Workshop 5 Wednesday, 19th September, 17:15-19:15 (Room B-1)

Path to Next-generation IMS: New Concepts, Advanced Instrumentation, and Leveraging the Ion-molecule Chemistry

Organizers: Toshiki Sugai (Toho Univ., Japan), Alexandre A Shvartsburg (PNNL, USA)

Over the last decade, IMS coupled to MS has grown into a mainstream analytical tool that now rapidly expands into diverse applications in proteomics, metabolomics, characterization of natural products, and industrial and environmental monitoring. In another major shift, differential or field asymmetric waveform IMS (FAIMS) that exploits the difference between ion mobilities at high and low fields has appeared as a broadly useful approach that is competitive and often superior to conventional IMS based on absolute mobilities at moderate fields. These trends have largely been due to introduction of conventional IMS/MS and FAIMS/MS systems by Waters, Thermo, and AB Sciex. On that trajectory, most high-end commercial MS instruments would in a few years include an (optional) IMS stage. This situation signifying successful integration of IMS into the repertoire of MS and thus analytical science, it is timely to think beyond the current paradigm to take IMS to the next level. Such emerging work will be the focus of our workshop.

The workshop will be appropriately opened by David Clemmer (Indiana Univ.) who had launched the transformation of IMS/MS from a niche physical chemistry technique of academic interest to a widely employed analytical method in 1990-s and forcefully pushed the frontier of this field since. His groundbreaking development of multistage IMS platforms and cyclotron IMS has enabled unprecedented resolving power that would be central to future IMS advances.

Since the invention in early 1990-s and until recently, conventional IMS (in both drift-tube IMS or DMA variants) employed static electric fields only. An innovative direction is use of dynamic fields, notably in the traveling-wave IMS implemented in the Synapt series. Here, Dr. Vidal de Miguel (SEADM) will present a novel IMS configuration employing orthogonal oscillatory and fixed fields. The first prototype already provides reasonable resolution in a compact footprint.

Next, Toshiki Sugai (Toho Univ.) will talk on the development of an ion trap/IMS system that enables one to monitor structural evolution of ions for hours. In particular, evaporation of water droplets and slow thermal deformation of polystyrene particles have been observed. Applications to nanomaterials and the new system with much higher resolving power will be discussed.

The quest for more specific ion separation and identification drives use of IMS to pre-separate isomers for various spectroscopic and chemical selectivity studies. Fuminori Misaizu (Tohoku Univ.) will lecture on the spectroscopy and reactions of isomer-selected clusters. His versatile apparatus coupling drift-tube IMS to ToF MS enables performing photodissociation, collision-induced dissociation, ion-molecule reactions, and negative-ion photoelectron spectroscopy for mobility-selected isomers, exemplified by carbon and silicon cluster cations and anions.

A major aspect of next-generation IMS will be buffer gases comprising vapors that interact with ions specifically rather than inert media that merely retards the ion motion. While such “shift reagents” have helped in some conventional IMS applications, they appear of most value for FAIMS where they generally expand both the overall peak capacity and resolution of targeted analytes. Utilization of vapor dopants is a key feature of the SelexION technology, and the latest highlights in this fast-evolving area will be communicated by Brad Schneider (AB Sciex).

The FAIMS resolving power scales roughly as the cube of field strength that was limited by electrical breakdown threshold. This constraint is essentially lifted in the FAIMS microchips by Owlstone, where fields up to 75 kV/cm permit ion filtering in <100 μs. Richard Yost (Univ. of Florida) will show first findings on the use of these chips with solvent vapors. While resolution gains resemble the effect in full-size FAIMS, the extreme fields in microchips cause intense ion heating that enables rich new chemistry leading to additional separation mechanisms.

A raising MS approach to structural elucidation of proteins and their complexes is chemical cross-linking, but enormous number and diversity of products greatly challenge their detection and identification. Separations by IMS have a major potential here, and Tara Pukala (Adelaide) will describe the use of novel negative-ion cleavable cross-linking reagents in this context.

Scope of Session: Ion mobility separations coupled to mass spectrometry have become a mainstream analytical tool, and both conventional IMS and FAIMS are available in commercial systems now applied in various areas. This workshop will look beyond established products and methods into qualitatively new approaches that would take IMS to the next level. Topics of presentations and discussion will include multi-stage platforms of much greater specificity and peak capacity, use of ion-molecule chemistry to expand the separation space and modify resolution of specific targets, and various integrative measurements incorporating the IMS dimension.