DATA MANAGEMENT PLAN (DMP) – QMI CORE FACILITIES (QMI-CF)

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Facilities Description

The Stewart Blusson Quantum Matter Institute (QMI) on UBC's Vancouver campus operates QMI-CF, which provides a comprehensive set of techniques to synthesize and characterize quantum materials (QM), fabricate them into devices, then test and optimize them. QMI-CF enables a complete quantum innovation cycle workflow that yields fundamental scientific discoveries and then guides them into applied development to realize novel technologies. QMI-CF encompasses 12 facilities:

1. High Performance Computing (HPC)
2. Quantum Materials Design Laboratory (QMDL)
3. Quantum Materials and Devices Foundry (QMDF)
4. 2D Heterostructure Fabrication Facility (2DH)
5. Quantum Materials Electron Microscopy Centre (QMEMC)
6. Laboratory for Atomic Imaging Research (LAIR)
7. UBC-Moore Centre for Ultrafast Quantum Matter (UQM)
8. Ultrafast Optical Spectroscopy Laboratory (UOSL)
9. Quantum Materials Spectroscopy Centre (QMSC)
10. Resonant Elastic/Inelastic X-ray Scattering (REIXS)
11. Quantum Science & Technology Lab (QSTL)
12. Advanced Nanofabrication Facility (ANF)

For details on these capabilities please go to: https://qmi.ubc.ca/research-services/facilities/

Guiding Principle

Data is managed using FAIR principles:

1. Findable
2. Accessible
3. Interoperable
4. Reusable

Data Collection generated within QMI-CF will consist of research output data such as publications and presentations (talks, posters), computational data, including quantum dynamics spectrum simulations and ab initio calculations, experimental data such as STM, SEM, ARPES, 2D spectroscopy, pump-probe experiments, amongst others, as well as fabrication process parameters (included in the experimental work as shown in Table 1) as well as 3D models for scientific devices and apparatus.

All data from QMI-CF projects will be generated by team members (from the QMI-CF group and/or collaborators) in experiments or modeling related to each group's research program. The data will be collected either manually, recorded in digital format, or automatically by the equipment software or custom computer codes. The collected data will be analyzed and processed by the team members of QMI-CF research groups.

Table 1 presents the format of the different types of data collected as well as the software that can be used to open the data and the typical location where the files are located. Wherever possible, all data will be saved in non-proprietary formats to foster collaborations. Software and code libraries to manipulate this data will be continuously developed in a private version control repository. Upon publication, the raw data as well as the code and the analyzed data would be open to the public.

Description (type of data collected)	File format(s)	Software(s)	Where is the file located?
Research Output Data			
Publications (scientific journals)	Manuscript: Overleaf Data (various formats) and python code for analysis and plotting. Final version: .pdf	Overleaf (group account for collaborative purposes). Final PDF manuscript: Adobe, Foxit, Okular, etc. Final TeX files can be compiled using any LaTeX compiler. Python.	Once submitted, the manuscript TeX file, data and code for analysis and plotting will be available on a QMI repository open to the public. Manuscript PDF available on open access archive (ArXiv) and QMI-CF member's research web page.
Presentation (poster or talk)	Powerpoint/Latex → PDF (final version).	PowerPoint, Overleaf. TeX files can be compiled using any LaTeX compiler. PDF presentation: Adobe, Foxit, Okular, etc. PDF presentation: Adobe, Foxit, Okular, etc.	Presentations available on QMI-CF member's scientific webpage.
Theoretical Work			
HPC: Ab initio calculation	.in, .input .out .txt .dat .struct INCAR, POSCAR, POTCAR, OUCAR electron density and potential files	WIEN2k,VASP,FPLO,Quantum Espresso, cp2k, elk, exciting, fleur, octopus, lamps, custom.	QMI clusters LISA, LISA2 and QUARC.

Experimental Work			
ANF: Fabrication process parameters	Written notebook (to be scanned and put online in .pdf format) .txt / .csv (digital format to be easily distributed amongst labs). Instrument control: .py, .exe.	Word/Notepad Excel Acrobat Python Vendor provided executables	The data is stored in the control computers and backed up periodically on QMI servers.
ANF: Designs/mask layouts	.gds/.dxf format PDKs (Process Development Kits) for KLayout	KLayout (open source) Also commercial software (Clewin, L-Edit)	Stored on lithography writing equipment (eg MLA) and backed up periodically on QMI servers. PDKs and Examples available on GitHub.
ANF: Process flowchart: Cleaning, Litho, Depositions, Etching, Testing at each level	.csv/.txt	Word/Notepad(.txt) Excel/Google sheet (.csv)	Stored in local computers and backed up periodically on QMI servers.
ANF, QMEMC: • Process testing • Profilometry • Reflectometry • Ellipsometry • SEM imaging • XPS	opdx/ .ascii .fmspe/.spe/.csv/.txt .SE .png/.jpg .csv	Python-Matlab=PyMa Vision64/ PyMa Filmeasure/Excel CompleEASE Imaging software Peakfit/PyMa	Equipment computer and local database backed up periodically to QMI servers.
LAIR: Scanning Tunneling Microscopy	data files: .Z_flat, .I(V)_flat, .sxm, .dat, .3ds, .txt	Nanonis Mimea Matlab LabVIEW WSxM Gwyddion	Dedicated control computers & external back-up hard drives and group's GitHub.
UQM: XUV Laser with misc. diagnostics (spectrometers, autocorrelators, locking diagnostics)	.txt: separate datafiles for each instrument. Lab data infrastructure SQL database format.	MATLAB and Python	Stored on the lab server and backed up periodically to QMI servers.
QMEMC: EDXS/EBSD	Aztec file (.oipx) Export to .h5	Aztec Python Igor Pro	Dedicated experiment PC and backed up periodically to QMI servers.

QMEMC: STEM/EELS	.tiff, .bmp, .jpg Meta file saved in separate .txt with the same filename.	ImageJ	Dedicated experiment PC and backed up periodically to QMI servers.
QMEMC: FTIR spectroscopy	OPUS files (.0) Export to .txt	OPUS RefFit Python	Dedicated experiment PC and backed up periodically to QMI servers.
QMEMC: Ellipsometry	CompleteEASE files (.se) Export to .txt	CompleteEASE RefFit Python	Dedicated experiment PC and backed up periodically to QMI servers.
QMEMC: Raman spectroscopy	Labspec files (.ls6) Export to .txt	Labspec 6 Origin Pro Python	Dedicated experiment PC and backed up periodically to QMI servers.
QMSC, UQM, QMDF: Angle-Resolved Photo-Emission Spectroscopy (ARPES)	Hierarchical Data Format (HDF5). The metadata is stored in the HDF5. A pdf copy of the lab book during acquisition is stored together with the hdf5 files. .txt	Interactive Data Language (IDL) Igor Pro Python C# Go	Stored in QMI-ARPES server.
QSTL: Quantum Electronics	HDF5	Igor Pro Python Matlab	Local computer and lab server.

Table 1. illustrates the formats of various types of collected data, along with compatible software for accessing the data, and file locations.

Research Notes

The design and planning of each experiment together with the contextual information will be recorded in digital notebooks. The parameters and status during the execution of the experiments are stored together with the raw data either as metadata or as a digital document. In cases where physical notebooks are used they will be scanned and stored digitally in QMI servers.

Additionally, all QMI-CF members will keep a digital log of their research including the details of experiments and analysis. This will facilitate collaborative work.

Research Output

The work performed at QMI-CF involves the generation, organization, and storage of three primary types of data:

1. publications
2. theoretical calculations
3. experimental data.

Each type of data is systematically organized to ensure it is easily searchable and accessible. Metadata is a critical component of this organizational framework, as it is generated and appended to all data at the time of its production or analysis. This metadata captures essential details such as the project name, date of creation, the facility where the data was generated, and additional data-specific descriptors. This comprehensive approach ensures that all data is well-documented and maintains its integrity throughout its lifecycle.

To enable efficient retrieval, a structured archive system is implemented. This system is designed to facilitate filtering and searching based on key metadata attributes, including the project, date, facility, and data-specific information. The archive's structure is optimized for intuitive navigation, ensuring that users can locate and access relevant data quickly and with minimal effort. By leveraging both detailed metadata and an organized archive, the plan supports robust data management practices, enabling seamless data discovery and fostering collaboration across projects and teams. This approach ensures that all data generated is not only preserved but also remains a valuable resource for future research and analysis.

Storage, backup, and volume

QMI-CF has three dedicated servers that are housed centrally at the UBC data Centre on campus. Data is uploaded to a storage system that is managed by QMI-CF dedicated staff and has ample capacity to be expanded to accommodate the anticipated volume of data.

1. **Theoretical work** - Data will be stored on local servers, and then uploaded to our main servers located at the UBC data centre.
2. **Experimental and research output work** - Every experiment has a dedicated computer where data will be locally saved. This data will be backed up to a local server accessible via an intranet. This server will be regularly backed up to our main servers located at UBC data centre. Individual team members will be responsible for saving their “research output data” and upload presentations, talks and other research output on their personal webpage.

Storage Schedule – Laboratory computers will be backed up daily to a local server accessible only via the lab’s intranet. The servers will be backed up monthly to our main server located at UBC’s data centre.

Access – Active collaborative projects will share data through the university’s OneDrive account. Once the project is finalized, the data will be backed up to QMI-CF’s servers that are housed at UBC’s data centre.

Preservation – Long-term conservation and access strategy – All data will be stored on QMI servers. Data will be exported in non-proprietary format that contains all relevant metadata. Datasets will be preserved by publishing them on Borealis, the Canadian Dataverse Repository. One of the key benefits of the Borealis platform is its support system and its reliability as a long-term solution.

Borealis UBC Dataverse Collection link: https://borealisdata.ca/dataverse/ubc

Sharing and reuse

All research output such as the raw data, analysis code, and metadata will be available to the community through scientific publications and Borealis. Data related to a particular publication will be included in a public git repository along with the TeX packages of the manuscript.

Safety and authority

Every QMI-CF user will be assigned a username and usergroup with suitable privileges and access for their functions within the facilities at QMI. The leadership team has administrator access to all IT infrastructure.

Responsibilities and resources

All members of the QMI-CF will generate data under the supervision of the facility group leader. The research scientists will be responsible for implementing the data management plan, its updates, and data storage. The research scientists will train new team members to ensure that the data management plan is followed.

Ethics and legal compliance

Data will be subjected to restrictions according to the best practices and protocols outlined by the University of British Columbia Office of Research Ethics. Only appropriate and approved metadata will be made available. Authorized personnel/users with sensitive data will be encouraged to ensure that files are encrypted. Any legal, ethical and intellectual property issues will be guided by the relevant policies of the University of British Columbia and the Laws of Canada.