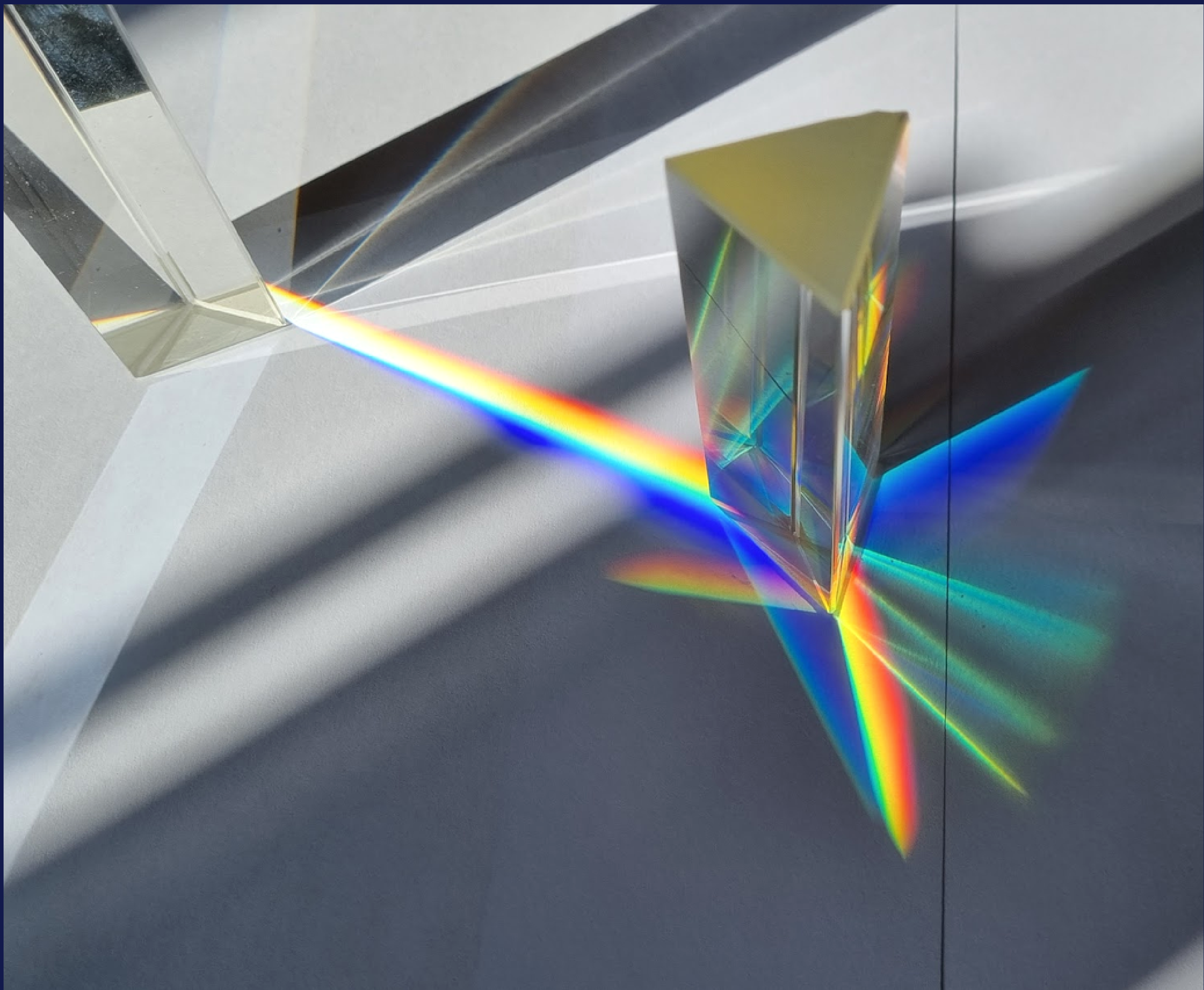
CHARISMA

Characterisation and Harmonisation for Industrial Standardisation of Advanced Materials



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CHARISMA In A Nutshell

CHARISMA aims to harmonise and standardise characterisation by Raman spectroscopy, including hardware, measurement protocols, and *in silico* methods, enabling end users to share digital spectral data through FAIR databases across domains and across the entire life cycle of diverse products. CHARISMA sets out to remove existing limitations on cross validation and data consistency, thus supporting fostering and implementing an open innovation environment in existing and developing industries through Raman spectroscopic characterisation techniques.

Why CHARISMA?

CHARISMA fundamentally focuses on the harmonisation of Raman spectroscopy for characterisation across the life cycle of a material, from product design and manufacture to lifetime performance and end-of-life stage. Thanks to its wide scope and topical agenda, the project will contribute to the *Industry Commons* concept and increase the marketability of materials with nanoscaled features engineered during the last decade. From microplastics control to pharmaceutic developments or security, it aims to respond to *Challenges of the Society*, too.

CHARISMA will have a strong impact in a number of different technological and scientific areas, including, but not limited to, producers of spectroscopy systems, industrial users of Raman spectroscopy, applications of Raman-active materials, and scientific research in physics, chemistry, materials science and biomedicine. Specifically, the project will demonstrate the feasibility of its concept in three industry cases in the areas of nanocatalysts, document security and active packaging for food.

Specific Objectives

Normalise the use of harmonised Raman spectroscopy

Develop and validate tools for Raman harmonisation, and make them accessible and useful for the NMBP and spectroscopy communities.

Develop models to harmonise Raman spectroscopy

Calculate the theoretical Raman responses to be used as reference for harmonisation. The simulated spectra, without measurement uncertainties, can be used to design standard reference materials for calibration, training of machine learning chemometric algorithms, or design of Raman-active products.

Harmonise Raman spectra

Provide calibration methods, acquisition protocols and harmonisation algorithms to make Raman spectra from different spectrometers quantitatively consistent and interoperable.

Harmonise Raman characterisation data

Generate an enhanced CHADA (**CHA**racterisation **DA**ta) structure that makes Raman data and chemometric models from different systems (spectrometers and samples) compatible through an algorithm.

Standardise Raman protocols

Generate pre-standards to harmonise Raman data acquisition and treatment protocols that contribute to data quality, traceability, and interoperability.

Demonstrate in industrial environments

Successfully implement the harmonisation strategy through representative case studies such as quality control in industrial production, authentication and traceability, and food safety monitoring. CHARISMA aspires to apply Raman characterisation systems adapted to IoT and delocalisation and to different stages of a product life cycle (design, manufacture, performance and end-of-use).

Generate a FAIR Raman data repository

Make Raman data **f**indable, **a**ccessible, **i**nteroperable and **r**eusable (fair) via websites or APIs with different levels of complexity, enabling distributed real-time characterisation of materials, processes and products.

Partners

Case Studies

SECURITY
Nanomarkers

Develop nanostructured tags with a digitalised code as tuneable Raman-active markers for documents (e.g. banknotes, passports, tickets, certificates) and goods (e.g. drug packaging, jewellery, paints, electronics) that can be monitored using IoT Raman equipment during their entire lifecycle for traceability.

FOOD
Active food packaging

Develop an active food packaging with a Raman fingerprint that can be correlated to the food quality to characterise the shelf life of food by in situ delocalised Raman measurements.

CHEMICAL INDUSTRY
Nanomaterial production

Develop a Raman-XRD correlation and a pilot testbed to control the synthesis of catalytic nanomaterials by real-time *in situ* Raman.

Harmonised Raman characterisation will be used for the development and evaluation of improved sustainability strategies in all relevant industries above.

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