

Effect of Vanadium Dopant on the Stability and Reactivity of Rhodium Clusters

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In recent years, nano-clusters and cluster based motifs have gained extensive popularity due to their unique properties and widespread applications. Despite the progress, the stabilization of the clusters has still remained one of the challenging tasks. To address this issue, we present an interesting case of small bimetallic mono-vandium doped rhodium clusters (Rh_mV , $1 \leq m \leq 8$). Our study suggested that a single vandium dopant structurally stabilizes all the selected clusters to significant extent, irrespective of their sizes. In addition, taking the C-H activation of CH_4 as a simple example, we have also observed that the single vandium dopant also make the rhodium clusters more reactive toward C-H activation by reducing the barrier and the endothermicity to a moderate extent.