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Dynamic and Chemical Disorder in Enzymatic Reaction Mechanisms

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This talk will address our most recent works devoted to understand enzyme reaction mechanisms using QM/MM methods [1-4].

The talk will not focus on specific applications but instead in will give an overview of the fields we are working in, with selected examples to illustrate the concepts. We will focus on the choice of the QM region and on the consequences in might have to the predicted reaction mechanism; on the choice of the theoretical levels, in particular the density functionals, and the expectable accuracy they might bring. The role of enzyme flexibility on catalytic rates will be discussed as well [5-6].

From a more broad point of view, we will discuss the insights that computer simulations brought on the general understanding on how enzymes work, and how the flexible enzyme machinery influences and dictates the reaction rate and controls the chemical pathway it catalyzes.

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