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This issue introduces Associate Professor Yuya Oaki, a scientist who enjoys chemically designing materials and finding useful functions for them in the world.

The pursuit for functional and soft 2D material structures

Having curiosity making new things and new ways to use them.

The term "applied chemistry" refers to the science of manipulating atoms and molecules to create substances that are useful in everyday life. There are endless possibilities for potential creations and their functions.
Associate Professor Oaki of the Department of Applied Chemistry focuses specifically on and finds joy in crafting "soft two-dimensional materials."
He says that they hold the possibility for "unexpected discoveries."

The blackened sample bottle "eureka" moment

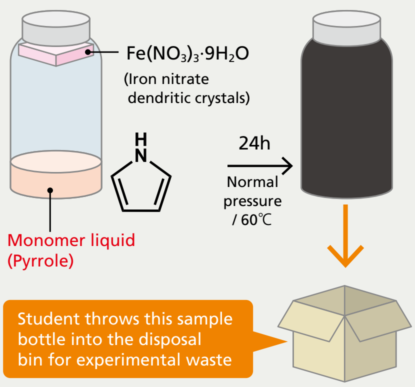
Throughout the research world, unexpected discoveries are often described as "serendipitous." Chemistry is no exception, with results from failed experiments sometimes leading to unexpected findings and useful data. Oaki of the Department of Applied Chemistry showed us a blackened sample bottle (Fig. 1, left) he says led to an "unexpected discovery" 10 years prior, explaining "I have been doing research for about 20 years, and have had an experience that I could call serendipitous on two occasions."

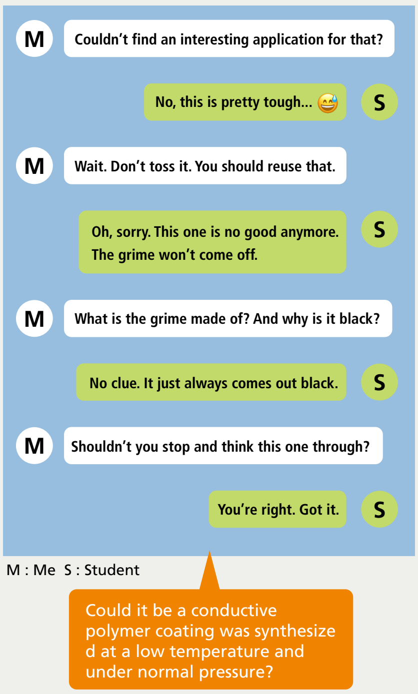
In university laboratories, students conduct research under the guidance of faculty members such as professors and associate professors. The faculty and students discuss and decide the direction and method of research together, but it is the students who carry out the experiments. Oaki likes to communicate with (or something like that...) how his students conduct their experiments and the results of their collected samples and then engage students in discussion. On one particular occasion, his attention was drawn by a student who was conducting an experiment to coat the surface of a dendritic crystal of iron nitrate with a conductive polymer in order to apply it to an electrical circuit. The student, thinking he had failed in his attempt, proceeded to dump the blackened sample bottle into the disposal bin for experimental waste.

"I instructed the student to reuse the bottle, given that normal grime can be removed from glass when washed. The student replied that it wouldn't come off," Oaki recalls. "I knew intuitively that something interesting was afoot as a coating on a glass bottle so black, even, and strong, should not have been produced by the planned experiment."

Following his instincts, he examined the black substance. The polypyrrole film they expected to form on the crystal surface of the iron nitrate had also adhered to the entire inner wall of the bottle. "Polypyrrole, which is a series of pyrroles (see the figure), is a 'conjugated polymer' in which double bonds and single bonds are alternately linked. They are incapable of mixing with solvent due to their rigid chemical structure. In other words, it should not be possible for them to form a paint-like coating. This means that while many conjugated polymers are highly functional in terms of conductivity, heat resistance, and redox activity, applying the substance can prove quite a challenge.

However, this failed experiment showed that conjugated polymers could easily be coated on various substrates and substrate surfaces," Oaki explained, emphasizing that the black sample bottle was a discovery, not a failure.





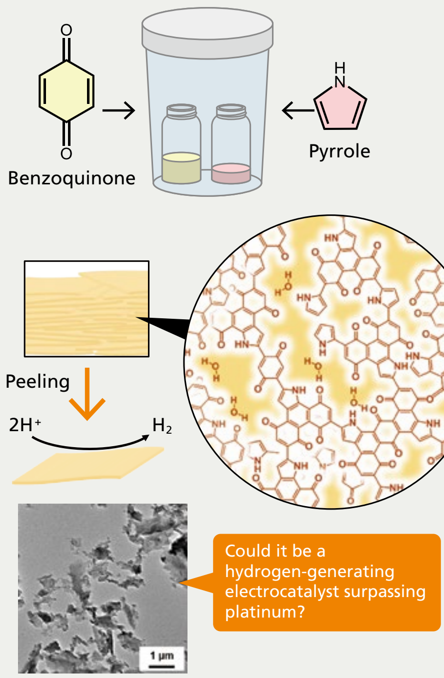
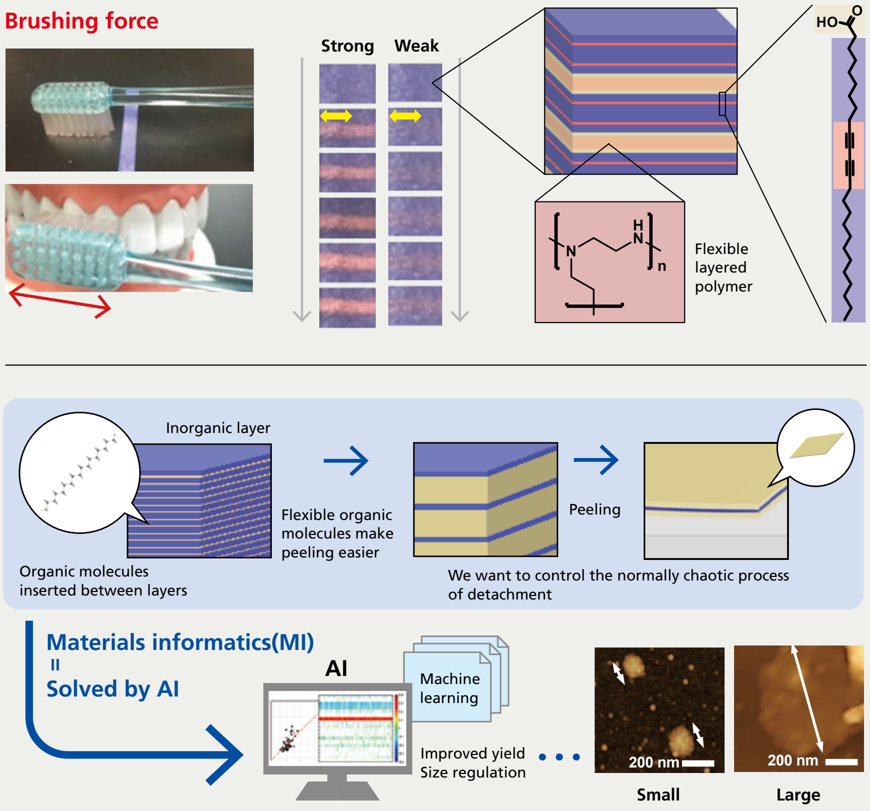


Fig.1 Two serendipities
Left side, middle: Reproduction of interaction with student at the time of the first "unexpected discovery," which is used when giving lectures on the topic. The student attached iron nitrate crystals to the lid of the sample bottle, added the monomer liquid which serves as the base of the coating, and closed the lid. It was thought that when this was allowed to stand at 60°C, the monomer liquid would evaporate and a polypyrrole coating would form solely on the surface of the iron nitrate crystals. In reality, the monomer vapor reacted with the iron nitrate, filling the bottle and creating a solid coating. Right: The second "unexpected discovery." A network structure is formed from a reaction between pyrrole with benzoquinone (middle). This could be easily delaminated (photo), and the produced nanosheets had the property of acting as a hydrogen-generating electrocatalyst.

Fig.2 Example of soft 2D material for which research and development is in progress

Above: Sensor material using layered polydiacetylenes that creates a visual of brushing force.

Bottom: Material development using "materials informatics (MI)" into his research since 2016 (Fig. 2, bottom). Artificial intelligence is used to work out factors (e.g., the properties required of a solvent used for dispersion) that are important for achieving a goal (in this case, wanting to control the exfoliation process).



A large step toward the development of a catalyst for hydrogen evolution reaction

The "coatability" of polypyrrole film is not the only factor to its viability; its quality also comes into question. At first the film was not sufficiently conductive to be used, but this problem was solved by changing the strength of the oxidant (a benzoquinone derivative) combined with pyrrole during its formation. "With that I thought that my research had reached its ending point, until one of my students said that they would attempt to synthesize the film by means of combining pyrrole and benzoquinone without substituents. Drawing from my own chemical knowledge, I warned the student that the reaction would not be feasible due to insufficient oxidizing power, but they proceeded with experiment anyway," Oaki remembers.

Their effort succeeded, resulting in the creation of a new polymer material consisting of a loosely stacked random network formed of pyrrole and benzoquinone (Fig. 1, right). Not only was it easily peeled off to produce thin nanosheets, but it was also found that the nanosheets function as a catalyst to electrochemically convert protons (H^+) into hydrogen (H_2). At present, hydrogen is of interest to researchers because it is an energy source that does not generate carbon dioxide. However, in general, since hydrogen production requires a platinum catalyst, there are inevitable cost and resource complications. This nanosheet has received a large amount of interest because it may present a possible alternative as a metal-free organic compound.

While Oaki claims that these two incidents were serendipitous, the story hints at Oaki's deep insight, chemical expertise, attentive ear when interacting with students, and ability to ignore "common sense" when pursuing an interesting lead that was necessary to capitalize on the fortunate turn of events.

Soft 2D materials are fascinating!

This is how Oaki's research focusing on conjugated polymers began. His methodology is to give flexibility (molecular mobility) to generally rigid conjugated polymers by various chemical methods, creating two-dimensional materials such as layered structures and nanosheets, and then explore their functionalities. Oaki's mindset is that "it is important to first enjoy creating substances; figuring out the new material's specific characteristics comes later." In the aforementioned case of a two-dimensional material made from polypyrrole and benzoquinone, "creating" was the important part of the process—its ability to catalyze hydrogen was a coincidental byproduct.

Oaki is also developing sensor materials that quantitatively detect heat, light, and force (Fig. 2, top) using a similar research methodology. When the diacetylene molecules arranged in layers are irradiated with ultraviolet light, the triple bond moieties polymerize with each other and turn blue. When this polydiacetylene is stimulated with heat, force, light, etc., the molecular chain is twisted and other subtle changes occur in the structure, causing the color to change. By manipulating what guest ions and molecules are inserted between the layers, scientists can adjust the material's responsiveness to external stimuli.

One of the materials developed using this process changes color depending on the frictional force created when brushing teeth. This then can be used to create a sensor that can gauge, based on color, an appropriate level of strength when using a toothbrush.

A new perspective on material development using artificial intelligence

Oaki due to his enjoyment of making new materials, has been incorporating "materials informatics (MI)" into his research since 2016 (Fig. 2, bottom). MI is said to accelerate research and development by utilizing informatics for material research. Specifically, he feeds the artificial intelligence a large amount of data about materials, and tasks it with finding possible factors necessary to discover new substances and improve their performance. However, in many cases, it is difficult to interpret exactly what the AI has done after processing the data.

Oaki is trying to prevent his AI from becoming a "black box" (an AI system that gives no view of its inner workings) by judging whether the computer-generated factors are important or correct based on his own chemical knowledge. "It is important for researchers to know when to take the lead," he says, "But artificial intelligence can also accomplish a large number of tasks, so it is our job is to make good use of it."

I am looking forward to the next "unexpected discovery," and how AI innovation will aid in sharpening Oaki's insight.

(Interview and text writer: Akiko Ikeda)