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Molecular Simulations of Methanol Valorisation to Sustainable Aviation Fuels over Zeolites

The methanol-to-olefins (MTO) process utilizes acidic zeolites to convert methanol into olefins and plays a pivotal role in the production of Sustainable Aviation Fuels (SAFs)1. This process involves a complex network of reactions, with multiple competing pathways and mechanisms2. The initial and critical step is the dehydration of methanol to form dimethyl ether (DME)3. Experimental and computational studies have revealed two main reaction pathways for this step, whose predominance depends strongly on the operating temperature4. Given the central role of this step in shaping the subsequent formation of the so-called hydrocarbon pool, it is essential to achieve a clear and detailed molecular-level description. However, current modeling approaches fall short of capturing the realistic complexity of the process under operando conditions, limiting their ability to provide accurate thermodynamic and mechanistic insights5. In addition, a systematic exploration of the broad physico-chemical space—defined by variations in temperature and zeolite topology—is still lacking, yet crucial for initiating an effective in silico screening aimed at process optimization. In this work, we address these challenges by employing metadynamics simulations coupled with machine learning potentials (MLPs), exploring a range of temperatures (600–800 K) and zeolite frameworks (chabazite, ZSM-5, and mordenite). This approach enables the investigation of reaction mechanisms with atomistic resolution, estimation of energy barriers, and construction of free energy profiles. Using metadynamics simulations powered by MLPs trained on accurate ab initio data, we elucidated both the associative and dissociative pathways involved in methanol dehydration. The resulting free energy profiles allowed us to determine the thermodynamic and kinetic parameters associated with each mechanism. By comparing these parameters, we identified the dominant reaction pathway for the methanol-to-DME conversion under different conditions. This study establishes a robust framework for mechanistic analysis of catalytic reactions in complex environments and provides fundamental insights into the MTO process. Our findings aim to support the development of more efficient catalytic systems and contribute to the broader goal of advancing sustainable and economically viable energy solutions. (1) Van der Mynsbrugge, J.; Moors, S. L. C.; De Wispelaere, K.; Van Speybroeck, V. ChemCatChem 2014, 6 (7), 1906 1918. https://doi.org/10.1002/cctc.201402146. (2) Wang, S.; Chen, Y.; Qin, Z.; Zhao, T.-S.; Fan, S.; Dong, M.; Li, J.; Fan, W.; Wang, J. J. Catal. 2019, 369, 382–395. https://doi.org/10.1016/j.jcat.2018.11.018. (3) Blaszkowski, S. R.; Van Santen, R. A. J. Phys. Chem. B 1997, 101 (13), 2292–2305. https://doi.org/10.1021/jp962006+. (4) Ghorbanpour, A.; Rimer, J. D.; Grabow, L. C. ACS Catal. 2016, 6 (4), 2287–2298. https://doi.org/10.1021/acscatal.5b02367. (5) Barducci, A.; Bussi, G.; Parrinello, M. Rev. Lett. 2008, 100 (2), 020603. https://doi.org/10.1103/PhysRevLett.100.020603.

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