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Mercury oxidation reaction mechanisms on halogenated activated carbon: a density functional theory study

The complete reaction mechanisms of elementary mercury (Hg) adsorption and oxidation on halogenated activated carbon (AC) models have been demonstrated for the first time using density functional theory (DFT) calculations. Two different halogenated AC models, namely X-AC and X-AC-X (X=Cl, Br, I), were used to compare the effect of degrees of halogenation on the reaction reactivity. The mechanism consists of (i) Hg adsorption, (ii) HgX formation, and (iii) HgX2 formation. The calculated potential energy surfaces reveal that Hg can be found both in the forms of Hg physisorption and mercury halide (HgX) chemisorption on the AC edge. Through the Hg physisorption energies are independent to the halide types of the halogenated AC, the activation energies required for the HgX formations increase as the order of HgI < HgBr < HgCl. The HgX is found to be stable state on the AC edge and its further desorption from the AC as HgX form or further oxidation to mercury-dihalides (HgX2) are energetically unfavorable. The trend of the calculated barriers for HgX formations are corresponded with the experimental observation. Therefore, the HgX formation is predicted as a crucial step in Hg oxidation of halogenated AC and in addition the halide concentration increases the reactivity of halogenated AC.

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