UniSysCat - Colloquium

Prof. Claudio Greco

University of Bicocca, Milan

Start Time: Wednesday, June 14, 2023 05:15 pm

End Time: Wednesday, June 14, 2023 06:30 pm

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or via Zoom

Theoretical description of the catalytic actions of CO-dehydrogenases and hydrogenases: tackling the challenges of reliable QM/MM modelling.

Prof. Claudio Greco

University of Bicocca, Milan

My talk will focus on recent advancements we obtained on the theoretical description of enzymes involved in the biotransformation of small gaseous molecules such as CO and H_2, a topic that has environmental relevance and can be inspiring for the development of greener processes for application in the energy and mobility sector. In the first part of the seminar, I will focus on the challenges posed by the hybrid quantum/classical (QM/MM) treatment of the catalytic mechanism of CO dehydrogenases (CODH), with specific reference to the Mo/Cu-dependent CODH. The picture coming from our QM/MM models of the latter will be compared with previous outcomes described in literature – mainly based on quantum chemical cluster models – keeping the available experimental data on the reactivity of such enzyme as a fundamental reference point. The second part of my talk will be devoted to the QM/MM study of hydrogenases, with focus on the functional interplay among iron-sulfur sites in the [FeFe]-hydrogenase by *D. desulfuricans*. Furthermore, I will present and discuss potential future steps in the investigation of these enzymes using computational chemistry approaches.

Prof. Dr. Kallol Ray

Organizer