Draft Project plan for the CEN Workshop on "Raman devices calibration, verification and twinning protocols"

Requests to participate in the Workshop and/or comments on the project plan are to be submitted by January 31st, 2024 to imoya@une.org[1]

Recipients of this project plan are kindly requested to name all patent rights known to them to be relevant to the Workshop and to make available all supporting documents.

November 30th, 2023 (Version 1)

[1] Applications for participating in the Workshop and comments on the project plan that are not received by the deadline do not need to be taken into consideration. Once constituted, the Workshop will decide whether or not to consider the comments received in good time.

Contents

Summary

Standardisation of Raman devices and Raman data spectroscopy is receiving strong interest in recent years due to the broad expansion in number and type of Raman devices and the need to assure data exchange and data consistency along devices and the across different units and sampling configurations.

Raman spectroscopy is very sensitive to the actual device configuration and physical characteristics of the spectrum acquisition. A bigger differentiation in device performance and the capability to reproduce data and transfer information between devices has been recognised by the users and institutions; for these reasons there is a raising interest to find ways to harmonise data sharing and protocols to calibrate and validate Raman devices.

1 Status of the project plan

Draft project plan for public commenting (Version 1.0)

This draft project plan is intended to inform the public of a new Workshop. Any interested party can take part in this Workshop and/or comment on this draft project plan. Please send any requests to participate or comments by e-mail to imoya@une.org.

All those who have applied for participation or have commented on the project plan by the deadline will be invited to the kick-off meeting of the Workshop on **<2024-02-28>**.

2 Workshop proposer and Workshop participants

2.1 Workshop proposer

Organisation	Short description and interest in the subject
CHARISMA	CHARISMA (Characterisation and HARmonisation for Industrial Standardisation of Advanced MAterials) is an European Union's Horizon 2020 research and innovation program funded project (grant agreement No. 952921) set to harmonise Raman Spectroscopy for characterisation across the life cycle of a material, from product design and manufacture to lifetime performance and end-of-life stage. CHARISMA is coordinated by CSIC (Spanish National Research Council). CSIC is the Spain's largest public research institution, generating 20% of the national scientific output, and ranks third among Europe's largest research organizations. CSIC is attached to the Spanish Ministry of Science and Innovation and plays a key role in scientific and technological policy in Spain and worldwide. ELODIZ Ltd will chair the WS and lead the CWA that originated the proposed work. ELODIZ is focused on the development of Raman spectroscopy instrumentation, offering knowledge solutions and distribution to a specialised line of products developed and manufactured in-house, reference materials, fibre coupled LED light sources and many other optoelectronics tools for spectroscopy users. An important part of its activity seeks the further development and spread of Raman spectroscopy through the harmonization of the different stages of the

	process. The outputs of this harmonization (validated in several round robins) are the base for the proposed work of the Workshop. CSIC will lead the second CWA proposed.

2.2 Other potential participants

This CWA will be developed in a Workshop (temporary body) that is open to any interested party. The participation of other experts would be helpful and is desired. It is recommended that:

- Industry companies
- Academic and research institutions
- Raman spectroscopy users

take part in the development of this CWA.

2.3 Participants at the kick-off meeting

The following persons or organisations are already expected to take part as Workshop participants at the kick-off meeting and to actively participate in the development of the CWA.

Person	**Organisation**
Workshop Chair Enrique LOZANO - Workshop Chair	ELODIZ LIMITED
Workshop secretariat Iván MOYA - Workshop secretariat	Spanish Association for Standardisation (UNE)
Miguel A. BANARES, Raquel PORTELA, Jose F. FERNÁNDEZ, María FERNÁNDEZ, Alberto MOURE	AGENCIA ESTATAL CONSEJOSUPERIOR DE INVESTIGACIONES CIENTIFICAS
Pablo BEATO	HALDOR TOPSOE AS
Julián REINOSA	ENCAPSULAE S.L
Vicente GARCIA JUEZ	FABRICA NACIONAL DE MONEDA Y TIMBRE-REAL CASA DE LA MONEDA
Afroditi NTZIOUNI	NATIONAL TECHNICAL UNIVERSITY OF ATHENS
Sara LIMBO	UNIVERSITA DEGLI STUDI DI MILANO
Mònica CALATAYUD	SORBONNE UNIVERSITE SU
Frederik TIELENS	VRIJE UNIVERSITEIT BRUSSEL
Dirk LELLINGER	FRAUNHOFER GESELLSCHAFT ZUR FOERDERUNG DER ANGEWANDTEN FORSCHUNG E.V.

James THOMSON	ELODIZ LIMITED
Nina JELIAZKOVA	IDEACONSULT LIMITED LIABILITY COMPANY
Yasemin ERTUGRUL	YORDAS GMBH
Hildegard LUHMANN	EUROPEAN RESEARCH SERVICES GMBH

2.4 Workshop secretariat

The Spanish Association for Standardisation (UNE) will hold the secretariat of the workshop.

3 Workshop objectives and scope

3.1 Background

Two CWAs are planned:

- CWA1: Raman devices calibration and verification protocols (lead by ELODIZ)

  This harmonisation protocol will focus on four parameters of the Raman instrument: x-axis positions, x-axis resolution, y-axis relative intensity. X-axis positioning is required for noting shift changes of materials, or successful identification. X-axis resolution is required for adjusting and comparing data between instruments of varying resolution. Y-axis relative intensity correction is required for comparing intensity ratios accurately and, particularly, visual laser instrument to NIR laser instruments, as the detectors have wildly different quantum efficiency profiles.

  The protocol has been developed by several studies utilising a wide range of Raman instrumentation with the collaboration of different companies. This data has allowed for an understanding of the range of variation that currently exists in Raman instrumentation, and how to correct for them. The harmonisation developed protocol is for post-acquisition calibration of the data with a goal to adapt it to make a version usable by manufacturers.

- CWA2: Raman device twinning protocol (lead by CSIC)

  This Raman twinning protocol will focus on using a reference sample to obtain a correction factor (CF) that accounts for the differences in the signal (intensity) between calibrated Raman devices to harmonize their Raman spectra. First the reference sample is measured to obtain raw Raman data at different laser powers for each Raman device. Data pre-processing is required for normalization and baseline removal of all Raman spectra. The correction factor is then calculated by power regression lines. Validation of Raman twinning is required for verifying that the CF allows obtaining harmonized Raman spectra.

  The Raman twinning protocol has been demonstrated for different sets of data/devices covering the most commons use cases: twinning non-confocal Raman devices of the same model for two different wavelengths and twinning confocal and non-confocal spectrometers.

3.2 Scope

- CWA1: Raman devices calibration and verification protocols

  The first planned CEN/CENELEC Workshop Agreement specifies a harmonization protocol for Raman devices that allows:

  - Recalibration of data or devices already calibrated by the manufacturer;
  - Calibration of devices without any previous calibration;
  - Verification of the calibration for devices that were calibrated with this protocol in the past;

The full protocol consists of the following stages that can be performed independently: x-axis positions, x-axis resolution and y-axis intensity correction.

The protocol is applicable to the Raman devices within certain specification and within defined boundaries that are described in the document.

- CWA2: Raman device twinning protocol

The second planned CEN/CENELEC Workshop Agreement provides a procedure for twinning Raman spectrometers to harmonize their spectra with a reference sample. This requires that the Raman device or the acquired reference sample data has already undergone a full calibration protocol on x and y axis prior to use for twinning.

This protocol will correlate different Raman devices to obtain similar intensities, improving comparability, reproducibility and reliability, thus promoting the use of this technique in different applications and industries.The protocol is applicable to Raman devices within certain specification and within defined boundaries that are described in the document.

3.3 Related activities

The subject of the planned CWA is not at present the subject of a standard and a specific standardization committee dedicated to this topic does not exist. However, there are committees, standards and/or other technical specifications that deal with related subjects and thus need to be considered during this Workshop:

- standardisation committees, working groups etc. and relevant standards or standard series:
  - IEC/TC 113 Nanotechnology for electrotechnical products and systems
    - IEC TS 62607-6-2:2023 Nanomanufacturing – Key control characteristics – Part 6-2: Graphene – Number of layers: atomic force microscopy, optical transmission, Raman spectroscopy
    - IEC TS 62607-6-6:2021 Nanomanufacturing – Key control characteristics – Part 6-6: Graphene – Strain uniformity: Raman spectroscopy
    - IEC TS 62607-6-11:2022 Nanomanufacturing – Key control characteristics – Part 6-11: Graphene – Defect density: Raman spectroscopy
    - IEC TS 62607-6-14:2020 Nanomanufacturing – Key control characteristics – Part 6-14: Graphene-based material – Defect level: Raman spectroscopy
  - CEN/TC 352 Nanotechnologies
  - ISO/TC 229 Nanotechnologies

- Other standards:
  - ASTM E1840-96 (2022) Standard Guide for Spectrometer Calibration and Validation of the Raman shift axis;
  - ASTM E2911-13 (2023) Standard Guide for Relative Intensity Correction of Raman Spectrometers;
  - ATSM E2529-06 (2022) Guide for testing Raman resolution with 785nm excitation;
  - ASTM E1683-02 (2022) Practice for testing the Performance of Scanning Raman Spectrometers.

4 Workshop programme

4.1 General

The kick-off meeting is planned to take place on 2024-02-28 online.

A total of two Workshop meetings (kick-off meeting and Workshop meeting) will be held, during which the content of the CWA(s) will be presented, discussed and approved.

The CWAs will be drawn up in English (language of meetings, minutes, etc.). The CWAs will be written in English.

4.2 Workshop schedule

Table 1: Workshop schedule (preliminary)

CEN/CENELEC Workshop	M01 DEC 23	M02 JAN 24	M03 FEB 24	M04 MAR 24	M05 APR 24	M06 MAY 24	M07 JUN 24	M08 JUL 24	M09 AGO 24	M10 SEP 24	M11 OCT 24
Initiation											
1. Proposal form and project plan submission and CCMC											
2. Open commenting period on draft project plan											
Operation											
4. Kick-off meeting											
5. CWA(s) development											
6. Open commenting period on draft CWA(s) (optional)											
7. CWA(s) finalised and approved by Workshop											
Publication											
8. CWA(s) publication											
Dissemination (see 7)											
Milestones			K		V				V/A	P	D

K Kick-off
M Workshop meeting
V Virtual Workshop meeting
A Adoption of CWA
P Publication of CWA
D Online distribution of CWA

5 Resource planning

Registration and participation at this CEN Workshop are free of charge, but each participant shall bear his/her own costs for travel, accommodation, and subsistence in the case of on-site meetings (at the moment of writing this document all meetings are planned to take place on-line).

The administrative costs of the CEN Workshop Secretariat will be financed within the framework of a research project: European Union's Horizon 2020 research and innovation program funded project CHARISMA (grant agreement No. 952921).

The copyright of the CWAs shall be with CEN. 8% secretariat costs will be provided by UNE to CCMC to cover the free download of the published CWAs.

6 Workshop structure and rules of cooperation

6.1 Participation in the Workshop

The Workshop will be constituted during the course of the kick-off meeting. By approving this project plan, the interested parties declare their willingness to participate in the Workshop and will be formally named as Workshop participants, with the associated rights and duties. Participants at the kick-off meeting who do not approve the project plan are not given the status of a Workshop participant and are thus excluded from further decisions made during the kick-off meeting and from any other decisions regarding the Workshop.

As a rule, the request to participate in the Workshop is closed once it is constituted. The current Workshop participants shall decide whether any additional members will be accepted or not.

Any new participant in the Workshop at a later date is decided on by the participants making up the Workshop at that time. It is particularly important to consider these aspects:

a. expansion would be conducive to shortening the duration of the Workshop or to avoiding or averting an impending delay in the planned duration of the Workshop;
b. the expansion would not result in the Workshop taking longer to complete;
c. the new Workshop participant would not address any new or complementary issues beyond the scope defined and approved in the project plan;
d. the new Workshop participant would bring complementary expertise into the Workshop to incorporate the latest scientific findings and state-of-the-art knowledge;
e. the new Workshop participant would actively participate in the drafting of the manuscript by submitting concrete, not abstract, proposals and contributions;
f. the new Workshop participant would ensure wider application of the CWA.

All Workshop participants who voted for the publication of the CWA or its draft will be named as authors in the European Foreword, including the organisations which they represent. All Workshop participants who voted against the publication of the CWA, or who have abstained, will not be named in the European Foreword.

6.2 Workshop responsibilities

The Workshop Chair is responsible for content management and any decision-making and voting procedures. The Workshop Chair is supported by the Workshop Vice-Chair (if exists) and the responsible Workshop secretariat, whereby the Workshop secretariat will always remain neutral regarding the content of the CWA(s). Furthermore, the Workshop secretariat shall ensure that CEN-CENELEC's rules of procedure, rules of presentation, and the principles governing the publication of CWA(s) have been observed. Should a Workshop Chair no longer be able to carry out her/his duties, the Workshop secretariat shall initiate the election of a new Workshop Chair. The list below covers the main tasks of the Workshop Chair. It is not intended to be exhaustive.

- Content related contact point for the Workshop
- Presides at Workshop meetings
- Ensures that the development of the CWA respects the principles and content of the adopted project plan
- Manages the consensus building process, decides when the Workshop participants have reached agreement on the final CWA, on the basis of the comments received
- Ensures due information exchange with the Workshop secretariat
- Represents the Workshop and its results to exterior

The Workshop secretariat, provided by a CEN/CENELEC national member, is responsible for organising and leading the kick-off meeting, in consultation with the Workshop proposer. Further Workshop meetings and/or web conferences shall be organised by the Workshop secretariat in consultation with the Workshop Chair. The list below covers the main tasks of the Workshop secretariat. It is not intended to be exhaustive.

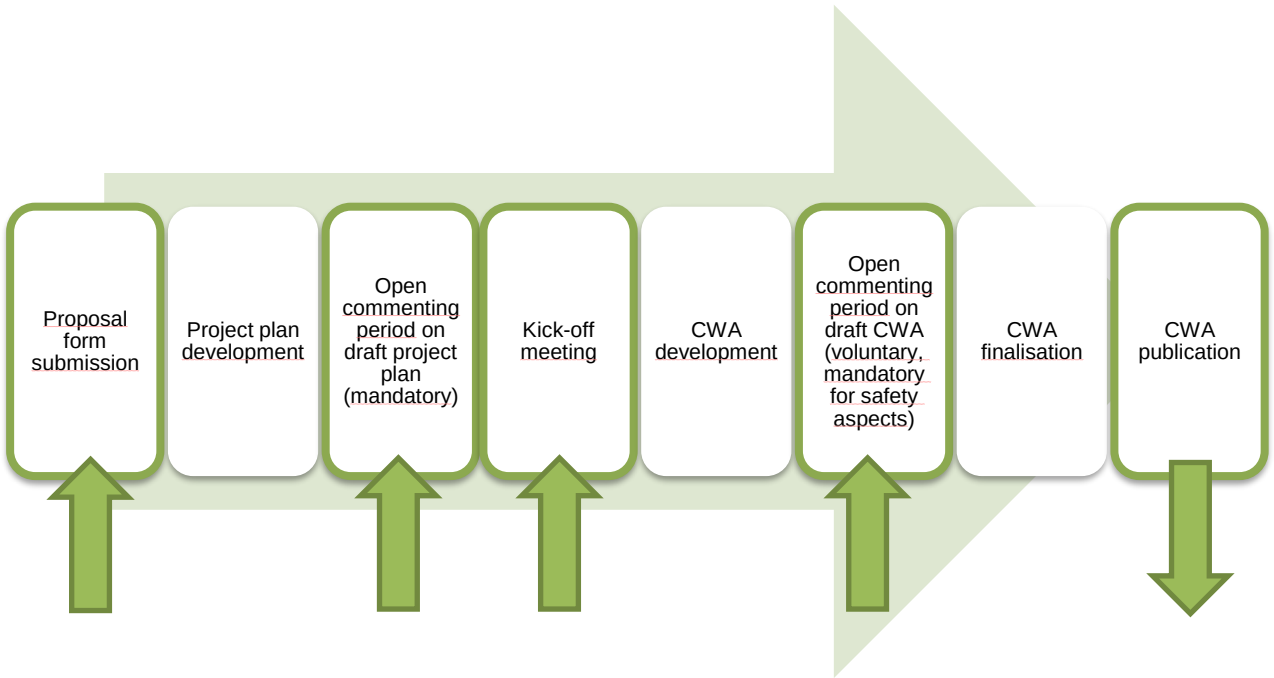
- Administrative and organisational contact point for the Workshop
- Ensures that the development of the CWA respects the principles and content of the adopted project plan and of the requirements of the CEN-CENELEC Guide 29
- Formally registers Workshop participants and maintains record of participating organisations and individuals
- Offers infrastructure and manage documents and their distribution through an electronic platform
- Prepares agenda and distribute information on meetings and meeting minutes as well as follow-up actions of the Workshop
- Initiates and manage CWA approval process upon decision by the Workshop Chair
- Interface with CEN-CENELEC Management Centre (CCMC) and Workshop Chair regarding strategic directions, problems arising, and external relationships
- Advises on CEN-CENELEC rules and bring any major problems encountered (if any) in the development of the CWA to the attention of CEN-CENELEC Management Centre (CCMC)
- Administrates the connection with relevant CEN or CENELEC/TCs

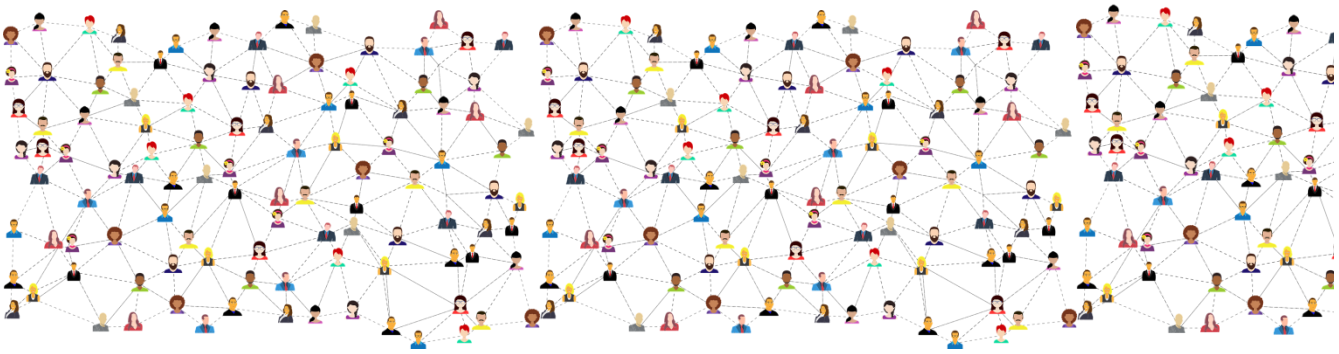
6.3 Decision making process

Each Workshop participant is entitled to vote and has one vote. If an organisation sends several experts to the Workshop, that organisation has only one vote, regardless of how many Workshop participants it sends. Transferring voting rights to other Workshop participants is not permitted. During voting procedures, decisions are passed by simple majority; abstentions do not count.

If Workshop participants cannot be present in the meetings when the CWA or its draft is adopted, an alternative means of including them in the voting procedure shall be used.

7 Dissemination and participation strategy





Dissemination of the announcement of the draft project plan and the date of the KOM

The announcement of the draft project plan and the date of the KOM will be disseminated to the following relevant stakeholders and bodies and will be invited to participate in the Workshop:

- standards committee, working group etc.
  - IEC/TC 113 Nanotechnology for electrotechnical products and systems
  - CEN/TC 352 Nanotechnologies
  - ISO/TC 229 Nanotechnologies
- R&I projects
  - NanoMECommons
  - CUSP cluster
- Raman communities
  - Raman metrology group (includes representatives from International Raman Metrology Team and VAMAS Technical Working Area (TWA) on Raman Spectroscopy and Microscopy)
  - Microplastics Standardization (VAMAS TWA 45)
- Manufacturers
  - BWTek
  - Wasatch Photonics
  - Avantes
- Scientists
  - To be identified

Open commenting period on draft CWA

The draft CWA will be disseminated to the following relevant stakeholders and bodies for commenting:

- standards committee, working group etc.
  - IEC/TC 113 Nanotechnology for electrotechnical products and systems
  - CEN/TC 352 Nanotechnologies
  - ISO/TC 229 Nanotechnologies
- R&I projects
  - NanoMECommons
  - CUSP cluster
- Raman communities
  - Raman metrology group (includes representatives from International Raman Metrology Team and VAMAS Technical Working Area (TWA) on Raman Spectroscopy and Microscopy)
  - Microplastics Standardization (VAMAS TWA 45)
- Manufacturers
  - BWTek
  - Wasatch Photonics
  - Avantes
- Scientists
  - To be identified

In addition to the CCMC website, the draft CWA will be advertised on CHARISMA web site (https://www.h2020charisma.eu/) and social media to raise awareness. Interested parties are requested to contribute through commenting of the draft CWA (short term).

CWA publication

The final CWA will be disseminated to the following relevant stakeholders and bodies:

- Standards committee, working group etc.
  - IEC/TC 113 Nanotechnology for electrotechnical products and systems
  - CEN/TC 352 Nanotechnologies
  - ISO/TC 229 Nanotechnologies
- R&I projects
  - NanoMECommons
  - CUSP cluster
- Raman communities
  - Raman metrology group (includes representatives from International Raman Metrology Team and VAMAS Technical Working Area (TWA) on Raman Spectroscopy and Microscopy)
  - Microplastics Standardization (VAMAS TWA 45)
- Manufacturers
  - BWTek
  - Wasatch Photonics
  - Avantes
- Scientists
  - To be identified

In addition to the CCMC website, the final CWA will be advertised on CHARISMA web site (https://www.h2020charisma.eu/)

- social media, such as
  - LinkedIn
  - Twitter/X

8 Contacts

- Workshop Chair:

Dr Enrique Lozano Diz
ELODIZ Ltd
Unit 29, Riverside Business Centre, Victoria Street, High Wycombe, Buckinghamshire, HP11 2LT, UK
+44 (0) 1494 708 810
enriquel@elodiz.com
https://www.elodiz.com/

- Workshop Secretariat:

Iván Moya Alcón
UNE, Spanish Association for Standardization
Génova 6, Madrid, Spain
(+34) 915 294 900
imoya@une.org
https://www.une.org//

- CEN-CENELEC Management Centre

<name>
CCMC
Rue de la Science 23
B - 1040 Brussels, Belgium
+32 2550xxxx
+32 2550xxxx
<e-mail>
https://www.cencenelec.eu/Pages/default.aspx

- Workshop proposer

Dr Raquel Portela
CSIC Agencia Estatal Consejo Superior de Investigaciones Científicas, CSIC (Spanish National Research Council)

c/ Marie Curie, nº 2. Lab T4
E-28049, Cantoblanco, Madrid (Spain)
Phone: +34 915854873
raquel.portela@csic.es
www.csic.es