Project Title: Implementation of Hybrid Multiscale Methods for Efficient Simulation of Non-adiabatic Dynamics of Complex Molecular Systems 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) An interface with the open source QM software NWChem which will provide an open source alternative to Gaussian for time-dependent density functional theory (TD-DFT) and access to core-spectroscopies (X-ray photoemission spectroscopy and near-edge X-ray absorption fine structure spectroscopy) at this level;
b) Transient spectroscopy protocols in the Visible, extreme UV and X-ray regimes on top of semi-classical non-adiabatic dynamics simulations scheme which treats a photoresponsive molecular system fully quantum-mechanically (through an interface with the software for multi-dimensional wave packet dynamics Quantics), coupled to a classical environment (bath);
c) A protocol for performing on-the-fly trajectory-based non-adiabatic dynamics simulations on machine learned potentials trained with single reference methods (e.g. TD-DFT) and fine-tuned around the S1/S0 conical intersection region with multireference methods to overcome the deficiency of single reference methods in describing the non-adiabatic coupling.

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