Project Title: Implementation Simulation Protocols for Transient X-ray spectroscopies on Top of of Non-adiabatic Dynamics in the COBRAMM package

Research Project: COBRAMM is a program package interfacing widely known commercial & academic software for molecular modeling (spanning from electronic structure and molecular mechanics computations) developed in the groups Prof. Garavelli and Prof. Nenov at the Department of Industrial Chemistry at the University of Bologna. It allows a problem-driven tailoring of computational chemistry simulations with effortless ground and excited state electronic structure computations within a combined quantum mechanical/molecular mechanical (QM/MM) framework to bridge the atomistic to the nano-scale.

The user can perform all necessary steps to simulate chemical reactions in complex environments (ranging from solvents to bio-polymers) and model the interaction of those systems with light to simulate their spectroscopy, as well as their photoinduced dynamics. Starting from ground state optimizations, reaction path computations, initial conditions sampling, spectroscopy simulation and photodynamics including deactivation events, COBRAMM is designed to assist the characterization and analysis of complex molecular materials and their properties as well as the interpretation of the recorded spectra ranging from steady-state to time resolved measurements. Various tools help the user to setup the system of interest and analyze the results.

COBRAMM's features regarding interfaces to QM codes, molecular dynamics protocols and spectroscopy techniques are constantly being enhanced. The current project aims at incorporating several novel features:

a) Enhancing the interface with the open source QM software NWChem for on-the-fly nonadiabatic dynamics at the time-dependent density functional theory (TD-DFT);
b) Protocol for simulation of transient spectroscopies (tr-XPS and tr-XAS) in the X-ray regime on top of mixed quantum-classical dynamics at the multireference and DFT level of theory

The implementation will include preparation of a tutorial and test / benchmarking cases for each protocol.