122c Computational Chemistry – a Tool for Gaining Insights into the Progress of Catalyzed Reactions

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During the past decade, it has become increasingly apparent that computational chemistry is a powerful tool for gaining insights into the pathways by which a catalyzed reaction may, or may not occur, and for assessing the effects of changes in the local structure of catalytically active sites on their activity and selectivity. Recent advances in methods for identifying transition states and determining the rate parameters of elementary reactions occurring at active sites have made it possible to determine what steps are most critical in determining the progress of a catalyzed reaction. The information gained from such analyses can provide a basis for thinking about how to modify the site composition and the composition and structure of the surrounding medium to "steer" the chemistry in a desired direction. This talk will present illustrations of the applications of computational chemistry to N2O decomposition over Fe-ZSM-5, CH4 oxidation to CH3COOH catalyzed by Pd2+ cations in sulfuric acid, and the oxidative carbonylation of methanol to dimethyl carbonate over Cu-ZSM-5. In each case comparison will be made between the computational and experimental results.