Caught in action: simulation of enzymatic reactivity

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As result of years of evolution, enzymes ended up as refined biocatalysts with (stereo)selective substrate scope and high catalytic activities. Fascinated with this molecular machinery, humankind has profited from their use to get valuable products by means of enzyme-based industrial synthesis. To tune enzyme substrate specificity, stability and/or proficiency, it is critical the understanding of the electronic and structural features that govern the catalytic steps. In this sense, the use of computational methods has been shown beneficial to speed up protein engineering campaigns. In the last years, quantum mechanics/molecular mechanics (QM/MM) methods have made possible the study of enzyme-catalyzed reaction within the active site. In this communication, I will explain our methodology to approach to the simulation of enzyme reactivity by means of QM/MM methods, illustrating this with recent examples of my research.[1-3]

References:

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