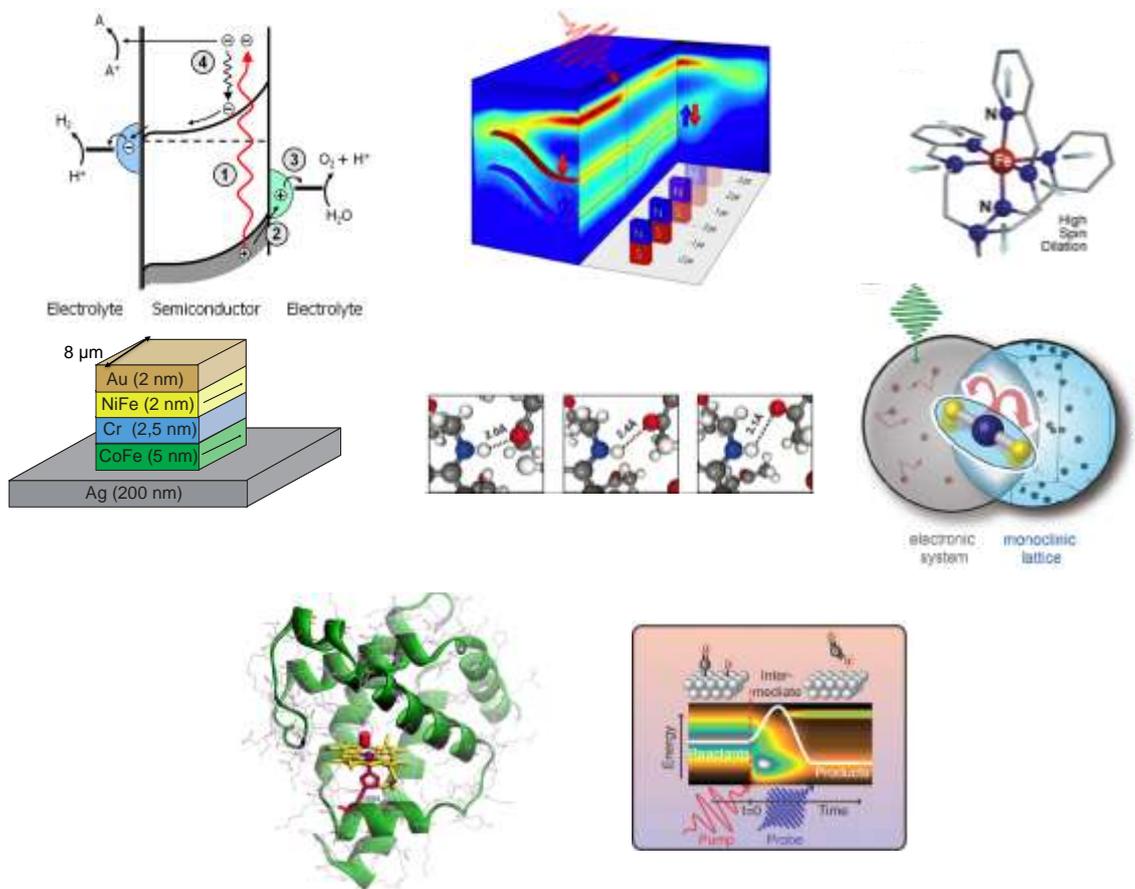


The variable pulse-length storage ring

Scientific Case



Executive Summary - April 2013

Helmholtz-Zentrum Berlin für Materialien und Energie GmbH

This summary is based on the “BESSY-VSR – Scientific Case” (April 2013) by the following contributors: M. Bär¹, M. Bargheer², M. Beye¹, U. Bovensiepen³, S. Eisebitt⁴, A. Erko¹, A. Föhlisch¹, P. Gaal², K. Holldack¹, N. Huse⁵, W. Kuch⁶, F. Kronast¹, N. Mårtensson⁷, E. Nibbering⁸, M. Odellius⁹, O. Rader¹, I. Radu¹, R. Shayduk², C. M. Schneider¹⁰, A. Schneegg¹, C. Schüssler-Langeheine¹, F. Sorgenfrei¹, S. Svensson⁷, R. van de Krol¹, A. Varykhalov¹, M. Weinelt⁶, Ph. Wernet¹, E. Weschke¹, M. Wietstruk⁶, H. Zabel¹¹ ¹HZB, ²U Potsdam, ³U Duisburg-Essen, ⁴TU Berlin, ⁵CFEL, U Hamburg, ⁶FU Berlin, ⁷Uppsala, University, ⁸Max-Born-Institut Berlin, ⁹Stockholm University, ¹⁰Forschungszentrum Jülich, ¹¹U Bochum

Executive Summary

BESSY-VSR – The variable pulse-length storage ring proposed by Helmholtz-Zentrum Berlin

BESSY-VSR is a novel approach to create in the Storage Ring BESSY II long and short photon pulses simultaneously for all beam lines through a pair of superconducting bunch compression cavities. Pulse-picking schemes will allow each individual user to freely switch between high average flux for X-ray spectroscopy, microscopy and scattering and picosecond pulses up to 500 MHz repetition rate for dynamic studies. Thus BESSY-VSR preserves the present average brilliance of BESSY II and adds the new capability of user accessible picosecond pulses at high repetition rate. In addition, high intensities for THz radiation with intrinsic synchronization of THz and X-ray pulses can be extracted from BESSY-VSR.

For the scientific challenges of **quantum materials for energy, future information technologies and basic energy science** BESSY-VSR is the multi-user Synchrotron Radiation facility that allows with the flexible switching between high repetition rate for picosecond dynamics and high average brightness to move classical 3rd generation Synchrotron Radiation science from the observation of static properties and their quantum mechanical description towards the function and the control of materials properties, technologically relevant switching processes and chemical dynamics and kinetics on the picosecond time scale.

Strategic relevance of BESSY-VSR for science with photons

BESSY-VSR creates for the highly productive Synchrotron Radiation community a uniquely attractive multi user storage ring adding the soft X-ray picosecond dynamics at MHz repetition rate. In particular investigations on reversible dynamics and switching in molecular systems and materials are accessible in a non destructive way. The investigations with X-rays from BESSY-VSR are highly complementary and compatible to dynamic studies conducted by users with optical lasers at their home universities and laboratories. BESSY-VSR represents also a missing link between the extreme average brilliance of ultimate storage rings like PETRA III and Free Electron Lasers. Ultimate storage rings are ideal for static spectroscopy, scattering and diffraction whereas the X-ray Free Electron Lasers XFEL and FLASH create for selected experiments highest peak brilliance in coherent, femtosecond X-ray pulses that excel in snap-shots and the detection of non-reversible dynamics in molecules, spontaneous order, non-linear X-ray processes and non reversible femtosecond dynamics. Technologically, the employed superconducting bunch compression cavities in BESSY-VSR are a direct synergy to the CW superconducting cavities developed for BERLinPro.

Unique science opportunities by BESSY-VSR for quantum materials for energy, future information technologies and basic energy science

BESSY-VSR users will excel to correlate chemical function with molecular dynamics on multidimensional potential energy surfaces and to determine principles underlying functional materials for reversible processes such as switching. The ability to determine through high quality Synchrotron Radiation Spectroscopy, Scattering and Microscopy the geometric and electronic structure as well as the nanoscale composition is the first step to then create and investigate transient states and their picosecond dynamics that govern materials' function.

For **future information technologies**, BESSY-VSR is a key facility for the science and technology of efficient and reversible **magnetic and all optical switching**. X-ray probes in combination with

picosecond dynamics will elucidate phonon and magnon driven processes, precessional magnetization dynamics, resistive switching dynamics, and the switching of nanostructures relevant for information storage. In a more general way, *phase transitions* determine materials functionality and BESSY-VSR will allow for the observation and the control of phases far from equilibrium in order to answer the key questions of “What is the most efficient way to control properties?” And “How fast can properties be changed, and how stable are the states?” Reversible switching extends far beyond the solid state toward molecular switches through e.g. isomerisation, tautomerisation or spin-cross over excitations that are the basis of *molecular electronics*. Here both X-ray probes and IR/ THz pulses from BESSY-VSR uniquely enable THz-EPR experiments with picosecond time resolution to reveal the structure-dynamic-function relationship of functional molecular systems.

BESSY-VSR will offer unique insight into the non-trivial low-energy excitation spectra arising from the coupling between different degrees of freedom in correlated materials that govern *quantum materials*. In *nanoscale materials*, BESSY-VSR will enable in an unprecedented way the investigation of direct spin-excitations in individual nanoparticles, the magnetic fluctuations in particle ensembles and nonlinear phononics by addressing the dynamics of phonons in anharmonic crystal potentials by time- and space-resolving X-ray methods. Investigations of *topological insulators* relevant for *spintronics* will benefit from novel opportunities for multidimensional X-ray spectroscopy at BESSY-VSR to elucidate the coupling of electronic structure, chemical environment and geometrical structure.

In *basic energy science* BESSY-VSR will address challenges in *photochemistry*, *photosynthesis*, *photovoltaics*, *catalysis* and the basic reaction steps underlying *solar fuels*. Understanding and controlling *photochemistry*, i.e., the correlated motion of electrons and nuclei holds the key to controlling the reaction kinetics and motivates the need for information on photoexcited electronic and structural changes in molecular systems. Following the structural dynamics and the valence charge density in ground and excited transient states with time-resolved X-ray spectroscopy at BESSY-VSR uniquely addresses fundamentals of charge-transfer reactions in metalloenzymes, photo-triggered proton-transfer reactions and nonequilibrium processes in hydrogen-bonded systems. For *photosynthesis*, the key process for oxygen regeneration on earth by photosynthetic water oxidation, BESSY-VSR will enable explaining the reaction kinetics resulting from the dynamic pathways of the photosystem II membrane protein complex *in vivo* in solution by X-ray spectroscopic characterization of the catalytic reaction center on nano- and millisecond time scales. In *photovoltaics*, time-resolved X-ray spectroscopy will reveal the coupling of charge carrier dynamics and interface properties, a key to understanding and controlling the efficiency of photovoltaic devices. For *catalysis* in general, time-resolved soft X-ray spectroscopy at BESSY-VSR will be used to address the pathways that govern chemical rate and selectivity in heterogeneous catalysis and surface chemistry. The catalyst or the adsorbate will be driven through external stimuli and the interplay between femtosecond charge transfer, local coordination and the electronic or vibrational excitations present in the system will be probed to pave the way towards insight-driven design of future catalysts with applications to solar fuels, clean combustion and green chemistry. For *solar fuels*, finally, photoelectrochemistry will be used to combine photovoltaic and electrocatalytic functionalities within a single material or composite. BESSY-VSR will be used to probe the generation, recombination and charge-transfer dynamics and charge-carrier lifetimes in solar fuel materials. In addition, BESSY-VSR will allow addressing the time scales and energy losses associated with charge transfer across semiconductor-catalyst interfaces to elucidate the complex four-electron proton-coupled electron transfer process in water oxidation in solar fuel devices.