DFT study of SO2 and CO2 on the activity of CaO surface for SeO2 capture

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Abstract

Selenium is a hazardous element in coal. During coal combustion, most of the selenium will convert to toxic SeO2 (gaseous). In 2011, US Environmental Protection Agency (EPA) issued the Mercury and Air Toxics Standards (US, MATS, updated in 2013). A selenium emission limit of 6.0×10^-2 lb/MWh (approximately 7.5 μg/m3) was set for existing coal-fired power plants, and 5.0×10^-2 lb/MWh (approximately 6.3 μg/m3) was set for new coal-fired power plants. Ca-based adsorbents, especially CaO, have been considered as a potential sorbent to adsorb SeO2 due to its low cost. SO2 and CO2, which are present in the flue gas, will react with CaO as well. Some researchers have found a simultaneous capture of SeO2, SO2, and CO2 using CaO sorbent. At the initial stage (dynamic control stage), SO2 and CO2 have a weak influence on the adsorption with SeO2, compared to the base case of SeO2 adsorption on CaO. It is the key stage for simultaneous removal of SeO2, SO2, and CO2 using CaO sorbent. However, the most likely adsorption mechanism has not been fully determined now.

In this paper, quantum chemistry calculation based on density functional theory (DFT) was applied to reveal the influence of SO2 and CO2 on SeO2 capture. The work mainly focused on the adsorption relationship between flue gas (SO2 and CO2) and SeO2. From the results, the influence of new adsorbed SO2 or CO2 on already adsorbed SeO2 are highly similar to that of new adsorbed SeO2 on already adsorbed SeO2. At the initial adsorption stage (the superficial O atoms are not mainly occupied), the adsorption of SeO2, SO2 and CO2 will be relatively independent, not affecting each other. Experimental data obtained from our previous study was used to validate some of the simulation results.