Contribution ID: **73** Type: **Invited talk**

Size-filtered Rotational Spectroscopy of Molecular Aggregates

Monday 15 September 2025 09:15 (45 minutes)

Rotational spectroscopy is a powerful technique for determining the precise three-dimensional structure of large and complex molecules. This method provides highly accurate data on molecular geometries and other key parameters. While recent advancements in spectrometer technology have boosted sensitivity and speed, they have also created a new challenge: interpreting the dense and intricate spectra that are now routinely generated.

To overcome these issues, we have developed new strategies to "disentangle" these complex spectra. One of the most effective approaches involves using cross-correlation techniques. By examining case studies, primarily focusing on clusters with water, we will demonstrate how these methods simplify the interpretation of complex spectra. These advancements broaden the application of rotational spectroscopy, allowing for deeper investigation into the structure, dynamics, and energy landscapes of molecular clusters and shedding new light on fundamental intermolecular forces.

Keywords

This abstract is submitted for....

HBond 2025 conference

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