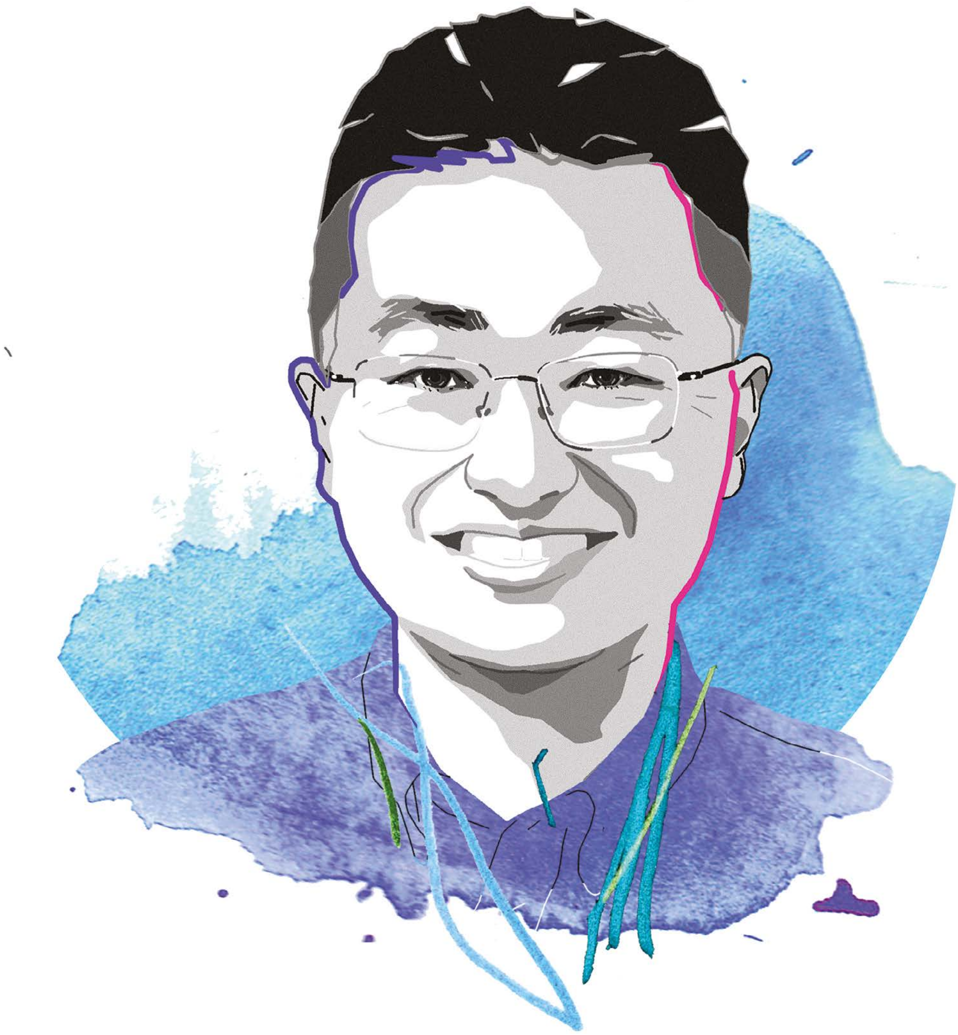
More than a decade on, Zanatta, a material chemist at Jaume I University in Castelló de la Plana, Spain, is focused on finding energy-efficient ways to convert carbon dioxide into sustainable materials that can be used in chemicals, fuels, and other useful products. "This can lead to a circular economy and a net-zero future," she says.

In October, the province of Valencia, near where Zanatta lives, experienced one of the deadliest flooding events in Spanish history. There were also devastating floods in May across Rio Grande do Sul, the Brazilian state where she had spent a significant part of her career. "These catastrophes are painful reminders that simply reducing carbon emissions is no longer enough to address the consequences of climate change," says Zanatta. "This reality underscores the urgency of my work."

She and her collaborators have invented ways to transform atmospheric carbon into compounds such as formate salts[4], which can be used as de-icing agents and fluids to aid drilling, and cyclic carbonates[5] — important materials in lithium batteries, cosmetics and industrial solvents.

The latter work, she says, is one of her biggest accomplishments to date. Producing cyclic carbonates from CO_2 is typically energy intensive, requiring temperatures above 100 °C, pressures 20 times greater than found in the atmosphere at sea level, and several hours to allow reactions to take place. But in 2023, Zanatta developed a more efficient method — one that takes place under mild conditions using inexpensive, commercially available organic salts such as tetrabutylammonium hydroxide. She's even used 3D printing to create bespoke reactors that enhance reaction rates by maximizing surface area and improving the distribution of reactants around the catalyst[6].

Enabling such reactions in ambient conditions has opened up other avenues, including decarbonization methods that combine both chemical and biological reactions. "Merging the two isn't so easy, because the second part involves microorganisms, which usually can't withstand harsh chemical conditions," Zanatta



Cong Xiao explores how quantum rules can predict the behaviour of materials.

explains. But harnessing such biological power – some microbes can metabolize simple carbon compounds – is crucial if scientists want to produce biodegradable materials based on biopolymers from CO_2. This year, Zanatta and her team successfully demonstrated how a green plastic called poly-3-hydroxybutyrate (PHB) could be produced using such a chemo-biocatalytic process, with formate salts as an intermediary – the first time PHB has been produced from captured atmospheric air[4].

Zanatta has received numerous recognitions for her work, including being named a 2023 Rising Star by the materials-science journal *ACS Materials Au*. But her journey hasn't always been easy, and Zanatta says female researchers face particular challenges.

"The years when we are close to securing a permanent position are often the same years many women are considering starting a family." A maternity break "can completely change a woman's career", she says.

Working in a male-dominated field also means that Zanatta frequently "hears sexist remarks or encounters 'mansplaining'", but she says it's important to try and speak up because "engagement and awareness are key". She offers her younger female counterparts the following advice: "Be persistent, resilient, and try not to take things personally. Always demonstrate your value, take initiative, and be confident in your leadership." **Sandy Ong**

Quantum explorer
Cong Xiao

Cong Xiao was drawn to the field of condensed-matter physics because he wanted to explore electron wavefunctions: mathematical descriptions of how electrons behave at the quantum-mechanical level.

The fact that it can be used to develop new electronic devices shows the wonder of how "the microscopic quantum-mechanical rules can be connected to the macroscopic devices in our daily life", says Xiao, a theoretical physicist.

As a PhD student at Peking University in Beijing from 2018 to 2021, for instance, Xiao learnt of the "power and beauty" of the Berry phase – an important unifying theory in the field. He says it cemented his decision to pursue an area of physics that underpins important products in materials science, such as liquid crystals and silicon chips.

Now an assistant professor at the Institute of Applied Physics and Materials Engineering at Macau University, Xiao is exploring new physical effects that can be predicted by quantum rules. For example, in sub-fields such as nonlinear transport and spintronics, he's looking at how electrons move and interact in unusual ways. Advances in these areas could inform the design of advanced technologies such as quantum computers.

Although his work is theoretical, Xiao says a characteristic of good research in his field is that it "not only reveals some new principle in the microscopy level but can also lead to developments in technology".

For example, some of Xiao's current work in nonlinear transport has potential use in rectifiers, electrical devices that convert alternating current into direct current, a common need in communications technology. "Nonlinear transport can be used to achieve such devices, and the underlying principle is truly quantum mechanical," says Xiao.

An important paper[7] in his career – published in 2021 – reported the first-principles calculations of the nonlinear Hall effect in antiferromagnets. The nonlinear Hall effect is the production, upon the application of an electric field, of a transverse voltage that scales nonlinearly with the applied field.

Xiao says the paper gave other researchers the tools to perform more research on nonlinear transport in magnetic systems, as manipulation of these systems has potential applications in information technology.

Xiao says it is sometimes difficult to decide which direction the field of condensed-matter physics is moving in. He says the biggest challenge for a theoretical researcher is "always keeping yourself always at the frontier of the research", because ideas and topics in condensed-matter physics "move very rapidly".

"We have to keep learning the theoretical skills just to help us to understand the questions in broader contexts, to help to study wider physical questions. I think this is the biggest challenge, to keep exploring wider and wider research" questions.

In the Nature Index, Xiao stands out from other early-career researchers for his relatively high materials science-related output. His Share of 3.53 for the period 2019 to 2023 places him among the leading 20 early-career researchers in the field. **Esme Hedley**

Biomolecule magician
Caio Otoni

At the State University of Campinas in São Paulo, Brazil, Caio Otoni studies the circular economy, where biological waste, such as fruit peels, coffee husks and crustacean shells, is upcycled into new products, materials and energy sources. This approach is particularly relevant to Brazil, a leading producer of sugarcane, coffee and other food crops.

In Otoni's lab, he and his colleagues break down waste material into its building blocks – cellulose, chitin and other polymers – and pair it with other compounds to create plastics with biodegradable and antibacterial properties.

In a 2019 paper[8], for example, Otoni and his colleagues described how they grafted cationic compounds, chemicals that contain positively charged ions, onto upcycled cellulose to create an antibacterial foam material for use in packaging, filtration and hygiene products. The foam's positively charged compounds adhere to and disrupt the negatively charged surface of bacterial cell membranes, leading to bacterial cell death. In tests, it displayed an 85% higher antimicrobial response to *Escherichia coli* compared with controls.

Otoni credits his botanist father, whose lab he would visit when he was growing up, for cultivating his appreciation for plants. But it was his time spent as an exchange student at the US Department of Agriculture's research facility in Berkeley, California, that solidified his passion for sustainably produced materials.

While working on a project with an Alaskan fishing company, Otoni realized how wasteful it was to throw fish skin back into the ocean. The young undergraduate devised a way to isolate collagen from the discarded skin, convert it to gelatin, and produce packaging material.

"That was the very first project I worked on that exploited not only biorenewable resources, but also waste biomass, as a source of polymers," says Otoni. As a PhD student and postdoc, he went on to create new materials from carrot and peach waste, as well as sugarcane bagasse – the pulpy residue left after sugarcane stalks are crushed to extract their juice.

Securing funding as a young scientist can be tough, he concedes, "because you are competing with the big fish, the established researchers". Working in Brazil "adds another level of complexity, because in most institutions, staff numbers are limited, meaning we have to deal with paperwork and administrative tasks in addition to our regular teaching, research and outreach duties", says Otoni.

"Also, in Brazil, almost everything is charged in dollars or euros, and the currency exchange makes it hard to afford some devices that are key to running competitive research."

It's also been a steep learning curve to launch his own lab in 2020. "You're trained to go to the bench and do research; you're not trained to supervise students and manage a team. That's something that comes with time and experience," says Otoni, who in 2023 was the sole researcher based outside Europe and North America to win the Materials Today Rising Star Award in 2023, an annual prize given to six early-career researchers in the field of materials science and engineering.

Otoni is keen to train other young researchers in his lab in how to upcycle waste products, as he sees it as work that can make a real impact.

"I really believe our research on circular plastics can make a difference and help diminish the burden of plastic pollution in the world," he says. **Sandy Ong**

Caio Otoni looks at new ways to upcycle biological waste into useful products.

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