

Utilization of the three-dimensional volcano surface to understand the chemistry of multi-phase systems in heterogeneous catalysis

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CO hydrogenation is used as a model system to understand why multi-phase catalysts are chemically important in heterogeneous catalysis. By including both adsorption and subsequent surface reactions, kinetic equations are derived with two fundamental properties, the chemisorption energies of C and O (ΔH_c and ΔH_o , respectively). By plotting the activity against ΔH_c and ΔH_o , a three-dimensional volcano surface is obtained, as illustrated in the figure. Because of the constraint between ΔH_c and ΔH_o on mono-phase systems (the black line in the figure), point B can be achieved. However, if multi-phase systems are used, such a constraint can be released and the global maximum may be achieved.

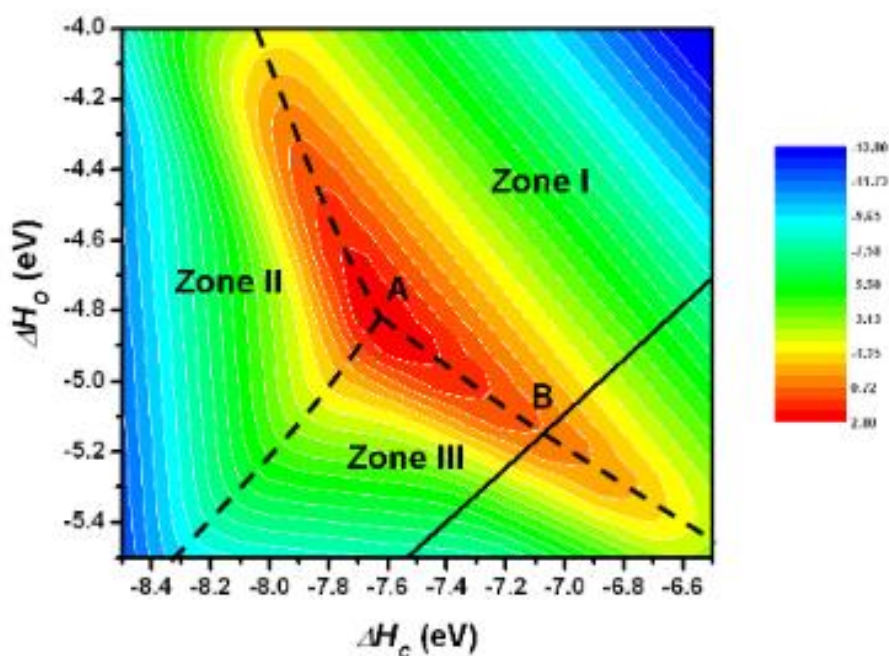


Figure 1. Two-dimensional contour of LogTOF as a function of ΔH_c and ΔH_o for CO hydrogenation.