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The interaction of mercury with halogenated graphene[1] ABIGAIL KIRCHOFER, ERDEM SASMAZ, JENNIFER WILCOX, Stanford University — The interaction of mercury with halogenated graphene was studied using plane-wave density functional theory. Various configurations of H, Hg, O and Br or Cl on the zigzag edge sites of graphene were investigated. Although Hg-Br (or -Cl) complexes were found to be stable on the surface, the most stable configurations found were those with Hg adjacent to O. The surface atoms Hg, O, and Br tend to repel each other during geometric optimization, moving towards an H atom nearest-neighbor where possible. The strength of the Hg-graphene interaction is very sensitive to the local environment. The Hg-graphene binding energy is strongest when the Hg is located next to a surface O but not immediately next to a bound Br. DOS analysis revealed that Hg adsorption involves a gain in Hg 6 p-states and a loss in Hg 5 s electron density, resulting in an oxidized surface-bound Hg complex. DOS analysis suggests that Br strengthens the Hg-graphene interaction by modifying the surface carbon electron density; however, when Br is adjacent to Hg, a direct Hg-Br interaction weakens the Hg-C bond. These investigations provide insight into the mechanism associated with enhanced Hg adsorption on Br-functionalized carbon materials for Hg emissions reductions from coal-fired power plant applications.

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