

Selective oxidation of propane by vanadium oxide sites supported on silica

Abstract:

With the development of modern chemical industry, the demand for olefins, such as ethylene, propene, is expected to increase significantly in the near future. Present main sources of olefins, such as steam cracking, fluid-catalytic-cracking (FCC) and catalytic dehydrogenation, are not enough to meet the increasing demands. Selective oxidation reaction is a potential solution, which functionalizes low molecular weight paraffin with oxidative dehydrogenation (ODH) to produce olefins instead of other more expensive materials.

We plan to study the selective oxidation of propane by vanadium oxide sites supported on silica using density functional theory as well as meta-dynamics simulation. Detailed mechanisms will be mapped out for the selective oxidation of propane to propene. Special attention will be paid to the selectivity problems by considering steps that lead to CO and CO₂ formation. A new method, which employs molecular-dynamics with a mechanical constraint along a reaction coordinate, will be used to evaluate the entropic effect.