Molecular Traffic Control inside TNU-9 Zeolite

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We study a reaction-diffusion system modeling the isomerisation reaction inside a catalytically active grain of TNU-9 zeolite. We are interested in the question: Is there any enhancement in the reactivity of the catalytic grain under the condition of molecular traffic control (MTC) when the reactant and product molecules show channel selectivity? Using dynamical Monte Carlo simulation, we compare the output current of MTC system with a reference system which does not show any channel selectivity. For a wide range of reactivity and the grain size, we find that inside this TNU-9 topology, there is a great enhancement of reactivity for the MTC system. MTC effect continues to remain strong as the grain size increases. The presence of MTC effect inside this realistic channel topology suggests possibilities of practical applications.