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PII: S1385-8947(17)30754-4
DOI: http://dx.doi.org/10.1016/j.cej.2017.05.013
Reference: CEJ 16911

To appear in: *Chemical Engineering Journal*

Received Date: 16 February 2017
Revised Date: 2 May 2017
Accepted Date: 3 May 2017

Please cite this article as: H. Zhang, K. Zhao, Y. Gao, Y. Tian, P. Liang, Inhibitory effects of water vapor on elemental mercury removal performance over cerium-oxide-modified semi-coke, *Chemical Engineering Journal* (2017), doi: http://dx.doi.org/10.1016/j.cej.2017.05.013

Inhibitory effects of water vapor on elemental mercury removal performance over cerium-oxide-modified semi-coke

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Abstract

A fixed-bed reactor was used to study the effect of water vapor on the efficiency of Hg^0 removal over CeO_2-modified semi-coke. Adsorption experiments showed that the oxidation activity, and therefore, the mercury adsorption efficiency decreased with increasing water vapor concentrations. Hydrogen temperature-programmed reduction (H_2-TPR) indicated that the oxidation activity of CeO_2 decreased after water vapor treatment. Fourier-transform infrared (FT-IR) studies revealed that CeO_2-H_2O showed new bending vibration peaks at 1110 cm^{-1} ascribed to Ce–OH groups. X-ray photoelectron spectroscopy (XPS) results showed that the content of Ce–OH increased from 20.85% to 39.99%, while the lattice oxygen content decreased from 68.21% to 45.83% after water vapor treatment. Density functional theory (DFT) calculations revealed that H_2O can be dissociated on clean and oxygen-defective CeO_2(111) surfaces to form H atoms and OH fragments. The H atoms associated with the adjacent oxygen atoms of CeO_2, and the OH fragments were bound directly with Ce atoms to form Ce–OH for the clean CeO_2 surface; or occupied the oxygen vacancies and were surrounded by three Ce atoms via van der Waals forces, without additional bond formation for

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