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The IJMS Young Scientist Feature: A special article collection featuring perspectives and critical insights from early career mass spectrometrists around the globe

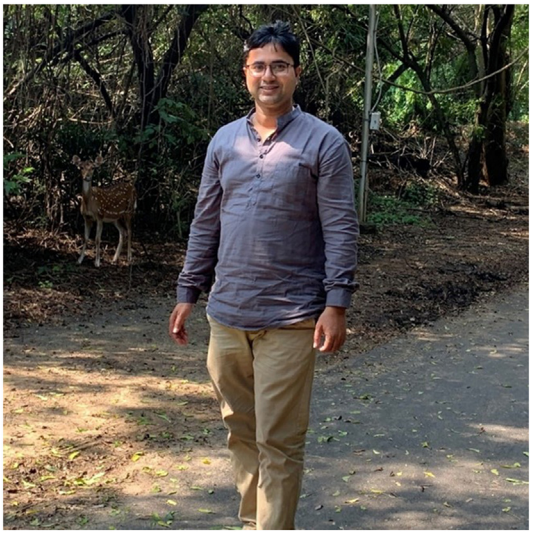
Continuing the tradition of celebrating the achievements of outstanding scientists in their early careers, we are excited to highlight two recent perspective articles in the Young Scientist Feature collection of the International Journal of Mass Spectrometry (IJMS) by Profs. Shibdas Banerjee (Indian Institute of Science Education and Research Tirupati) and Liang Qiao (Fudan University). The Young Scientist Feature promotes early career researchers by providing them with an opportunity to present their research accomplishments and highlight future perspectives in their respective areas of research.

Shibdas Banerjee received his Ph.D. in Chemical Sciences in 2014 from the Tata Institute of Fundamental Research in Mumbai, working with Prof. Shyamalava Mazumdar. His graduate research focused on studying gas-phase properties of analytes using electrospray ionization mass spectrometry and applications in protein engineering for cytochrome P450 biocatalysis. From 2014 to 2017, he was a postdoctoral researcher in Richard Zare's group at Stanford University, where he applied microdroplet-based mass spectrometry for clinical diagnostics (cancer and renal disorder) and for studying mechanisms of organic reactions. In 2017, he joined the Indian Institute of Science Education and Research Tirupati as an assistant professor and was promoted to associate professor in 2022. His group specializes in the real-time, *in-situ* analysis of chemical and biological transformations and discovery of disease biomarkers by correlating molecular and biological abnormalities.

Liang Qiao received his B.S. degree in Chemistry from Fudan University in 2006, M.S. degree in Chemistry from Fudan University in 2009, and Ph.D. degree in Chemistry from École Polytechnique Fédérale de Lausanne (EPFL) in 2013. He then continued as a Postdoctoral Research Associate with Prof. Hubert Girault at EPFL from 2013 to 2015. In 2015, he was appointed a professor in the Department of Chemistry at Fudan University. His current research interests mainly focus on proteomics, microbial mass spectrometry, coupling of microfluidics and mass spectrometry, metabolomics, and bioinformatics.

We asked Shibdas and Liang several questions about their research.

Shibdas Banerjee



Shibdas Banerjee, Associate Professor at the Indian Institute of Science Education and Research Tirupati.

What excites you the most about your research?

As a mass spectrometrist, I feel privileged to have the right tool or probably one of the most powerful analytical techniques in science that can solve the mystery of molecular transformations, be it in a living organism or a reaction vial. As mass spectrometry deals with atoms and molecules, the fundamental building blocks of all matters, I am much excited to solve problems in chemistry and biology relating to molecular makeup in elucidating the mechanisms of transformations, such as disease progression or a chemical reaction. Knowing how molecules change empowers chemists and

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biologists in various ways, including the development of novel methods for chemical and biochemical synthesis, fine-tuning of chemical and biological functions, development of therapies and diagnostics, harnessing renewable energy, combating climate change, etc.

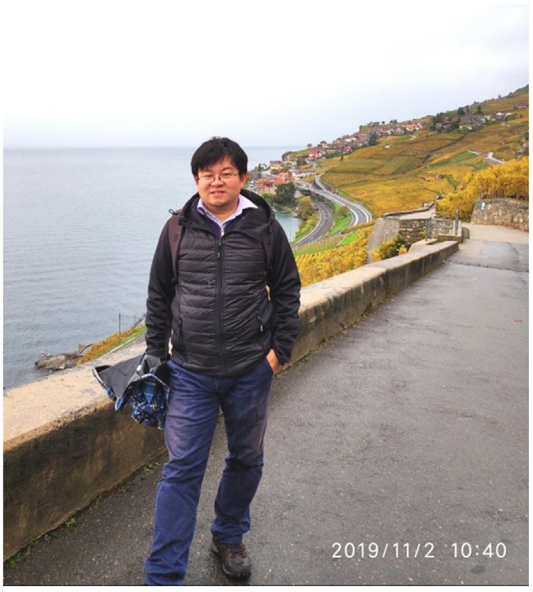
What do you consider the most interesting study that you performed in your independent career?

We have tamed water microdroplets to capture and stabilize reactive intermediate species, such as carbocations, carbanions, and protein unfolding intermediates, followed by detecting those using mass spectrometry. Often the lifetime of such species in the reaction medium is so fleeting that most spectroscopic techniques fail to detect those as the associated measurement timescale is longer than the lifetime of those transient intermediate species. We are now translating this success to harness the chemistry of such reactive species in aqueous microdroplets, especially for sustainable developments in organic synthesis in the aqueous medium. As we have found that water microdroplets promote unusual reactions at the air/water interface, we are also currently exploiting such interfacial reactions for developments in disease diagnostics.

What are the key challenges that must be addressed in your field moving forward?

We observed that the property of water changes, and it becomes a “wonder chemical” when it forms microdroplets. Understanding chemistry in microdroplets is still in its infancy. The chemical reactivity at the air/water interface is believed to be guided by the cumulative effect of multiple factors, such as partial solvation, confinement, alignment of reagents, the ultrahigh electric field in the interface, probable pH gradient, and high surface-to-volume ratio. Not necessarily all interfacial reactions have to experience these effects equally. Therefore, quantifying the role of each factor or revealing any other hitherto unknown properties of water microdroplets in this aspect is crucial to predict chemical reactivity at the interface accurately. I am pretty optimistic about the great future of microdroplet chemistry. It will likely play a dominant role in molecular/material synthesis, understanding of reaction mechanisms, disease diagnostics, disinfections, and environmental studies (and many more) in the future.

Liang Qiao



Liang Qiao, Professor in the Chemistry Department of Fudan University.

What excites you most about your research?

There are many exciting things in research: first discovery of a phenomenon, first publication in a top journal, first independent grant, graduation of the fist student, etc. Among all of these, I think the most exciting thing is to grow up with students and to learn with students. I have gained a lot of knowledge during my independent research. To guide students, I need to push myself to learn a lot. I like the feeling of acquiring knowledge and coming up with new ideas. Working with students always brings me passion and energy.

What do you consider the most interesting study that you performed in your independent career?

We use deep learning to analyze mass spectrometry data. From 2017, we started developing deep learning based MS/MS spectra prediction, retention time prediction, and detectability prediction for peptides, with which we achieved prediction-

based spectral library for data independent acquisition (DIA) proteomics analysis. More recently, we realized deep learning prediction-based protein PTMs analysis. It is amazing to see how a revolution in science and technology changes the state-of-the-art of a field. Before deep learning, scientists also worked on MS/MS prediction, but could hardly reach the performance of experiments. Now, in many fields deep learning can replace experiments, and specifically in proteomics deep learning has greatly boosted the data mining ability.

What are the key challenges in your field moving forward?

The key challenge is to remain competitive and generate new ideas. It is important to discuss with researchers in other fields, and to collaborate with others. Some of my best studies involve collaborations.

Julia Laskin*, Zheng Ouyang, Isabelle Fournier, Stephen Blanksby

* Corresponding author.
E-mail address: jlaskin@purdue.edu (J. Laskin).

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