Tiny sensors rapidly detect trace 'forever chemicals' in drinking water

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"Forever chemicals" are notoriously difficult to detect, but a collaboration between the University of Chicago Pritzker School of Molecular Engineering and Argonne National Laboratory has yielded a novel detection method. The method, which they plan to share via a portable, handheld device, uses unique probes to quantify levels of PFAS "forever chemicals," some of which are toxic to humans. Credit: John Zich

They linger in our water, our blood, and the environment—"forever chemicals" that are notoriously difficult to detect.

But researchers at the UChicago Pritzker School of Molecular Engineering (UChicago PME) and Argonne National Laboratory have collaborated to develop a novel method to detect minuscule levels of per- and polyfluoroalkyl substances (PFAS) in water. The method, which they plan to share via a portable, handheld device, uses unique probes to quantify levels of PFAS "forever chemicals," some of which are toxic to humans.

"Existing methods to measure levels of these contaminants can take weeks, and require state-of-the-art equipment and expertise," said Junhong Chen, Crown Family Professor at the UChicago Pritzker School of Molecular Engineering and Lead Water Strategist at Argonne National Laboratory. "Our new sensor device can measure these contaminants in just minutes."

The technology, described in the journal *Nature Water*, can detect PFAS present at 250 parts per quadrillion (ppq)—like one grain of sand in an Olympic-sized swimming pool. That gives the test utility in monitoring drinking water for two of the most toxic PFAS—perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS)—for which the U.S Environmental Protection Agency (EPA) recently proposed limits of 4 parts per trillion.

"PFAS detection and elimination is a pressing environmental and public health challenge," said Andrew Ferguson, Professor of Molecular Engineering at UChicago PME. "Computer simulations and machine learning have proven to be an incredibly powerful tool to understand how these molecules bind to molecular sensors and can guide experimental efforts to engineer more sensitive and selective molecular probes."

"Even though they are typically present at minuscule concentrations, PFAS do have certain molecular characteristics that differentiate them from other things dissolved in water, and our probes are designed to recognize those features," said Seth Darling, a Senior Scientist at both Argonne and UChicago.

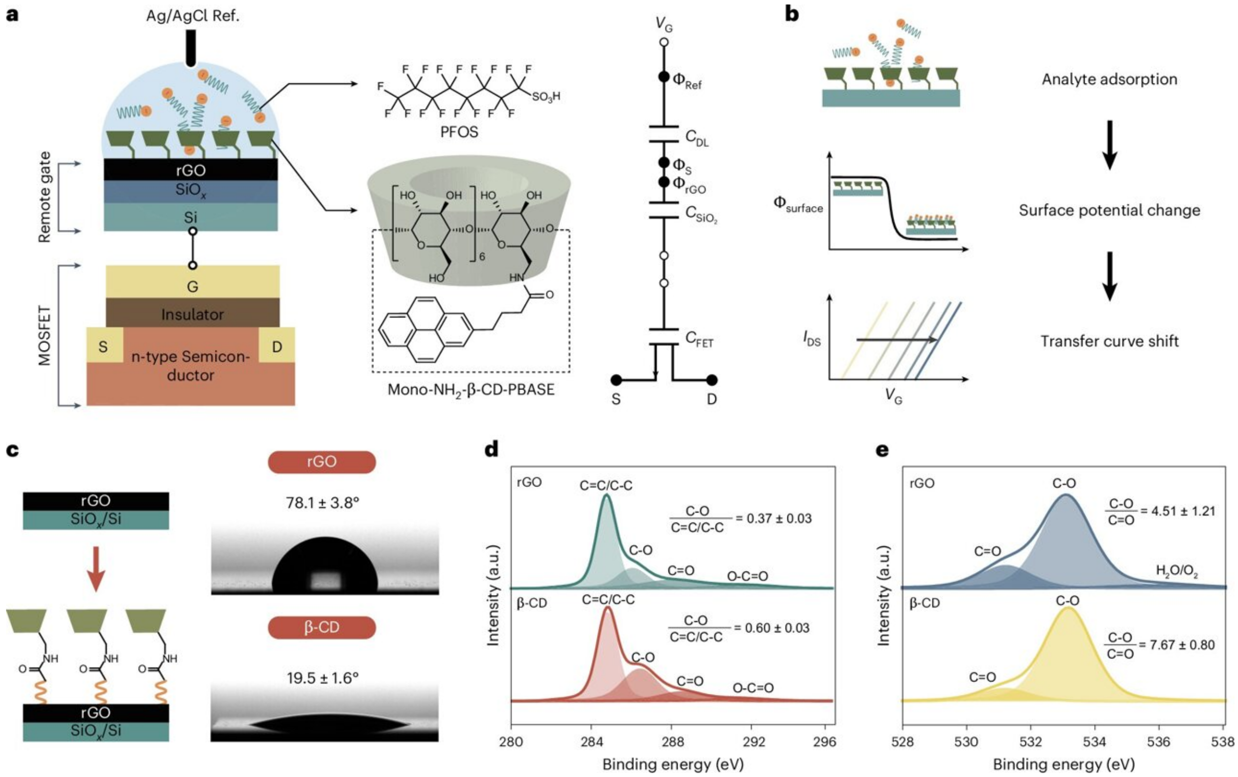
A detection challenge

PFAS are oil- and water-resistant chemicals that are used for a wide range of consumer and industrial products, including nonstick pots and pans, fast food packaging, firefighting foam, raincoats, and stain-resistant carpeting. Often called "forever chemicals," they are incredibly long-lasting and do not naturally degrade, but instead accumulate in the environment and people's bodies over time.

In recent years, studies have linked PFAS to health concerns, including cancers, thyroid problems and weakened immune systems. In light of some of these findings, the EPA proposed the new limits for PFOS and PFOA.

"The problem with enforcing these limits is that it's very challenging and time-consuming to detect PFAS," said Chen. "You currently can't just take a sample of water and test it at home."

The gold standard for measuring PFAS levels is an expensive laboratory test known as liquid chromatography/tandem mass spectrometry, which separates chemical compounds and provides information on each one.



Credit: Sensor design and characterization of RG electrodes.

Researchers attempting to make their own faster and cheaper PFAS tests face a few challenges: for one thing, PFAS chemicals are often present in water at much lower concentrations than dozens of other, more common contaminants. In addition, there are thousands of different PFAS chemicals with only slight variations between their chemical structures—but important differences in their health effects and regulations.

But Chen's team has been developing highly sensitive, portable sensors on computer chips for the last fifteen years. Chen is already using the technology in a lead sensor for tap water, and his lab group suspected that the same method could be used in PFAS sensing. Their proposal to adapt the technology for PFAS became part of the National Science Foundation Water Innovation Engine in the Great Lakes.

Designed by AI

The gist of Chen's sensor is that if a PFAS molecule attaches to his device, it changes the electrical conductivity that flows across the surface of the silicon chip. But he and his colleagues had to figure out how to make each sensor highly specific for just one PFAS chemical—such as PFOS.

To do this, Chen, Ferguson, Darling, and team turned to machine learning to help select unique probes that could sit on the sensing device and ideally bind only the PFAS of interest. In 2021, they won a Discovery Challenge Award from the UChicago Center for Data and Computing (CDAC) to support their use of artificial intelligence in designing PFAS probes.

"In this context, machine learning is a tool that can quickly sort through countless chemical probes and predict which ones are the top candidates for binding to each PFAS," said Chen.

In the new paper, the team showed that one of these computationally-predicted probes does indeed selectively bind to PFOS—even when other chemicals common in tap water are present at much higher levels. When water containing PFOS flows through their device, the chemical binds to the new probe and changes the electrical conductivity of the chip. How much the conductivity changes depends on the level of PFOS.

To ensure that the readings from the new device were correct, the team collaborated with EPA and used EPA-approved liquid chromatography/tandem mass spectrometry methods to confirm concentrations and verified that the levels were in line with what the new device detected. The team further showed that the sensor could maintain its accuracy even after many cycles of detection and rinsing, suggesting the potential for real-time monitoring.

"Our next step is to predict and synthesize new probes for other, different PFAS chemicals and show how this can be scaled up," says Chen. "From there, there are many possibilities about what else we can sense with this same approach— everything from chemicals in drinking water to antibiotics and viruses in wastewater."

The end result may eventually be that consumers can test their own water and make better choices about their environment and what they consume.

More information: Reversible parts-per-trillion-level detection of perfluorooctane sulfonic acid in tap water using field-effect transistor sensors, *Nature Water* (2025). DOI: 10.1038/s44221-025-00505-9.

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