

Università degli Studi di Padova Dipartimento di Scienze Chimiche

Ciclo di Seminari 'Frontiers in Chemistry'

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Proton Relays and Local Concentration Effects in Molecular Catalysis

Giovedì 6 Febbraio 2020, ore 14.30 Aula A, Dipartimento di Scienze Chimiche Via Marzolo 1 - Padova

Abstract:

Several examples of remarkably bidirectional or even reversible catalysis with small overpotentials have been recently described in the case of the electrochemical H2 oxidation and production. This is the occasion to show that such challenging achievements are made possible by local concentration effects allowed by the installation of fast proton relays inside the catalyst molecule close to its metal center. A satisfactory kinetic model consists of two fast proton-coupled electron transfer square schemes linked together by means of two slower reactions involving changes in the metal coordination sphere. This leads to an equivalent description of the problem by means of a much more compact reaction scheme after definition of the connections with the parameters of electron and proton reactivity of the actual catalytic system. The treatment provides expressions for the catalytic cyclic voltammetric responses revealing the factors that govern the local concentration effects and the transition between bi-directionality and reversibility.

La presenza della S. V. sarà molto gradita.

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