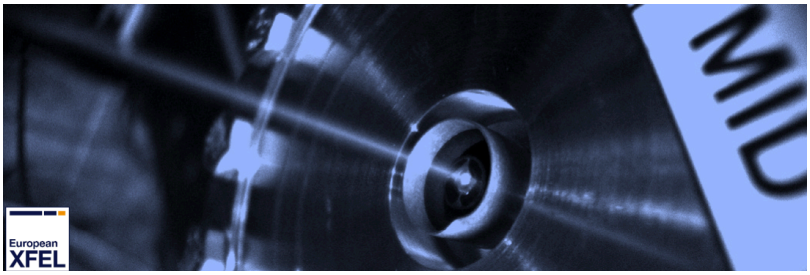

Contribution ID: **1** Type: **Talk**

Understanding functionality in molecular photo-catalysis with high-energy XFELs

Thursday 19 January 2023 10:45 (20 minutes)

A key aspect of molecular (photo-) catalysis is to optimize how much of the input energy is useful towards forming the desired photoproducts. For rational design of novel catalysts it is therefore of high importance to be able to determine how the input energy is re-distributed on internal and external Degrees of Freedom such as vibrational excitations and energy loss to the surroundings. Using the well-studied Pt2POP4 and related transition metal systems as cases, this talk will address how very hard X-rays with femtosecond time resolution can enable detailed mapping of the flow of energy from the initially well-defined vibrational (wave packet) excitations, through inter-system crossings and couplings to the environment to the final and hopefully energy-rich catalytically active state.

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Session Classification: Dynamics of functional materials

Track Classification: Dynamics of functional materials