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Complete reaction mechanisms of mercury oxidation on halogenated activated carbon

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Highlights

- Hg oxidation on halogenated activated carbon were investigated by DFT method
- Halide type has less effect to Hg adsorption energy
- Halide type strongly affects activation energy of mercury halide formation.
- Energy barrier of Hg oxidation is a sorbent reactivity descriptor.

Abstract

The reaction mechanisms of mercury (Hg) adsorption and oxidation on halogenated activated carbon (AC) have been completely studied for the first time using density functional theory (DFT) method. Two different halogenated AC models, namely *X*-AC and *X*-AC-*X* (*X=Cl, Br, I*), were adopted. The results revealed that Hg*X* is found to be stable-state on the AC edge since its further desorption from the AC as Hg*X*, or further oxidation to HgX_2, are energetically unfavorable. Remarkably, the halide type does not significantly affect the Hg