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Small-Pore Molecular Sieves SAPO-34 with Chabazite Structure: Theoretical Study of Silicon Incorporation and Interrelated Catalytic Activity HONG WANG, JAMES LEWIS, West Virginia University, ZHONGMIN LIU, Dalian Institute of Chemical Physics — The catalytic conversion of methonal to olefin (MTO) has attracted attention both in industrial and academic fields. Strong evidence shows that small-pore molecular sieves with certain amount silicon incorporated (SAPO) present promising high catalytic activity in MTO conversion. Using DFT, we study the structural and electronic properties of chabazite SAPO-34. Although there are extensively experimental results show that silicon incorporation does not change the overall structure as the original AlPO structure, local structural changes are still created by silicon substitution, which probably accounted for the high catalytic activity. It is noted that the catalytic activity of SAPO-34 presents increasing trend along with the silicon incorporation amount increasing and maintain a flat peak even with more silicon incorporated. Hence, there is an optimal silicon incorporation amount which possibly yields the highest catalytic MTO conversion.

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