Efficient nickel-based catalysts for amine regeneration of CO2 capture: From experimental to calculations verifications

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Abstract

High heat duty is an urgent challenge for industrial applications of amine-based CO2 capture. In this work, we report a novel, stable, efficient, and inexpensive Ni-HZSM-5 catalyst to reduce the heat duty. The density functional theory (DFT) calculations successfully explain the catalytic performance. The catalytic activity associates with the combined properties of MSA × B/L × Ni2+. The 7.85-Ni-HZ catalyst presents an excellent catalytic activity for the CO2 desorption: it increases the amount of desorbed CO2 up to 36%, reduces the heat duty by 27.07% compared with the blank run, and possesses high stability during five cyclic tests. A possible catalytic mechanism for the Ni-HZSM-5 catalysts through assisting carbamate breakdown and promoting CO2 desorption is proposed based on experimental results and theoretical calculations. Therefore, the results present that the 7.85-Ni-HZ catalyst significantly accelerates the protons transfer in CO2 desorption and can potentially apply in industrial CO2 capture.

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