A DFT Study of Mercury Capture on Paper Waste Derived Sorbents

Xinxin Li[†] and Paul Blowers*
Department of Chemical and Environmental Engineering
The University of Arizona
Tucson, AZ 85719
[†]Speaker, *Corresponding Author

Introduction

Control of mercury emissions in post-combustion gases from coal-burning power plants and other industrial sources has been extensively investigated over the last several decades. The purpose of our research is to find out the mechanisms of interaction of Hg and HgCl2 with a kind of efficient Mercury capture sorbents - paper waste derived (kaolinite and calcium based) sorbents.

Results and Discussions

In this work, density functional theory (DFT) was used to investigate the structure of the PWDS using program DMOL at both the LDA and GGA functional and DNP basis set. The choice of method and basis set combination was validated through a detailed comparison of theoretical geometry and heats of reaction predictions to experimental data available in the literature. The Hg and HgCl2 adsorption energy on the sorbents surface, enthalpy and other thermodynamic properties was calculated.

In addition to this, the cluster structure of PWDS was built to simulate the Hg and HgCl2 adsorption process. Meanwhile, the effect of temperature changes on the adsorption ability was evaluated. This work not only allows for a more thorough understanding of mercury's speciation adsorption on PWDS in the flue gas environment, but also set a basis for finding out more efficient dry sorbents in the future.

Author Contact Information

Phone: (520) 626-5319
Fax: (520) 621-6048
Email: blowers@engr.arizona.edu