Contribution ID : **22** Type : **Poster**

Development of a new open-source “4+ Angle Polarisation” QUASAR widget for orientation analysis of FTIR hyperspectral images

Determination of molecular orientation using linearly polarised Fourier transform infrared (p-FTIR) spectroscopy has been an established method for decades. However, the accuracy of the orientational information obtained when using the traditional approach based on an orthogonal pair of polarisation angles, relies largely on a good understanding of the orientation of molecules within the sample prior to analysis. Alternatively, the azimuth of the vibrational transition dipole moment can be determined for the vibrational mode specific to the measured sample. A relatively new method utilising 4 or more polarisation angles has been developed for determining the azimuth of the vibrational transition dipole moment of certain vibrational modes in the measured sample [1]. Whilst this 4-angle polarisation approach significantly reduces the necessity of prior knowledge, the calculations required are significantly more laborious and computationally intensive. To alleviate this burden and thus improve the accessibility of this method, a software tool to analyse p-FTIR data collected at 4 or more polarisation angles is introduced. This tool is implemented as a “widget” within the open-source spectroscopic data analysis package, QUASAR, which is built on the Python programming language. It requires minimal input from the user and implements parallel computations of the algorithm to produce simple and rapid results. An overview of the 4-angle polarisation method will be presented, along with the basic use of the new widget and examples of its applications in determining orientational information in polymeric materials , as well as fibres in biological tissue samples.

Reference:
[1] Hikima et al. Macromolecules, 44, 3950 (2011).

Level of Expertise

Student

Presenter Gender

Man

Pronouns

He/Him

Do you intend to attend UM2022

Unsure at this stage

Students Only - if available would you be interested in student travel funding

No

Students Only – Do you wish to take part in the Student Poster Slam

No

Terms and conditions (Please confirm that you have read all the requirements and agree to the conditions)

Yes

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Session Classification : Poster

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