2024

# WaPoDe

Water pollutants detection by ZnO-modified electrochemical sensors:
From computational modeling via electrochemical testing to real
system application

| HISTORY OF CHANGES | | |
|---|---|---|
| Version | Publication date | Changes |
| 1.0 | 2024-05-16 | Initial version |
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## Document status sheet

| PROJECT | |
|---|---|
| Funder | Science Fund of the Republic of Serbia |
| Program name | PRISMA 2023 |
| Project title | Water pollutants detection by ZnO-modified electrochemical sensors: From computational modeling via electrochemical testing to real system application |
| Project acronym | WaPoDe |
| Grant number | 7377 |
| Project start date | 2023-12-01 |
| Project end date | 2026-11-30 |
| Participating Scientific and Research Organization (SRO) | Institute of Technical Sciences of SASA (ITS SASA)<br>Vinča Institute of Nuclear Sciences; University of Belgrade (VINS)<br>Faculty of Physical Chemistry; University of Belgrade (FFHUB)<br>Faculty of Engineering Management; University Union – "Nikola Tesla" (FIM UNION) |
| Principal Investigator | Smilja Marković (ITS SASA) |
| Project web-site | www.wapode.rs |

**Document status sheet**

| DELIVERABLE | |
|---|---|
| Deliverable title | D7.3 - Data Management Plan |
| Brief description | The Data Management Plan describes what data the WaPoDe project will generate, and how the data will be handled during and after the project. |
| Work package number | 7 - Project management |
| Deliverable due date | 2024-05-31 |
| Responsible person | Ana Umićević |
| Contact | umicev@vin.bg.ac.rs |
| Comments | Will be updated regularly and when major changes occur. |
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| Reviewed by | Smilja Marković, Jelena Belošević-Čavor, Ana Umićević, Vladimir Tomašević |
| Approved by | Smilja Marković |
| Dissemination level | Public use. |
| License | CC-BY |

# Table of Contents

## 1. Executive Summary

This document describes the initial version of the Data Management Plan (DMP) for the WaPoDe project. The overall objective of the WaPoDe project is to synthetize materials with enhanced sensitivity, selectivity, and response time as electrochemical sensors (ECS) for detection and monitoring of different pharmaceutical and pesticide pollutants in water and to reduce ECS manufacturing costs. The focus of the WaPoDe project is on ZnO-based electrochemical sensors. The database will be developed under the WaPoDe project with the main purpose to summarize the WaPoDe research results on the types, properties, and application of ZnO-based nanoparticles as selective ECS.

This initial DMP provides information on the data management principles that will be implemented during and for a certain period after the WaPoDe project completion. It is based on the Data Management Plan template ([https://enspire.science/wp-content/uploads/2021/09/Horizon-Europe-Data-Management-Plan-Template.pdf](https://enspire.science/wp-content/uploads/2021/09/Horizon-Europe-Data-Management-Plan-Template.pdf)) which follows the guidelines from Europe Horizon calls. This DMP will be regularly updated as the implementation of the project progresses. The draft DMP was developed within the project work packages. Further development and updating of DMP will specify how project data and datasets that are generated will be curated and made findable, accessible, interoperable and re-usable (FAIR). Dr. Smilja Marković and Prof. Dr. Vladimir Tomašević will manage DMP and its revisions. Dr. Ana Umićević will be the person responsible for data management and protection in line with the FAIR principles, intellectual property rights (IPR) and data protection legislation, as well as for contact. This DMP version, as well as all revised versions will be publicly available.

## 2. Data Summary

In this section, it is explained which data and datasets are expected to be generated or re-used during the project, their types, origin, format and size. The WaPoDe project consists seven work packages (WPs). A re-evaluation of the generated data and datasets will be provided during the course of completion of each WP. The purpose of the project's data generation/re-use, relation to the project objectives and their utility to the project beneficiaries and third-parties is also stated.

**QUESTION**: Will you re-use any existing data and what will you re-use it for? State the reasons if re-use of any existing data has been considered but discarded.

The existing crystallographic data of the studied initial compounds are needed as a starting point for preparing input files for the calculations within WP3. These data are available scientific database Materials Project in open access under the Creative Commons Attribution 4.0 License.

Existing data, e.g. from collection of reference X-ray diffraction data from ICDD database; synthesis protocols from research articles as well as our own previously generated/collected data will be used in order to verify syntheses and characterization of ZnO-based nanoparticles in the WP1 and for their testing in the WP2. The licence of the existing crystallographic data will be taken into account when determining the licence of the resulting datasets.

The primary collected project data are raw data obtained by planned experimental and calculation methods. The new data and datasets that will be generated are in direct relation with the overall project objective on synthetizing enhanced ZnO-based electrochemical sensors for the detection and

monitoring of different pharmaceutical and pesticide pollutants in water with reduced manufacturing costs.

**QUESTION**: What types and formats of data will the project generate or re-use?

The Project will generate crystallographic and electronic structure data for different ZnO-based systems. The types of research data to be generated are experimental data and data calculated using commercial and free codes. Data will be collected directly through various characterization techniques (XRD, Raman, FESEM, TEM, BET, TG/TGA-DSC, FTIR, XPS, UV Vis DRS and PL spectroscopy) and appropriate experimental and computational methodologies with the participation and interaction of researchers in research organizations involved in the project. Where possible, the raw data of instrument and program specific format will be transformed, stored and distributed to users in open formats (e.g. TXT, PNG, or JPEG).

**Raw data generated by the project**

**Research data**

Folder and file names will only use allowed ASCII characters.

The primary collected project data are raw data obtained by planned experimental and calculation methods.

Raw data: naming convention

The file naming convention for the raw data generated by the WaPoDe project is dependent on the WPs:

WP1 naming convention:

Folders naming convention

Parent folder [Project Acronym]_[work package number] i.e. wapode_WP1

Subfolders naming convention

[Characterization Technique] e.g. XRD, FESEM, Raman, etc.

Files naming convention

[Project Acronym]_[Name of the characterization technique]_[Name of the sample]_[Author Acronym]_[Specific detail]_[Date YYYY-MM-DD].[extension]

e.g. WaPoDe_FTIR_ZnO_SM_2024-02-11.txt


WP2 naming convention:

Folders naming convention

Parent folder [Project Acronym]_[work package number] i.e. wapode_WP2


Subfolders naming convention

[Characterization Technique] e.g. CV, DPV, etc.

Files naming convention

[Project Acronym]_[Name of the characterization technique]_[Name of the sample]_[Author Acronym]_[Specific detail]_[Date YYYY-MM-DD].[extension]

e.g. WaPoDe_CV_ZnO_ISS_2024-02-11.txt


WP3 naming convention:

Due to the complexity of the planned calculations, there is no general naming convention for the WP3, but rather a tree of subfolders with naming convention logic explicitly related to the specific details of the calculation.


Parent folder naming convention

The parent folder for WP3 will be named "wapode_wp3".


Main folders within parent folder naming convention

The main folders will be named by "[Year]_[Semester]_[Semester number]".

For example, "2024_semester_1", "2024_semester_2", etc.


The folders within one of the main folders "[Year]_[Semester]_[Semester number]" will be named after the specific case related to the ZnO "[ZnO]_[Specific case]".

For example, ""ZnO_clean_surfaces", "ZnO_surface_10-10_vacancy_O", etc

Subfolders within one of the "[ZnO]_[Specific case]" folders naming convention

The subfolders within one particular "[ZnO]_[Specific case]" folder will be named after one more specific detail of the ZnO specific case being processed "[One_more specific_detail]".

For example, within "ZnO_clean_surfaces" folder, the subfolders will be named by the ZnO particular surfaces, for example "10-10", "11-20", etc.


Files naming convention

Files will be named by "[Code specific detail].[Specific case]" or "[Code specific detail].[Specific case].[extension]".

The VASP code specific files formats by default do not have extensions, but mostly they are ASCII (TXT) files. Where necessary, VASP code specific file formats will be transformed to ASCII files and therefore will have in addition "[extension]" in the file name.

WP5 naming convention:

Folders naming convention

Parent folder [Project Acronym]_[work package number] i.e. wapode_WP5

Subfolders naming convention

[Brief description] e.g. published papers, patent documentation, conferences abstracts, material for workshop, etc.

Files naming convention

[Project Acronym]_[Name of the activity]_[Number]_[Specific detail]_[Date YYYY-MM-DD].[extension]

e.g. Wapode_Paper_1_2024-05-01.odt


WP6 naming convention:

Folders naming convention

Parent folder [Project Acronym]_[work package number] i.e. wapode_WP6

Subfolders naming convention

[Brief description] e.g. list of stakeholders, reports from the meetings, material for stakeholders, etc.

Files naming convention

[Project Acronym]_[Name of the activity]_[Number]_[Specific detail]_[Date YYYY-MM-DD].[extension]

e.g. Wapode_Report_1_2024-02-22.pdf


WP7 naming convention:

Folders naming convention

Parent folder [Project Acronym]_[work package number] i.e. wapode_WP7

Subfolders naming convention

[Brief description] e.g. Administrative reports, Financial Reports, Data Management Plan, Final Report.

Files naming convention

[Project Acronym]_[Name of the activity]_[Number]_[Specific detail]_[Date YYYY-MM-DD].[extension]

e.g. Wapode_Administrative_Report_1_2024-05-31.pdf


Raw data: formats

Expected generated datasets will be named by [DS].[WP number].[Specific detail]

WP1: Laboratory and personal Notebooks, TXT, TIFF, JPEG, CSV.

Expected generated datasets within WP1 are:

- specific experimental characterization methods datasets:
  XRD dataset (TXT);
  Raman dataset (TXT);
  FESEM dataset (TIFF, JPEG);
  TEM dataset (TIFF, JPEG);
  BET dataset (JPEG, TXT);
  TG/TGA-DSC dataset (CSV, JPEG);
  FTIR dataset (CSV);
  XPS dataset (TXT, JPEG);
  UV-Vis DRS dataset (TXT, CSV);
  PL dataset (TXT).

WP2: Laboratory and personal Notebooks, TXT.

Expected generated experimental testing methods datasets within WP2 are:

- specific testing experimental methods datasets:
  amperometric/chronoamperometric dataset (TXT);
  linear sweep voltammetry (TXT),
  cycling voltammetry (TXT),
  square wave voltammetry (TXT),
  differential pulse voltammetry (TXT),
  stripping voltammetry (TXT);
  electrochemical impedance spectroscopy dataset (TXT);

WP3: code specific formats from density functional theory (DFT) calculations (VASP commercial code files formats are mostly ASCII type file).

Expected generated datasets within WP3 are:

- input files for DFT calculations (VASP-files formats which are ASCII type files)
- output files from DFT calculations (VASP-files formats which are mostly ASCII type files and where necessary VASP specific file formats will be transformed to TXT)

WP4:

Expected generated datasets within WP4 are:

- Metadata in the DAIS and Vinar institutional repositories that will be stored in the repository, exposed in the xml format via the OAI-PMH public endpoint under the CC0 1.0 Universal Public Domain Dedication licence (see Metadata describing a dataset in the repository provided by depositors / collection manager below).
- Archival Information Packages (including data files, readme files and the distribution licence) in the DAIS and Vinar institutional repositories that will be handled in line with the

preservation plan: https://repowiki.rcub.bg.ac.rs/index.php/DAIS_-_Digital_Archive_of_the_Serbian_Academy_of_Sciences_and_Arts:_Preservation_plan

WP5:

Expected generated datasets within WP5 are:

- accepted papers (DOCX, ODT)
- patent documentation (DOCX)
- conferences abstracts (DOCX, PDF)
- material for workshop (DOCX, PDF)

WP6:

Expected generated datasets within WP6 are:

- list of potential stakeholders (TXT)
- reports from the meetings with potential stakeholders (TXT, PDF)
- material for potential stakeholders (PDF)

WP7:

Expected generated datasets within WP7 are:

- project website (HTML)
- project administrative and financial reports (PDF),
- project scientific reports (PDF)
- project data management plan (PDF)

Research data will be described using rich metadata. To ensure the consistency of practices across partners, a shared table accessible to all project partners will be used to describe the raw data collected:

Metadata for raw data

| Field | Description | Status |
|---|---|---|
| Title | A descriptive title of the dataset | mandatory |
| Persons who obtained the data | The person(s) responsible for data creation (person performing analysis) | mandatory |
| Device | Devices used to obtain data (full name of the device and the manufacturer) | mandatory if applicable |
| Description | Description of the dataset<br>information about synthesis methods<br>information about analysis methods<br>any specific circumstances of data creation | mandatory |
| Content format | File format | mandatory |
| Content version | Version of the file | mandatory |
| Keywords | Free-style keywords | recommended |

| Institution | Name of the organization(s) or entities where the data were created | mandatory |
|---|---|---|
| Creation date | The date when the data were created Format: YYYY-MM-DD. | mandatory if applicable |
| Identifiers | If deposited data have been assigned a DOI in another repository, it will be mentioned. Otherwise, this field will be empty. | mandatory if applicable |
| Dataset contents | List of files in the dataset | mandatory |
| Location | Information about the physical location of the dataset (address, computer name, path; URL or PID in case it is stored on a cloud server) | mandatory |
| Backup status | Is the dataset backed up? | mandatory |
| Availability in the repository | Handle, DOI or other PID of the dataset in a repository. If it is available in multiple repositories, list all. | mandatory if applicable |
| Link to a different version of the resource | Handle, DOI, other PID of a different version of the dataset, in case such a version is available | mandatory if applicable |
| Link to related materials | Handle, DOI, other PID or URI of any publications, supplementary materials, research data related to the dataset | recommended |
| Access | Who has access to data (groups or individuals) | mandatory |
| License | The license under which the resource (data files) is or will be distributed. A Creative Commons license or All rights reserved. | mandatory |
| Note | Any annotation or comment | optional |

**QUESTION**: What is the purpose of the data generation or re-use and its relation to the objectives of the project?

The generated project data will be used to deepen the knowledge about the Project topic. The overall objective of the Project is to synthetize materials with enhanced sensitivity, selectivity and response time as electrochemical sensors (ECS) for detection and monitoring of different pharmaceutical and pesticide pollutants in water and to reduce ECS manufacturing costs. The research data generated within the synthesis protocols (WP1), testing protocols (WP2) and modelling (WP3) of surface modified ZnO nanoparticles, ZnO-based composites and heterojunction particles, are directly related to the main objective of the project to identify the best ECS ones for monitoring the specified pollutants in water and make it commercially available. The generated project data that will be curated within the WaPoDe database (WP4) are related directly to the others objectives of the project such as raising visibility of the research team and enabling collaboration with wider scientific community and stakeholders.

**QUESTION**: What is the expected size of the data that you intend to generate or re-use?

The original raw data occupy less than 10 MB per sample per technique and less than 20 MB per calculation specific case. Where possible, the raw data will be transformed, stored and distributed to users in ASCII, TXT, PNG or JPEG format. These storage formats will occupy in general no more than 3 MB and are accepted standards.

**QUESTION**: What is the origin/provenance of the data, either generated or re-used?

The Project will generate crystallographic and electronic structure data for different ZnO-based systems. The research data to be generated are experimental data and data calculated using commercial and free codes. Data will be collected directly through various experiments (XRD, Raman, FESEM, TEM, BET, TG/TGA-DSC, FTIR, XPS, UV Vis DRS and PL spectroscopy) and appropriate experimental and computational methodologies with the participation and interaction of researchers in research organizations involved in the project.

The project will generate research datasets: 10 specific experimental characterization methods datasets (XRD, Raman, FESEM, TEM, BET, TG/TGA-DSC, FTIR, XPS, UV-Vis DRS, PL); 7 specific testing experimental methods datasets (amperometric/chronoamperometric, linear sweep voltammetry, cycling voltammetry, square wave voltammetry, differential pulse voltammetry, stripping voltammetry, electrochemical impedance spectroscopy) and 2 code specific datasets (DFT calculations input and output files).

The project will also generate dissemination and management specific datasets: accepted papers, patent documentation, conferences abstracts, material for workshop, list of potential stakeholders, reports from the meetings with potential stakeholders, material for potential stakeholders, project website, project administrative and financial reports, project scientific reports, and project data management plan.

The project may potentially re-use some of the crystallographic data from Materials project database (https://next-gen.materialsproject.org/) and reference X-ray diffraction data from ICDD Database.

**QUESTION**: To whom might your data be useful ('data utility'), outside your project?

The generated project data will be curated within the project database which will include accumulated knowledge on the types, properties and application of ZnO-based ECS for detection of pharmaceutical and pesticide pollutants in water. Drawbacks and advantages of each case will be presented. The research data created might be useful to the WaPoDe team, scientific community, education and industry. The dissemination and management datasets might be useful to researchers, education, industry, public, decision makers and stakeholders involved in the field of water pollution.


## 3. FAIR Data


**Publishing data in the institutional repository and access to data**

The data underlying publications will be deposited in the institutional in the DAIS (Digital Archive of SASA) upon creation. Where appropriate, data will be made publicly available under an open licence after publication. Otherwise, data will be available upon request. Metadata will always be available, to ensure that potential users can locate data.

DAIS (Digital Archive of SASA) repository is a joint repository of the Serbian Academy of Sciences and Arts and its institutes. It is based on the DSpace open-source software. ITS SASA has a dedicated collection in this repository and is able to create and manage sub-collections. The repository is certified under CoreTrustSeal as a trusted digital repository and it enables compliance with FAIR principles. The repository enables sophisticated access control and ensures long-term preservation (https://repowiki.rcub.bg.ac.rs/index.php/DAIS_-_Digital_Archive_of_the_Serbian_Academy_of_Sciences_and_Arts:_Preservation_plan).

The repository also has a detailed security policy: https://repowiki.rcub.bg.ac.rs/index.php/DAIS_-_Digital_Archive_of_the_Serbian_Academy_of_Sciences_and_Arts:_Security

A dedicated sub-collection will be created for the project outputs, including data. A team responsible for data management will be established. A collection manager will be assigned and team members will be granted adequate privileges enabling them to deposit and curate data in the repository. All submissions will be reviewed by the collection manager to ensure metadata quality and completeness, the compliance of data formats, best practice and preservation requirements, data integrity and quality, and resolve potential legal issues. Once the deposit is approved, only authorized collection managers are able to change the metadata and data. Upon deposition and later, periodically, fixity checks (md5 checksums) are performed to verify that data files have not been altered or corrupted. Special attention will be paid to naming conventions for data files and data formats, making sure that formats suitable for long term preservation are used

(https://repowiki.rcub.bg.ac.rs/index.php/DAIS_-_Digital_Archive_of_the_Serbian_Academy_of_Sciences_and_Arts:_General_information#Preferred_file_formats).

The repository enables compliance with the FAIR principles (Findable, Accessible, Interoperable, Reusable)

**Findable**

Upon approval by a repository manager, deposited items are assigned unique persistent identifiers (PIDs) - handles. The repository supports the integration of ORCID identifiers for authors and contributors. Data are described with rich metadata that make it possible to locate data. Along with descriptive dataset titles, keywords, abstracts providing information about synthesis or analysis methods and parameters and information about devices used will be provided. For each dataset deposited in the repository a landing page displaying metadata is created. Metadata are also included in a README file, which contains the list of all files in the dataset. The unique PID resolves to the landing page and is included in the README file. The repository supports browsing and searching and exposes machine readable metadata (as HTML meta tags and coded in Dublin Core via the OAI-PMH protocol), making it easy for generalist search engines like Google and aggregators (OpenAIRE, BASE, CORE, EOSC Marketplace) to capture and index them.

**Accessible**

Metadata are openly accessible, without authentication, through the HTTPS protocol and displayed on the user interface. Metadata are also exposed via an open OAI-PMH protocol and are distributed under the CC0 license. Data in Open Access are available to users without authentication. Access to data files can be restricted and accessible to authorized groups of users after login into the system. The repository enables sophisticated access control. In line with the repository policy, metadata remain accessible even when data are no longer available. Standard procedures (request/feedback forms in the repository) are available for those who want to request access to data. More information about access can be found in the repository policy: https://repowiki.rcub.bg.ac.rs/index.php/DAIS_-_Digital_Archive_of_the_Serbian_Academy_of_Sciences_and_Arts:_General_information#Access_and_licences

**Interoperable**

Metadata conform to the Qualified Dublin Core Schema, which is a formal, accessible, and broadly applicable language for knowledge representation. The Dublin Core "Relation" metadata element is

used to show various types of relations between data, e.g. IsVersionOf, IsPartOf, HasPart, IsReferencedBy, IsReplacedBy, Replaces, IsRequiredBy, Requires, etc.), e.g. https://hdl.handle.net/21.15107/rcub_dais_14608.

**Reusable**

To enable proper reuse data are always released with clear conditions of use – license; license information is provided in metadata in a machine-readable format. If necessary, a new version of data can be deposited. Each version is assigned a unique PID and relations between versions are established in the metadata. Provenance information is saved for each dataset.

Metadata describing a dataset in the repository provided by depositors / collection manager

| Field | Description | Status | Dublin Core Mapping |
|---|---|---|---|
| Title | A descriptive title of the dataset | mandatory, repeatable | dc.title |
| Contributor | The person(s) responsible for data creation (person performing analysis) Device used to obtain data | mandatory if applicable, repeatable | dc.contributor |
| Description | Description of the dataset, including information about synthesis and analysis methods used and any specific circumstances of data creation. List of files in the dataset. | recommended, repeatable | dc.description.abstract |
| Content type | Dataset | mandatory, non-repeatable, controlled | dc.type |
| Content version | Version of the resource (draft, submitted, accepted, published, corrected), controlled, aligned with the DRIVER-version info:eu-repo version terms. vocabulary. | mandatory, non-repeatable, controlled | dc.type.version |
| Subject | Free-style keywords Subject controlled vocabularies are currently not implemented in the repository but users are encouraged to define keywords relying on controlled vocabularies relevant for their discipline. | recommended, repeatable | dc.subject |
| Institution | Name of the organization(s) or entities where the data were created | recommended, repeatable | dc.publisher |
| Creation date | The date when the data were created Format: YYYY-MM-DD. | mandatory if applicable, non-repeatable | dc.date.issued |
| Publication date | The year when the resource was published (deposited in the repository) Preferred format: YYYY | mandatory, non-repeatable | dc.date.issued |

| Field | Description | Status | Dublin Core Mapping |
|---|---|---|---|
| Embargo end date | This field is used when there is a plan to keep data files only temporarily closed. This is the date when the resource (data files) will be automatically made publicly available. | optional, non-repeatable | dc.date.available |
| Funding information | Sponsors and funding that supported the research. The project name and code will be mentioned in this field. | mandatory if applicable, repeatable | dc.relation |
| Identifiers | If deposited data have been assigned a DOI in another repository, it will be mentioned. Otherwise, this field will be empty. | mandatory if applicable, repeatable | dc.identifier.doi |
| Link to a different version of the resource | Handle, DOI, other PID of a different version of the dataset, in case such a version is available | recommended, repeatable | dc.relation.isversionof |
| Link to related materials | Handle, DOI, other PID or URI of any publications, supplementary materials, research data related to the dataset | recommended, repeatable | dc.relation.isreferencedby |
| Access level | The access to the resource in the repository; controlled values aligned with the info:eu-repo-Access-Terms vocabulary. | mandatory, non-repeatable | dc.rights |
| License | The license under which the resource (data files) is distributed. A Creative Commons license or All rights reserved should be selected from the drop-down list | mandatory, non-repeatable | dc.rights.license |
| Note | Information about any specific software or other technical requirements necessary to open and use the dataset. Any annotation or comment | optional, repeatable | dc.description.other |
| Copyright holder | The name of the person or entity holding the copyright. | optional, repeatable | dc.rights.holder |
| Content language | Language of the data | mandatory, repeatable, controlled | dc.language.iso |

Metadata created automatically when the submission is approved by the collection manager

| Field | Description | Status | DC mapping |
|---|---|---|---|
| Accession date | The date when the item is accessioned in the repository, in the format YYYY-MM-DD | mandatory, non-repeatable | dc.date.accessioned |
| Provenance and changes to the record | This field records an administrative event in the lifecycle of the item in the repository. The information is accessible to repository managers. | mandatory, repeatable | dc.description.provenance |
| URI | Permanent URL to the item landing page. It is displayed as an interactive link on the item page. | mandatory, non-repeatable | dc.identifier.uri |
| Handle - persistent identifier | Unique and persistent Handle URL to the item landing page | mandatory, non-repeatable | dc.identifier.rcub |
| Licence URI | URL to the licence website, generated automatically for Creative Commons licences based on the information provided in the field dc.rights.license, to ensure the machine readability of the licence information. In case all rights are reserved, the URL will not be generated. | mandatory if applicable, non-repeatable | dc.rights.uri |
| Format | File format | mandatory | Not mapped to DC |
| File size | In bytes, Kbyes, MB (automatically assigned) | mandatory | Not mapped to DC |

## 4. Other Research Outputs

QUESTION: In addition to the management of data, beneficiaries should also consider and plan for the management of other research outputs that may be generated or re-used throughout their projects. Such outputs can be either digital (e.g. software, workflows, protocols, models, etc.) or physical (e.g. new materials, antibodies, reagents, samples, etc.).

We will deposit the description of the synthesis protocols together with datasets in the repository to provide context and make it easy to interpret data. Physical outputs of the project, such as samples produced by the project, will be safely stored where possible at ITS SASA for at least 5 years after the completion of the project for validation and verification of the related project results.

QUESTION: Beneficiaries should consider which of the questions pertaining to FAIR data above, can apply to the management of other research outputs, and should strive to provide sufficient detail on

how their research outputs will be managed and shared, or made available for re-use, in line with the FAIR principles.

Other research products such as protocols and publications will be deposited in the dedicated collection in the repository along with research data and links will be established among them using a dedicated metadata field. The same procedures to ensure FAIRness will be applied as for research data.

## 5. Allocation of Resources

**QUESTION**: What will the costs be for making data or other research outputs FAIR in your project (e.g. direct and indirect costs related to storage, archiving, re-use, security, etc.)?

There will be no additional costs. We already have all necessary external hard disks for local back-up. The transformation of the specific code files formats to ASCII files suitable for long-term preservation will be done by the individual authors.

**QUESTION**: How will these be covered? Note that costs related to research data/output management are eligible as part of the Horizon Europe grant (if compliant with the Grant Agreement conditions)

The costs of data curation and preservation will be covered from the Institutional costs.

**QUESTION**: Who will be responsible for data management in your project?

Dr. Ana Umićević will be the person responsible for data management, protection and contact.

**QUESTION**: How will long term preservation be ensured? Discuss the necessary resources to accomplish this (costs and potential value, who decides and how, what data will be kept and for how long)?

The data will be long-term preserved in DAIS and VinaR trusted institutional repositories. The costs of data curation and preservation will be covered from the Institutional costs. Both repositories have long-term preservation policies.

A decision about what data will be kept and for how long will be brought by the authorized representatives of the partners: Dr. Smilja Marković and WPs leaders.

## 6. Data Security

**QUESTION**: What provisions are or will be in place for data security (including data recovery as well as secure storage/archiving and transfer of sensitive data)?

**Raw data: data security**

All team members (authors) will contribute to the raw data collecting and provision of the meta-data according to their expertise. Each individual team member (author) is responsible for the implementation of data management policy stated within this DMP and for the local storage of the raw data during the 5 years after the end of the project. Dr. Ana Umićević will be the person

responsible for data management, protection and contact. Dr. Ana Umićević will be responsible for back-up of the raw data across the partners SROs on the two external hard disk drives dedicated only for the project and the data and files exchange will be done on the weekly base through the Google platform and Google drive. The two external HDDs dedicated only for the project will be stored in two different SROs (VINS and FIM UNION) which will provide physical mode of security.

During the project, raw data will be stored on local computers and local personal USBs of the partner institutions, making sure that only the authorized representatives of the partners have access to data. ITS SASA will ensure data protection according to the 3-2-1 rule (at least three copies of data, stored on two different types of media, with one copy kept off-site): external hard drive, institutional backup server and an off-network computer in a secure room with CCTV monitoring.

The authors of the raw data and the authorized representatives of the partners (Dr. Smilja Marković and WPs leaders) will have access to the secondary copies of the raw data.

The Google Drive and pCloud storage will be used for data and file exchange.

The back-up of the raw data on the local personal USBs will be done weekly and each individual team member (author) is responsible for the back-up on the regular basis. Dr. Ana Umićević will be the person responsible for data management, protection and contact. Dr. Ana Umićević will be responsible for back-up of the raw data across the partners SROs on the two external HDDs dedicated only for the project and the data and files exchange will be done on the weekly base through the Google platform, Google drive and USBs.

For the WPs, the back-up of the raw data on the external HDDs/USBs will be done after specific characterization/calculation is completed and each individual team member (author) from SROs will be responsible for the back-up of their own results. Back-up of results will be done weekly in SROs.

The project participants will have access to the raw data through the contact persons which are the authorized representatives of the partners (Dr. Smilja Marković and WPs leaders). The Google Drive and pCloud storage will be used for data and file exchange.

QUESTION: Will the data be safely stored in trusted repositories for long term preservation and curation?

The data will be long-term curated and preserved in DAIS and VinaR trusted Institutional repositories.


## 7. Ethical Aspects


QUESTION: Are there, or could there be, any ethics or legal issues that can have an impact on data sharing? These can also be discussed in the context of the ethics review. If relevant, include references to ethics deliverables and ethics chapter in the Description of the Action (DoA).

The project is not dealing with animals, human participants or personal data. There will be stated an embargo period in the metadata where needed for time to publish the project results or to protect intellectual property.

QUESTION: Will informed consent for data sharing and long-term preservation be included in questionnaires dealing with personal data?

Research data collected and used in the project do not contain any personal data. Personal data in the project and event reports will be handled in line with the project privacy policy. Minutes containing personal data will not be shared publicly.

## 8. Other Issues

QUESTION: Do you, or will you, make use of other national/funder/sectorial/departmental procedures for data management? If yes, which ones (please list and briefly describe them)?

Code of Conduct in Scientific Research, National Council for Science and Technological Development, date 21.06.2023.

https://nitra.gov.rs/images/nauka/dokumenta/kodeks-ponasanja-u-naucnoistrazivackom-radu.pdf

Rulebook on the implementation of the Open Science Platform of the Ministry of Education, Science and Technological Development at the Institute of Technical Sciences SASA, ITS SASA, date 21.09.2018.

https://www.itn.sanu.ac.rs/images/Pravilnik_o_sprovodjenju_Platforme_za_otvorenu_nauku_MPN TR-2018.pdf

Code of conduct in scientific research work at the Vinča Institute of Nuclear Sciences, VINS, number 110-1/2018-300/000, date 25.04.2018.

Contract on financing the realization of a scientific research project, Science Fund of the Republic Serbia, 2023.

https://fondzanauku.gov.rs/wp-content/uploads/2022/04/Etika-Prirucnik-naucnoistrazivackog-rada-Fond-za-nauku.pdf

## 9. List of Abbreviation

| | |
|---|---|
| BET | Brunauer-Emmett-Teller analysis |
| CV | cycling voltammetry |
| DFT | density functional theory |
| DMP | data management plan |
| DPV | differential pulse voltammetry |
| DS | dataset |
| ECS | electrochemical sensor |
| ICDD | International Centre for Diffraction Data |
| IPR | intellectual property right |
| ITS SASA | Institute of Technical Sciences of Serbian Academy of Science and Art |
| FAIR | Findable, Accessible, Interoperable, Reusable |
| FESEM | Field emission scanning electron microscopy |
| FIM UNION | Faculty of Engineering Management; University Union – "Nikola Tesla" |
| FFHUB | Faculty of Physical Chemistry; University of Belgrade |
| FTIR | Fourier Transform Infrared Spectroscopy |
| PL | Photoluminescence Spectroscopy |

| | |
|---|---|
| SRO | Scientific Research Organization |
| TEM | Transmission electron microscopy |
| TG/TGA-DSC | Thermogravimetric/ Thermogravimetric Analysis-Differential Scanning Calorimetry |
| UV Vis DRS | Ultraviolet–Visible Diffuse Reflectance Spectroscopy |
| VASP | Vienna Ab Initio Simulation Package |
| VINS | Vinča Institute of Nuclear Sciences; University of Belgrade |
| WP | work package |
| XPS | X-ray photoelectron spectroscopy |
| XRD | X ray diffraction |
| ZnO | zinc oxide |