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The MxCuBE2/ISPyB environment for remote data collection at the ESRF

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MxCuBE, is a beamline control graphical user interface (GUI) for macromolecular crystallography (MX) experiments that was developed by the ESRF and has been in use since 2005. The GUI provides the user with a friendly interface to electronic devices, permitting to carry out experiments in a intuitive environment while benefiting from the increasing automation. Since its release, MxCuBE has become the preferred MX data acquisition software, also installed at other European synchrotron sites [SOLEIL, EMBL@PETRAIII, BESSY and MAXLAB].In September 2013, after intense recoding, experiment design and testing, the ESRF has deployed MxCuBE2 on all the ESRF's MX beamlines. This new generation of GUI is capable of interfacing with a variety of low level control systems. MxCuBE2, written in the Python programming language, has a radical new appearance and provides an updated environment for performing complicated multi-crystal/multi-position MX experiments in a modular, logical and automatic fashion. ISPyB is a Laboratory Information Management System (LIMS) conceived to record experimental parameters and basic reporting of the data obtained. Since 2009 ISPyB has been a collaboration between ESRF and Diamond Light Source (DLS) and the LIMS is now a multi-site, generic system for synchrotron-based (MX) experiments. The current version allows users to track their sample location (to/from & at the synchrotron), facilitates transmission of information from and to other LIMS, records experiment details, and provides the results - including reflection files - of automatic data processing protocols. Indeed as experiments have become more complex and automated ISPyB has become more than just a repository for project histories - it has become a support for rapid decision making during experiments. The combination of these two indispensable tools in every day users life at the European Synchrotron Radiation Facility will be presented and discussed.

Keywords: ESRF, MxCuBE, ISPyB