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CAREER: Time-Resolved Studies of Charge Transfer and Chemical Reactivity at Photoelectrode-Electrolyte Interfaces

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Data Management Plan

Data to be generated in the proposed project include experimental details recorded by hand in laboratory notebooks as well as digital data. Data are saved as ASCII format from Labview or other software. Discussions and experimental setups should be taken as photos and saved as jpeg format in a weekly report.

1) Management of laboratory notebooks

Experimental details will be recorded on a daily base. The main experimental data must be printed and pasted on notebooks. Files names in the notebooks will be consistent with those in the digital data. The images of every experimental setup for the data will be taken and pasted on notebooks.

2) Management of digital data

Digital data includes raw digital data from instrument outputs, analyzed data, and figure data. Each data must include metadata that describes the parameters used to generate the data and any calibration of equipment. In addition, experimental setups must be pictured and included in order for another researcher to reproduce your results.

Raw digital data from instrument outputs are stored on laboratory workstations at Utah State University, which are synchronized under a directory of Original Data with your file on Box and the personal computers of the experimental performers and the PI. The data are transferred to the department's server biweekly. Thus, both the experimental performers and the PI could see the data immediately. The transfer ensures three local copies and two remote copies for redundancy. The file folders for raw data are named in date. The file names for raw data are named as the following: Date_Key words_Who. For example, 07_-10_2020_SFG on 10 uM aerosols_Rao.

Analyzed data are divided into preliminary analyzed data and further analyzed data. Analyzed data are also stored under a directory of Analyzed Data with your file on Box, which are synchronized automatically and uploaded to the department server biweekly. The workstations and server are backed up daily to external hard drives. The analyzed data will be analyzed and archived using Igor, Microsoft Excel, or Matlab. For data which require additional programs, the original codes for the data analysis should be kept in a same file.

Preliminary analyzed data: File folders and file names for the preliminary analyzed data follow those described above for *Raw Digital Data from Instrument Outputs*. In other words, these are organized in order of *Date*.

Further analyzed data: A) File folders for the further analyzed data are organized in *Topic*. B) File names for the further analyzed data should keep both dates which the data are analyzed and acquired. For example, Rao is analyzing the data on 07_08_2020 (today is 07_20_2020). The file name should be 07_20_2020_key words_07_08_2020_Rao. Therefore, the data and analysis could be tracked.

Figure data are chosen from the further analyzed data. The file names are the same as the further analyzed data. Final versions of analyzed data will be published in the peer-reviewed literature. After the closing of the project, analyzed data, filed according to the corresponding peer-reviewed publication, will be archived through Utah State University Libraries in the Institutional Repository Digital Commons@USU, as described below.

3) Deposit and storage of data

Utah State University, through the Merrill-Cazier Library, provides institutional repository services. Data files are fully described and published articles can link to the data sets via persistent URLs or a DOI. All files are backed up at multiple sites, including cloud storage. Preservation copies are stored in Amazon Web Services, with redundant storage across multiple facilities and are regularly verified for integrity of data using checksums. Data are freely and openly accessible to the public, and all file types are accepted.

During the research project, files deposited in Box and the department's server are written to a disk cache in an Oracle SAM-FS file system once a year and is stored at the PI's office. <u>Box.com</u> is a cloud storage system used by Utah State University. Files are backed up nightly at multiple sites. <u>Box.com</u> ensures data integrity, includes version control, and is password controlled and encrypted. The data can be shared upon request. The data will only be made available after journal publication.

Hard-copy laboratory books remain in the PI's office at all times for security reasons for a minimum of five years after the end of the project.

4) Professionalism committee for data management

A professionalism committee in the Rao laboratory has been established. The committee members are assigned by the PI and reassigned every year. The primary job of the committee is to assist to educate new group members, to check both the data every month, and to advise new data management to the PI. The execution of backups in Box is conducted by the laboratory personnel. The department server is maintained by a professional staff. The PI, Yi Rao, holds primary responsibility for data management.