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**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<sup>0</sup> removal over CeO<sub>2</sub>-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<sub>2</sub>-TPR) indicated that the oxidation activity of CeO<sub>2</sub> decreased after water vapor treatment. Fourier-transform infrared (FT-IR) studies revealed that CeO<sub>2</sub>-H<sub>2</sub>O showed new bending vibration peaks at 1110 cm<sup>-1</sup> 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<sub>2</sub>O can be dissociated on clean and oxygen-defective CeO<sub>2</sub>(111) surfaces to form H atoms and OH fragments. The H atoms associated with the adjacent oxygen atoms of CeO<sub>2</sub>, and the OH fragments were bound directly with Ce atoms to form Ce-OH for the clean CeO<sub>2</sub> 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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