Selective Conversion of CH_4 to CH_3Cl with Cl_2 Gas Using Ion-exchanged Zeolites: Electrophilic Chlorination Controlled by Surface Properties of Catalysts

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CH_4 chlorination is one of the energy-efficient conversion pathways of CH_4 using the reactive chlorine gas molecule, which produces various chlorinated methane products (i.e., CH_3Cl, CH_2Cl_2, $CHCl_3$, CCl_4). Among them, CH_3Cl has higher industrial value because it can be further used as an intermediate material that can be converted to hydrocarbon. For the selective production of CH_3Cl, CH_4 should be chlorinated by ion-mediated pathway. This requires superacid catalysts that can induce polarization of chlorine molecules. In this work, ion-exchanged zeolites and hence having controlled surface acidity and polarity were investigated in CH_4 chlorination. The CH_3Cl yield was remarkably changed according to the cations on the zeolite surface, which could be correlated with chemical properties of elements such as electron affinity and standard reduction potential in the zeolite framework. Furthermore, physical adsorption enthalpy of CH_3Cl and natural-bond-orbital charges of cations derived by DFT calculations suggested strong electrostatic interaction between CH_3Cl and the zeolite cluster model. The details of CH_4 chlorination and the results are going to be discussed in this poster.