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Correlations between vapor-phase Na/K/As adsorption capacities of kaolinite and temperature-dependent derivation of its Al-containing groups

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Abstract

Kaolinite is a commonly used additive, which has been proven to be capable of in-furnace capturing the vapor-phase Na, K, and As, so as to alleviate the fouling and slagging on the heat-exchange surface, the poisoning of selective catalytic reduction (SCR) catalyst, and to reduce related environmental pollution. Considering that temperature-dependent derivation of kaolinites significantly influence the collaborative removal of these vapors, the present study quantified the Na/K/As adsorption capacity of kaolinites using a self-designed device over a wide temperature range to explore the temperature window for high adsorption efficiency. By analyzing Al-coordination of kaolinites before and after adsorption, fixation pathway of Na/K/As vapor was revealed. Effect analysis of single adsorbed atom combined with adsorption energy calculation based on density functional theory (DFT) was performed to demonstrate the difference of adsorption sites for Na/K/As vapors. The results showed that kaolinites had high Na/K/As adsorption capacity at 1073 K–1173 K, 723 K–1273 K, and 1173 K, respectively. When the temperature was between 723 K and 1173 K, the primary hexa-coordinated $^{[VI]}$Al of kaolinites transformed into penta-coordinated $^{[V]}$Al/tetra-coordinated $^{[IV]}$Al. The newly formed $^{[IV]}$Al atoms bonded with Na/K/As atoms. Specifically, both of center sites and bridge sites of $^{[IV]}$Al-O rings can offer position for the fixation of Na and K atoms, and Na atoms were prone to be fixed at the former sites, while K atoms were easy to locate at the latter. In contrast, almost only the center sites of $^{[IV]}$Al-O rings contributed to As adsorption. Thus, with the segmented injection of kaolinites at different temperature within 723 K–1273 K, development of two kinds of modified kaolinites

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