UCD Impact Case Study

Getting up close with chemistry – new perspectives on life's interactions

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SCIENTIFIC · HEALTH · TECHNO-LOGICAL · ACADEMIC · ECONOMIC

SUMMARY

Water is the most abundant molecule in the known Universe and it is vital for life, yet we understand precious little about it.

Associate Professor Aoife Gowen is changing that thanks to her expertise in a branch of science called hyperspectral imaging, which looks at minute changes within molecules as they interact.

Her current project, which secured prestigious European Research Council funding, is examining how water interacts with surfaces and how that can affect important processes such as the breakdown over time of materials grafted into the body to repair bone.

She is also applying her expertise to help improve the diagnosis of prostate cancer in patient samples and to monitor the growth of bacteria on surfaces.

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Research to 'see' chemistry

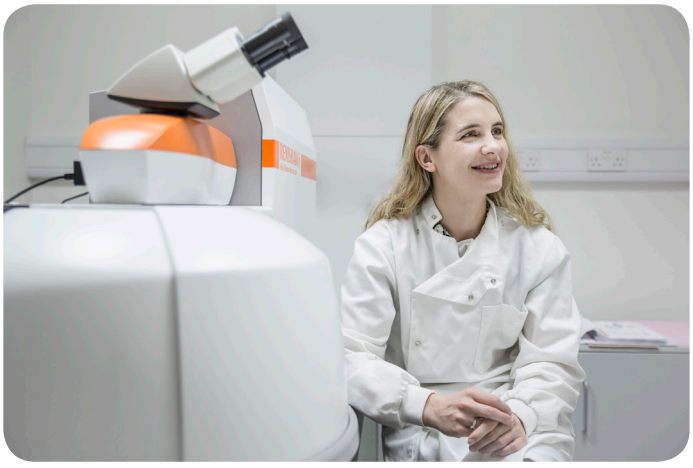
Much of what drives life forward happens without us seeing it. Unaided, our eyes have no way of registering the billions of chemical interactions that make things happen in our bodies, in our food and in our environment but which shape our health.

What if we could get a closer look at those all-important interactions? It's a tall order, but Associate Professor Aoife Gowen is on the case.

Associate Professor Gowen, of the UCD School of Biosystems & Food Engineering is an expert in the field of hyperspectral imaging, a technique that captures images of objects and extracts information about wavelengths from each pixel. The results can give insights into the 'unseen' properties and chemistry of the object.

"I'm particularly interested in what we can learn about water by using hyperspectral imaging," said Associate Professor Gowen. "Because even though water is a really familiar substance, there's a lot we don't know yet about how it changes chemically when it interacts with other molecules"

Knowing more about the tiny but important chemical changes in water could tell us more about how processes in living systems work and also how living systems interact with surfaces.



Associate Professor Gowen's current research, which is funded by the European Research Council, is using hyperspectral imaging to probe the interactions between water and silicon (a relatively simple material) and between water and materials used to artificially repair damaged bones in the body. She is also applying her knowledge of chemical imaging to several other problems in medicine and food monitoring.

Benefits for medicine and food safety

Opening new views on the 'invisible' chemistry of water and other molecules will build our understanding of how that chemistry works, and deliver new insights into events that may have previously been unreachable.

Associate Professor Gowen **secured prestigious European Research Council funding** to carry out her fundamental research on hyperspectral imaging of water and surface interactions. The nature of ERC grants is that they support excellent basic research that has potentially large benefits for society. Her lab's work to observe the chemical changes in water as it interacts with surfaces will have many applications.

One aspect of the project is looking at how water interacts with cement materials that are used to make bone repair grafts. Bone grafts are surprisingly common: after blood, bone is the second-most transplanted tissue, and the market for bone graft substitutes is expected to grow to the region of 3 billion Euro by 2022. The longevity of these grafts, or the length of time that they can maintain their structure in the body, is an important and practical factor for their use.

By analysing how water interacts with these materials under a range of conditions, Associate Professor Gowen's work will help **to inform the development of future materials that can be implanted into the body** and can 'weather' the environment while continuing to maintain their structure and function.

She is also using her expertise in another type of chemical imaging – Raman spectroscopy - to devise new ways for computers to 'see' information in patient samples and **help doctors as they search for signs of disease.**

Associate Professor Gowen is currently working with colleagues on a Health Research Board-funded project to analyse samples from patients with prostate cancer. "Computers will not replace a doctor's expertise, but by being able to scan lots of samples automatically it makes use of the computer's ability to crunch large datasets and **help doctors to pinpoint important changes** in those samples," explains Associate Professor Gowen.

Her work could also revolutionise monitoring in the food industry. She is leading a project funded by Science Foundation Ireland to explore hyperspectral imaging of bacteria on surfaces. This could ultimately lead to the development of **hand-held technology to chemically scan foods** for signs of spoilage or contamination.

Throughout her work, Associate Professor Gowen has needed to handle large datasets and mathematical models, and she has **developed computational tools** that are now used by other researchers and also in a commercial software package used for chemical analysis.

Associate Professor Gowen has **raised the profile of women in engineering** by taking part in public engagement and outreach projects. Her work was featured in the Science Apprentice book series for children aged 8-12 (distributed with the Irish Independent newspaper). Aoife was also selected as 1 of 8 Irish Scientists to have her portrait painted as part of the Women on Walls project. This project was run by Accenture and the Royal Irish Academy to increase the visibility of female researchers within STEM.

"What we do is very challenging, we are probing really tiny changes and interactions on one hand and we are dealing with massive amounts of data and computational science on the other," says Associate Professor Gowen. "But the challenge is there to be met and it will allow us to understand some fundamentally important chemistry that can have an impact on medicine, food and engineering design."

Research References

Gowen, A.A., Dorrepaal, R.M. (2016) Multivariate Chemical Image Fusion of Vibrational Spectroscopic Imaging Modalities. Molecules. 21(7), 870; doi:10.3390/molecules21070870

Burger, J., Gowen, A. (2015) 'Classification and Prediction Methods in Hyperspectral Imaging' In: Park, B (eds). Technology in Food and Agriculture. New York: Springer. DOI 10.1007/978-1-4939-2836-1

Achata, E., Esquerre, C., O'Donnell, C., Gowen, A. (2015) A study on the application of near infrared hyperspectral chemical imaging for monitoring moisture content and water activity in low moisture systems. Molecules. Feb 3;20(2):2611-21. doi: 10.3390/molecules20022611.

Gowen AA., Marini, F., Esquerre, C., O'Donnell, C., Downey, G., Burger, J. (2011) Time series hyperspectral chemical imaging data: challenges, solutions and applications. Analytica Chimica Acta Oct 31;705(1-2):272-82. doi: 10.1016/j.aca.2011.06.031.

Women on Walls: https://www.ucd.ie/biosystems/newsandevents/ucdsbfeassocprofaoifegowenfeaturedinwomenonwallscampaign/