# Nanocluster-based electrochemical sensing: an interdisciplinary approach towards Durable Glucose Monitors (DuGluMo)

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# Project abstract:

Diabetes mellitus is a group of metabolic diseases characterised by chronic hyperglycaemia resulting from defects in insulin secretion, action or both. It is a major public health problem causing high costs for individuals and society. If left untreated, the chronic hyperglycaemia will lead to long-term damage, dysfunction and failure of various organs. In the last decades, several technologies have been developed to monitor glucose in diabetics (e.g., finger-stick blood tests and lately continuous glucose monitors). Such sensors are unpleasant, show a limited operational time window and expose patients to a high risk of infection and scarring if conceived for a real-time control. DuGluMo aims at overcoming the above-mentioned limitations using original electrochemical nanotechnologies based on size- and composition-controlled metal nanoclusters. The proposed synthesis methods are wafer-compatible and enable a fine control of particle size, composition and density. These experimental features guarantee the establishment of a synergistic approach to develop nanocluster layers on the electrodes breaking new ground in the development guidelines of glucose monitors for lifelong functional duration and high user-acceptability. The results of this interdisciplinary research will also lead to new scientific insights in the field of chemical sensing and bioengineering

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### **Research Data Summary**

List and describe all datasets or research materials that you plan to generate/collect or reuse during your research project. For each dataset or data type (observational, experimental etc.), provide a short name & description (sufficient for yourself to know what data it is about), indicate whether the data are newly generated/collected or reused, digital or physical, also indicate the type of the data (the kind of content), its technical format (file extension), and an estimate of the upper limit of the volume of the data.

Primary data (generated by researcher and research group):

- 1) Analogue data:
- 1.1) Samples
- 1.2) Laboratory logbooks.
- 1.3) Researchers' notebooks
- 2) Digital data
- 2.1) Experimental data (as directly measured): data files in an output format dictated by the specific software, containing numerical data (measurement output) and text metadata (describing experimental/instrumental parameters). Different formats, depending on instrument used for the measurements.
- 2.2) Electronic laboratory logbooks containing detailed information on the samples, sample treatment, conditions and specifications, technical problems, main results...
- 2.3) Processed and analysed experimental data: text documents, spreadsheets and graphical representation of data, used for (or resulting from) data analysis.

Dataset name / ID	Description	New or reuse	Digital or Physical data	Data Type	File format	Data volume	Physical volume
		Indicate: <b>N</b> (ew data) or <b>E</b> (xisting data)	Indicate: <b>D</b> (igital) or <b>P</b> (hysical)	Indicate: Audiovisual Images Sound Numerical Textual Model SOftware Other (specify)		Indicate: <1GB <100GB <1TB <5TB >5TB NA	
MS	Time-of-flight mass spectra	new	Digital	Experimental	.txt, .csv	1-10 GB	
Inputs and outs of computer Simulations	simulations	new	Digital	Software	Specialized formats	10 GB	
Computer codes and scripts	simulations	new	Digital	Software	Specialized formats	10 GB	
XPS	surface chemistry analysis	new	Digital	Experimental Software	.vms,.emf,.csv	<100MB	
	Glucose transport in cell lines & primary cultures	New	Digital & physical	Experimental	xlsx	<1 GB	<100 samples
In vivo	Glucose measurements in type 1 & type 2 diabetic mice	New	Digital & physical	Experimental	xlsx	<1 GB	<100 samples
XRD/XRR	crystallographic characterization	new	Digital	Experimental Software	.xrdml,.csv	<100MB	
Electrochemical techniques	chronoamperometry, cyclic voltammetry, impedance spectroscopy	new	Digital	Experimental	.txt,.csv,.nox	<1GB	
SEM	sample morphology characterization	new	Digital	Experimental	.tif	<100MB	
AFM	roughness estimation	new	Digital	Experimental	.jpg	<100MB	
RBS	near-surface characterization	new	Digital	Experimental		< 100 Mb	
Ion implantation	Implantation of clusters in solid surfaces	new	Digital + physical	Experimental	.xlsx	< 100 Mb	Parameters written down on physical/electronic logbook
	Sputtering of thin films and clusters on solid surfaces	new	Digital & physical	Experimental	.xlsx	<100MB	Parameters written down on physical/electronic logbook

If you reuse existing data, please specify the source, preferably by using a persistent identifier (e.g. DOI, Handle, URL etc.) per dataset or data type:

All data will be initially generated new and analyzed data will work as basis for new ones

Are there any ethical issues concerning the creation and/or use of the data (e.g. experiments on humans or animals, dual use)? If so, refer to specific datasets or data types when appropriate and provide the relevant ethical approval number.

• Yes, animal data (Provide ECD reference number below)

Yes

- -Human primary cultures: S57826 (obese patients), S56978 (multi-organ donors)
- -Animal studies in vivo: we will submit applications for ethical approval in due time

Will you process personal data? If so, please refer to specific datasets or data types when appropriate and provide the KU Leuven or UZ Leuven privacy register number (G or S number).

No

NA

Does your work have potential for commercial valorization (e.g. tech transfer, for example spin-offs, commercial exploitation, ...)? If so, please comment per dataset or data type where appropriate.

Yes

This work has a clear commercial potential. Both the raw and analyzed data will be kept confidential and shared when appropriate only with the members of the research group. On a case by case basis we will evaluate whether to patent (LRD office) or publish an article on our work.

Do existing 3rd party agreements restrict exploitation or dissemination of the data you (re)use (e.g. Material or Data transfer agreements, Research collaboration agreements)? If so, please explain in the comment section to what data they relate and what restrictions are in place.

No

NA

Are there any other legal issues, such as intellectual property rights and ownership, to be managed related to the data you (re)use? If so, please explain in the comment section to what data they relate and which restrictions will be asserted.

No

NA

#### **Documentation and Metadata**

Clearly describe what approach will be followed to capture the accompanying information necessary to keep data understandable and usable, for yourself and others, now and in the future (e.g. in terms of documentation levels and types required, procedures used, Electronic Lab Notebooks, README.txt files, codebook.tsv etc. where this information is recorded).

All protocols and methodology are kept in Excel spreadsheets and shared among the team members. The files are kept on a personal computer and on two different cloud services (Onedrive). Accompanying .readme files explaining the electronic filing system will always be kept in the main directory. Data collected directly from certain equipment with no possible digital data format(s), are kept in a physical and electronic laboratory notebook (Evernote).

For the research data concerning the simulation work (D. Escudero):

During research, data will be stored on computers belonging to the Quantum Chemistry and Physical Chemistry Division (QCPC) and to the Flemish Supercomputing Centre. Key data will always be backed up regularly to avoid loss of data (i.e., this is done on a daily basis in our cluster at the QCPC). Generally to unambiguously trace and organize data; the data arising from the simulations (inputs&outputs) will be collected in separate folders per simulation test, including a txt file with a clear description of what the data represent and how they were generated. A common protocol to name and store data for this project will be set up among all project members. Scripts, codes, input&output files will unambiguosly display date of creation and who generated the data.

Will a metadata standard be used to make it easier to find and reuse the data? If so, please specify which metadata standard will be used.

If not, please specify which metadata will be created to make the data easier to find and reuse.

No

The names of the files will be structured in a comprehensible way:

system studied/date/main parameters used

In addition, data will be stored in a folder per experimental setup, the type of investigated system and the corresponding date. In this way, by tracking the corresponding logbook notes, each file can be easily found on the local computers controlling the setup and on the server of the laboratory.

The analysis files will contain notes describing the analysis procedure and mention which original data files are included. A readme file describing the goal of the experiment and the analysis procedure will be stored in the folder where the data are saved.

# Data Storage & Back-up during the Research Project

Where will the data be stored?

- OneDrive (KU Leuven)
- Shared network drive (J-drive)
- Personal network drive (I-drive)

All physical logbooks will be stored in a cabinet at the institute. Once each logbook is full, it will be stored in a central storage cabinet of the institute, for a period of 15 years after the last registered experiment. Parts of the physical logbooks will be regularly scanned and stored digitally.

The electronic data, including the physical logbook scans, electronic logbooks, raw data and analysis files, as well as reports, will be saved on local computers. The data stored on these computers are backed-up daily on a central server. A mirror copy of this server is made on a back-up server located in a different building. All researchers involved in the project will have access to the corresponding folder.

Concerning the simulation work (D. Escudero): Full output from all calculations is very voluminous, but the field has standard protocols for collecting the key data. Specifically, data will be stored in our computers belonging to the Quantum Chemistry and Physical Chemistry Division (QCPC, KU Leuven) and on the data storage services of the Flemish Supercomputing Centre (VSC)The PI

has considerable expertise in curating computational chemistry research data with these types of approach. All data (appropriately collected and classified with a clear description of what the data represent and how they were generated) will be preserved for at least 10 years (this is the standard protocol at the QCPC division). Automatic daily back-up procedures are ensured at both our QCPC cluster as well as at the VSC facilities.

#### How will the data be backed up?

- Standard back-up provided by KU Leuven ICTS for my storage solution
- · Personal back-ups I make (specify below)

Additional backups will be archived in the protected ESAT cloud. Long-term data preservation (after research) will occur in Zenodo. Every 6 months, all data is backed-up into a physical pen-drive.

Is there currently sufficient storage & backup capacity during the project?

If no or insufficient storage or backup capacities are available, explain how this will be taken care of.

Yes

How will you ensure that the data are securely stored and not accessed or modified by unauthorized persons?

Data on Onedrive is encrypted and requires authentication to access it. Every team member has a unique link that allows access from his/her account. Data on the personal workstation is protected by an access password. The data on the pendrive is zipped in a password protected archive.

What are the expected costs for data storage and backup during the research project? How will these costs be covered?

Every KU Leuven employee has 2TB of storage free to use. J-drive: 51,9€ per year. Sharepoint online: free. One drive: free

### Data Preservation after the end of the Research Project

Which data will be retained for 10 years (or longer, in agreement with other retention policies that are applicable) after the end of the project?

In case some data cannot be preserved, clearly state the reasons for this (e.g. legal or contractual restrictions, storage/budget issues, institutional policies...).

All data will be preserved for 10 years according to KU Leuven RDM policy

NA

Where will these data be archived (stored and curated for the long-term)?

KU Leuven RDR

NA

What are the expected costs for data preservation during the expected retention period? How will these costs be covered?

NA

## **Data Sharing and Reuse**

Will the data (or part of the data) be made available for reuse after/during the project? Please explain per dataset or data type which data will be made available

- Yes, as open dataYes, as restricted data (upon approval, or institutional access only)

Some data could remain confidential due to the potential for commercialization.

If access is restricted, please specify who will be able to access the data and under what conditions.

Team members and LRD

Are there any factors that restrict or prevent the sharing of (some of) the data (e.g. as defined in an agreement with a 3rd party, legal restrictions)?

Please explain per dataset or data type where appropriate.

• Yes, intellectual property rights Where will the data be made available? If already known, please provide a repository per dataset or data type. • KU Leuven RDR (Research Data Repository) When will the data be made available? • Upon publication of research results Which data usage licenses are you going to provide? If none, please explain why. • Other (specify below) To be discussed with LRD Do you intend to add a persistent identifier (PID) to your dataset(s), e.g. a DOI or accession number? If already available, please provide it here. • Yes, a PID will be added upon deposit in a data repository What are the expected costs for data sharing? How will these costs be covered? By the project and afterwards to be defined Responsibilities Who will manage data documentation and metadata during the research project? Who will manage data storage and backup during the research project? Who will manage data preservation and sharing? The team members Who will update and implement this DMP? Prof. Taurino