Università degli Studi di Padova

DiSC

Venerdì **28 giugno 2024** alle ore **11:30** presso l'aula L1

il **Prof. Fahmi Himo**

Department of Organic Chemistry
Arrhenius Laboratory
Stockholm University

terrà il seminario dal titolo:

Modeling Homogeneous and Enzymatic Catalysis

Using modern density functional theory it is today possible to routinely and accurately treat relatively large systems. The calculated energies can be used to rule out or substantiate reaction mechanisms and have also been shown to be sufficiently accurate to satisfactorily reproduce various kinds of selectivities. These developments have made it possible to tackle increasingly difficult problems in homogeneous catalysis and supramolecular chemistry. It also allows to model enzyme active sites in a more realistic way. This talk will give a brief account of the methods used in these fields and a number of recent examples from our work will be discussed.

La presenza della S. V. sarà molto gradita

Il Direttore del Dipartimento
Stefano Mammi

Marilena Di Valentin