Identification of the driving forces in methanol-to-olefin conversion by modeling the zeolite cage and contents

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The rapidly increasing demand of oil-based chemicals calls for the development of new technologies based on other natural sources. Among these emerging alternatives, the methanol-to-olefin process (MTO) in acidic zeolites is one of the most promising. However, unraveling the reaction mechanism of such an extremely complex catalytic process like MTO conversion has been a challenging task from both experimental and theoretical viewpoint. For over 30 years the actual mechanism has been one of the most discussed topics in heterogeneous catalysis.[1] Instead of plainly following *direct* routes,[2-3] the MTO process has experimentally been found to proceed through a *hydrocarbon pool* mechanism, in which organic reaction centers act as cocatalysts inside the zeolite pores, adding a whole new level of complexity to this issue.[4-5] Therefore, a more detailed understanding of the elementary reaction steps can be obtained with the complementary assistance of theoretical modeling.

In this work, a complete supramolecular complex of both the zeolite framework and the co-catalytic hydrocarbon pool species is modeled through state-of-the-art quantum chemical techniques [6-7]. This approach provides a more detailed understanding of the crucial interactions between the zeolite framework and its contents, which form the driving forces for successful methanol-to-olefin conversion.

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