Special Issue

Quantum Chemical Modelling of Enzymatic Reactions

Message from the Guest Editors

DFT studies of mechanisms for enzymes and metalloenzymes over the past 15 years have increased a great deal, becoming of equal importance compared to traditional spectroscopic studies. Lately, the QM/MM approach also achieved a significant role in the field of theoretical methodologies devoted to the untangling of different aspects of enzymatic catalysis. This Special Issue aims to cover recent progress and advances in elucidating the catalytic role of important members of enzymatic families, implicated in important biological processes, as well as of artificial enzymes that will be involved in technological and industrial applications. http://www.mdpi.com/journal/catalysts/special_issues/quantum_model

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