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REACTION KINETICS, CATALYSIS AND....

绝氧条件下β-$Bi_2Mo_2O_9$晶相上丙烯氧化反应的Monte Carlo模拟研究

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摘要 A random walk Monte Carlo（RWMC）simulation model of catalytic particle was established on the basis of the structures of bismuth molybdate catalysts and mechanisms of catalytic reactions with propylene selective oxidation and ammoxidation. The simulation results show that rationality of the RWMC model is proved on the basis of pulse experimental data. One of the most remarkable factors affecting catalytic behavior is the transfer of bulk lattice oxygen, which decides the rate of ammonia-consuming and propylene-consuming. The selectivity of main products reaches the maximum after the reduction of catalysts to a certain degree. It is inferred that catalytic performance improves greatly if the ratio of capacity for dehydrogenation from adsorbed propylene molecule on catalytically active site of molybdenum metal-imido group（Mo=NH）to that on catalytically active site of molybdenum metal-oxo group (Mo=O) becomes much higher.

关键词 绝氧条件 β-Bi2Mo2O9 晶相 丙烯氧 氧化反应 Monte Carlo模拟 指晓力

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Monte Carlo Simulation of Propylene Selective Oxidation and Ammoxidation overβ-$Bi_2Mo_2O_9$ Catalyst under Anaerobic Condition

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Abstract A random walk Monte Carlo（RWMC）simulation model of catalytic particle was established on the basis of the structures of bismuth molybdate catalysts and mechanisms of catalytic reactions with propylene selective oxidation and ammoxidation. The simulation results show that rationality of the RWMC model is proved on the basis of pulse experimental data. One of the most remarkable factors affecting catalytic behavior is the transfer of bulk lattice oxygen, which decides the rate of ammonia-consuming and propylene-consuming. The selectivity of main products reaches the maximum after the reduction of catalysts to a certain degree. It is inferred that catalytic performance improves greatly if the ratio of capacity for dehydrogenation from adsorbed propylene molecule on catalytically active site of molybdenum metal-imido group（Mo=NH）to that on catalytically active site of molybdenum metal-oxo group (Mo=O) becomes much higher.

Key words catalyst; modeling; Monte Carlo simulation; selective oxidation and ammoxidation of propylene; bismuth molybdate; random walk Monte Carlo model;

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