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A Comparative Density Functional Theory Study of Hydrocarbon Combustion on Metal Surfaces

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Abstract : Catalytic combustion of hydrocarbons is an important technology developed to produce energy with minimum pollutant formation. The catalyst plays a key role in this process which operates at lower temperatures compared to conventional flame combustion. The energetics of the direct combustion of hydrocarbons (CH → C + H) on a series of metal surfaces including Ag, Au, Al, Cu, Rh, Pt, Pd, Ni, Fe and Co were investigated using density functional theory (DFT). Brønsted-Evans-Polanyi (BEP) and transition state scaling (TSS) correlations were proposed based on DFT calculations on the Ag, Au, Al, Cu, Rh, Pt and Pd surfaces. These correlations were then used to estimate the energetics on Fe, Ni and Co surfaces. Results showed that the estimated reaction and activation energies by BEP and TSS correlations on Fe, Ni and Co surfaces are in an excellent agreement with those obtained by DFT calculations. Therefore these correlations can be efficiently used to predict energetics of similar reactions on these surfaces without doing computationally costly transition state calculations. It was found that the activation barrier for CH dissociation follows the order Ag ˃ Au ˃ Al ˃ Cu ˃ Pt ˃ Pd ˃ Ni > Co > Rh > Fe. Also, BEP (with R2 value of 0.96) and TSS correlations (with R2 value of 0.99) support the results.

Keywords : BEP, DFT, hydrocarbon combustion, metal surfaces, TSS
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