Contribution ID: **161** Type: **Talk (20 min + 5 min discussion)**

Science case and concepts of a macromolecular diffractometer for the High Brilliance Neutron Source (HBS)

Monday, 4 December 2023 15:50 (25 minutes)

Enzymes are a sub class of proteins which act as natural catalysts and reduce the activation energy of chemical reactions necessary to keep up the metabolism of life. This renders enzymes important drug targets. To elucidate their structure is often the key to understand certain diseases. X-ray protein crystallography contributed by far the largest number of structures but methods like transmission electron microscopy start to yield also atomic resolution. However, those techniques lack the ability to locate hydrogen atom positions since they scatter from the electron shells. Hydrogen has only one electron and is therefore a weak scatterer for electrons or x-rays but it often plays a crucial role in the enzymatic process. Here, neutrons provide a solution since they scatter from the nuclei. Neutron protein crystallography is now an established technique and has elucidated many enzymatic processes by pointing out important protonation states of amino acid side chains. But it requires a large neutron flux and good resolution in reciprocal space. Therefore, the number of instruments accessible to the user community is limited. Mostly, these instruments reside at powerful reactor or spallation neutron sources. In this contribution we would like to asses how one can design such an instrument at a High current proton accelerator-based Neutron source (HiCANS). Using Vitesse simulations on potential instruments we discuss their potential for the future user community.

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Session Classification: Structure Research

Track Classification: Structure Research